Continuum-kinematics-inspired peridynamics. Mechanical problems

A. Javili [a,*], A.T. McBride [c], P. Steinmann [b,c]

[a] *Department of Mechanical Engineering, Bilkent University, Ankara, 06800, Turkey*
[b] *Chair of Applied Mechanics, University of Erlangen-Nuremberg, Egerland Str. 5, Erlangen,91058, Germany*
[c] *Glasgow Computational Engineering Centre, School of Engineering, University of Glasgow, Glasgow, G12 8QQ, United Kingdom*

A R T I C L E   I N F O

A B S T R A C T

The main objective of this contribution is to develop a novel continuum-kinematics-inspired approach for peridynamics (PD), and to revisit PD's thermodynamic foundations. We distinguish between three types of interactions, namely, one-neighbour interactions, two-neighbour interactions and three-neighbour interactions. While one-neighbour interactions are equivalent to the bond-based interactions of the original PD formalism, two- and three-neighbour interactions are fundamentally different to state-based interactions in that the basic elements of continuum kinematics are preserved exactly. In addition, we propose that an externally prescribed traction on the boundary of the continuum body emerges naturally and need not vanish. This is in contrast to, but does not necessarily violate, standard PD. We investigate the consequences of the angular momentum balance and provide a set of appropriate arguments for the interactions accordingly. Furthermore, we elaborate on thermodynamic restrictions on the interaction energies and derive thermodynamically-consistent constitutive laws through a Coleman–Noll-like procedure.

1. Introduction

Peridynamics (PD) is an alternative approach to formulate continuum mechanics (Silling, 2000) the roots of which can be traced back to the pioneering works of Piola (dell'Isola et al., 2015; 2016; 2017) which prepared the foundations for nonlocal continuum mechanics and peridynamics. PD has experienced prolific growth as an area of research, with a significant number of contributions in multiple disciplines. PD is a non-local continuum mechanics formulation. However, it is fundamentally different from common non-local elasticity (e.g. Eringen, 2002) in that the concepts of stress and strain are not present. As a non-local theory, the behaviour of each material point in PD is dictated by its interactions with other material points in its vicinity. Furthermore, in contrast to classical continuum mechanics, the governing equations of PD are integro-differential equations appropriate for problems involving discontinuities such as cracks and interfaces.

While the discretized format of PD bears a similarity to discrete mechanics formulations such as molecular dynamics (MD), it is still a continuum formulation and only takes advantage of basic MD concepts such as the cutoff radius and

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* Corresponding author.
  E-mail address: ajavili@bilkent.edu.tr (A. Javili).

Table 1

Major applications and selected key contributions of PD.

| PD application	Important contributions
Quasi-static problems	Dayal and Bhattacharya (2006), Mikata (2012), Breitenfeld et al. (2014), Huang et al. (2015), and Madenci and Oterkus (2016)
Coupled problems	Gerstle et al. (2008), Bobaru and Duangpanya (2010), Oterkus et al. (2014a, 2014b, 2017)
Multiscale modeling	Bobaru et al. (2009), Shelke et al. (2011), Rahman and Foster (2014), Talebi et al. (2014), Ebrahimi et al. (2015), Tong and Li (2016), and Xu et al. (2016)
Structural mechanics	Silling and Bobaru (2005), Diyaroglu et al. (2016), O'Grady and Foster (2014), Taylor and Steigmann (2015), Chowdhury et al. (2016), and Li et al. (2016)
Constitutive models	Aguiar and Fosdick (2014), Sun and Sundararaghavan (2014), Tupek and Radovitzky (2014), Silhavý (2017), and Madenci and Oterkus (2017)
Material failure	Kilic and Madenci (2009), Foster et al. (2011), Silling et al. (2010), Agwai et al. (2011), Dipasquale et al. (2014), Chen and Bobaru (2015), Han et al. (2016), Emmrich and Puhst (2016), De Meo et al. (2016), Sun and Huang (2016), and Diyaroglu et al. (2016)
Biomechanics	Taylor et al. (2016), Lejeune and Linder (2017a, 2017b, 2018a, 2018b)
Wave dispersion	Zingales (2011), Vogler et al. (2012), Wildman and Gazonas (2014), Bazant et al. (2016), Nishawala et al. (2016), Silling (2016), and Butt et al. (2017)
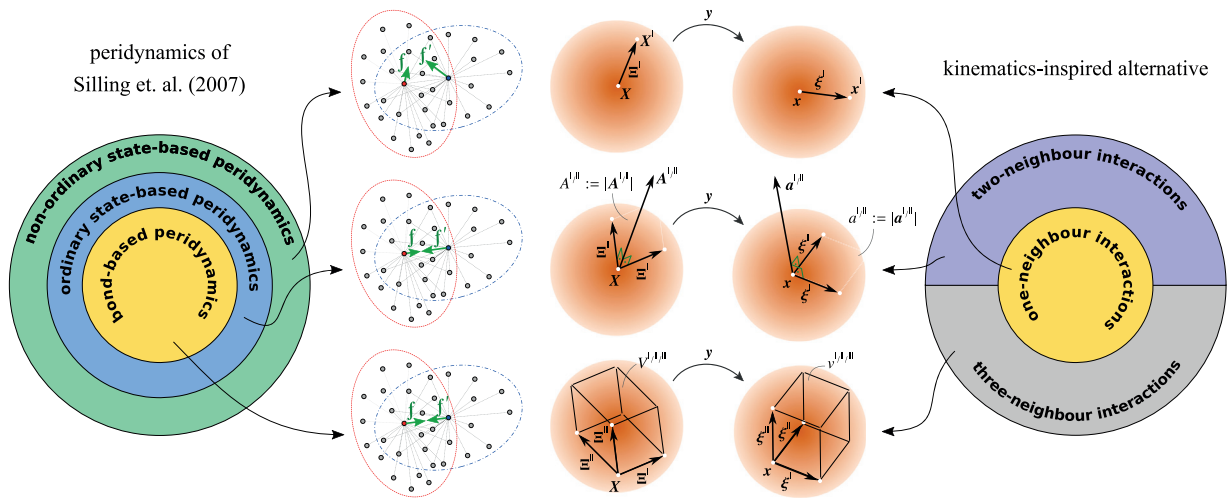
Fig. 1. Schematic illustration and comparison between the standard PD formulation (left) and the proposed continuum-kinematics-inspired alternative (right). One-neighbour interactions in our framework are identical to bond-based interactions in the PD formulation of Silling (2000). Two and three-neighbour interactions corresponding to Eq. (4) and Eq. (5), respectively, are alternatives to state-based interactions. The difference between the bond-based, ordinary state-based, and non-ordinary state-based PD formulations lies in the magnitude and direction of the interaction forces (green arrows) between the materials points. In our approach, the difference between the one-, two- and three-neighbour interactions lies in their kinematic descriptions. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

point-wise interactions. For further connections and differences between PD theory, continuum mechanics and particle systems see the fundamental contributions by Fried (2010), Murdoch (2012), Fosdick (2013), and Podio-Guidugli (2017), among others. PD inherently accounts for geometrical discontinuities, hence it is readily employed in fracture mechanics and related problems. However, the applications of PD extend far beyond fracture and damage. For an extensive study of the balance laws, applications, and implementations, see Madenci and Oterkus (2014), and for a brief description of PD together with a review of its applications and related studies in different fields to date, see Javili et al. (2018). Table 1 categorises various PD applications and the associated key contributions in the literature. It is clear that the range of PD applications is broad and not limited to fracture mechanics.

The original PD theory of Silling (2000) was restricted to bond-based interactions. This limited 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 finally rectified by Silling et al. (2007) via the introduction of the notion of *state* and categorising the interactions as bond-based, ordinary state-based and non-ordinary state-based as schematically illustrated in Fig. 1 (left). Despite the large amount of research on PD, its thermodynamic foundations have not been fully investigated. Fundamental works on PD are limited in number but include those of Silling and Lehoucq (2010), Ostoja-Starzewski et al. (2013), and Oterkus et al. (2014a). The starting point of these contributions is the PD theory and constitutive formulation of Silling et al. (2007). The goal here is to adopt a continuum-kinematics-inspired approach and thereby bridge the gap between classical continuum thermodynamics and PD. More precisely, we propose an alternative PD formulation whose underlying concepts are reminiscent of classical continuum mechanics. In particular, we firstly propose to decompose the interaction potentials into three parts corresponding to *one-neighbour interactions*, *two-neighbour interactions* and

three-neighbour interactions within the horizon, as illustrated in Fig. 1 (right). Note, one-neighbour interactions are identical to bond-based interactions in the PD formulation of Piola (dell'Isola et al., 2015) and Silling (2000). Secondly, we derive the balance of linear and angular momentum corresponding to our interaction potentials and identify the fundamental properties of these potentials such that angular momentum balance is a priori fulfilled. Finally, we derive the dissipation inequality and propose thermodynamically-consistent constitutive laws. Crucially, we postulate the virtual power equivalence as the key requirement of our approach and build our entire framework solely on this variational assumption.

Remark. Before proceeding, we revisit the notions of a "localization procedure" and a "point-wise equation" since in the current context they serve a broader purpose than they usually do in classical continuum mechanics. Localization refers to the process of deriving a point-wise relation from an integral form over a domain. The resulting point-wise relation itself may or may not be an integral form. Applying the localization procedure on global forms in CCM renders point-wise relations at each X that are not integrals and thus are local. On the contrary, point-wise equations at each X in CPD include integrals over the horizon and are hence non-local. It is possible to apply a localization procedure on these non-local forms to derive neighbour-wise equations that are point-wise forms at each neighbouring particle's location $X^|$. Henceforth, we use the term "local form" exclusively to indicate the point-wise quantities and equations of CCM. The term "non-local form" on the other hand refers to point-wise integral forms associated with CPD. Finally, the term "neighbour-wise form" refers to non-integral quantities and relations in CPD obtained via localization of their non-local forms. □

The manuscript is organized as follows. Section 2 introduces the notation, elaborates on the kinematics of the problem and presents the geometrical aspects of the proposed framework. Here the novelty is to introduce two- and three-neighbour interactions inspired by basic elements of classical continuum kinematics. Firstly, as a motivation, we derive the governing equations using the Dirichlet principle in Section 3 via minimizing the total energy functional, for the special case of a quasi-static, conservative problem. Next, for the general case, thermodynamic balance laws are discussed in Section 4. In particular, we detail the kinetic energy, energy and entropy balance equations. Afterwards, through a Coleman–Noll-like procedure based on the dissipation inequality, we provide thermodynamically-consistent constitutive laws. Section 5 concludes this work.

2. Kinematics

Consider a continuum body that occupies the material configuration $\mathcal{B}_0 \in \mathbb{R}^3$ at time $t = 0$ and that is mapped to the spatial configuration $\mathcal{B}_t \in \mathbb{R}^3$ via the nonlinear deformation map y as

$$\boldsymbol{x} = \boldsymbol{y}(\boldsymbol{X}, t) \; : \; \mathcal{B}_0 \times \mathbb{R}_+ \to \mathcal{B}_t \qquad \Rightarrow \qquad \mathcal{B}_t = \boldsymbol{y}(\mathcal{B}_0)$$

in which X and x identify the points in the material and spatial configurations, respectively illustrated in Fig. 2. Central to the PD theory, and in contrast to standard local continuum mechanics, is the non-locality assumption that any point X in the material configuration can interact with points within its finite neighbourhood $\mathcal{H}_0(\boldsymbol{X})$. The neighbourhood $\mathcal{H}_0$ is referred to as the *horizon* in the material configuration. The *measure* of the horizon in the material configuration is denoted δ_0 and is generally the radius of a spherical neighbourhood at X. The spatial horizon $\mathcal{H}_t$ is the image of the material horizon $\mathcal{H}_0$ under the deformation map y and its measure is denoted δ_t, that is

$$\mathcal{H}_t = \boldsymbol{y}(\mathcal{H}_0, t) \qquad \text{with} \qquad \delta_0 := \text{meas}(\mathcal{H}_0) \quad \text{and} \quad \delta_t := \text{meas}(\mathcal{H}_t) = \boldsymbol{y}(\delta_0) \,.$$

Note that the horizon $\mathcal{H}_0$ coincides with the point X in the limit of an infinitesimal neighbourhood and therefore

$$\lim_{\delta_0 \to 0} \mathcal{H}_0 \to \boldsymbol{X} \qquad \text{and} \qquad \lim_{\delta_0 \to 0} \mathcal{H}_t \to \boldsymbol{x}$$

recovering the kinematics of the local continuum mechanics formalism.

To be more precise and to better distinguish the PD formalism from conventional continuum mechanics, we identify the points (neighbours) within the horizon by a superscript. For instance the point $\boldsymbol{X}^| \in \mathcal{H}_0(\boldsymbol{X})$ denotes a neighbour of point X
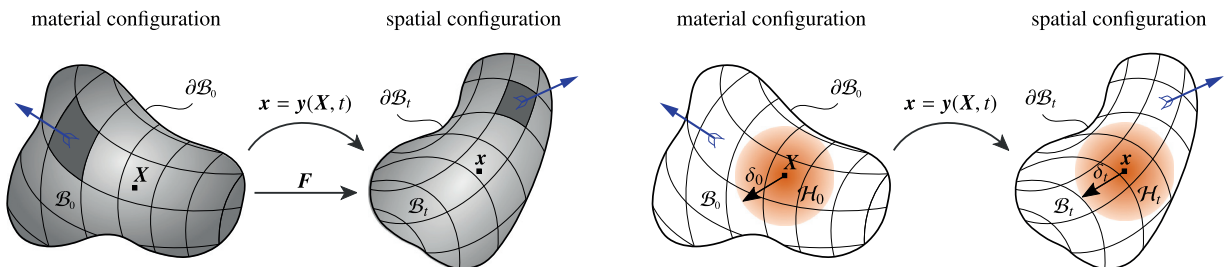

Fig. 2. Motion of a continuum body. Illustration of classical continuum mechanics formalism (left) and the peridynamics formulation (right). The continuum body that occupies the material configuration $\mathcal{B}_0 \in \mathbb{R}^3$ at time $t = 0$ is mapped to the spatial configuration $\mathcal{B}_t \in \mathbb{R}^3$ via the nonlinear deformation map y.

in the material configuration. The point $\boldsymbol{x}^{|}$ within the horizon of $\boldsymbol{x}$ is the spatial counterpart of the point $\boldsymbol{X}^{|}$ defined through the nonlinear deformation map $\boldsymbol{y}$ as

$$\boldsymbol{x}^{|} := \boldsymbol{y}(\boldsymbol{X}^{|}, t) \,. \tag{1}$$

For our proposed framework, we identify the neighbour set of point $\boldsymbol{X}$ as

$$\left\{ \boldsymbol{X}^{|}, \boldsymbol{X}^{||}, \boldsymbol{X}^{|||} \right\} \quad \forall \quad \boldsymbol{X}^{|} \in \mathcal{H}_0(\boldsymbol{X}) \quad , \quad \boldsymbol{X}^{||} \in \mathcal{H}_0(\boldsymbol{X}) \quad , \quad \boldsymbol{X}^{|||} \in \mathcal{H}_0(\boldsymbol{X}) \,.$$

These neighbours of $\boldsymbol{X}$ denoted $\boldsymbol{X}^{|}$, $\boldsymbol{X}^{||}$, $\boldsymbol{X}^{|||}$ are mapped onto $\boldsymbol{x}^{|}$, $\boldsymbol{x}^{||}$, $\boldsymbol{x}^{|||}$, respectively. The relative positions, i.e. the finite line elements, in the material and spatial configurations are denoted as $\boldsymbol{\Xi}^{\{\cdot\}}$ and $\boldsymbol{\xi}^{\{\cdot\}}$, respectively, where the superscript $\{\cdot\}$ identifies the neighbour, that is

$$
\begin{aligned}
\boldsymbol{\Xi}^{|} &:= \boldsymbol{X}^{|} - \boldsymbol{X} & \text{and} \quad & \boldsymbol{\xi}^{|} := \boldsymbol{x}^{|} - \boldsymbol{x} & \text{where} \quad & \boldsymbol{\xi}^{|} = \boldsymbol{\xi}(\boldsymbol{X}^{|}; \boldsymbol{X}) = \boldsymbol{y}(\boldsymbol{X}^{|}) - \boldsymbol{y}(\boldsymbol{X}) \,, \\
\boldsymbol{\Xi}^{||} &:= \boldsymbol{X}^{||} - \boldsymbol{X} & \text{and} \quad & \boldsymbol{\xi}^{||} := \boldsymbol{x}^{||} - \boldsymbol{x} & \text{where} \quad & \boldsymbol{\xi}^{||} = \boldsymbol{\xi}(\boldsymbol{X}^{||}; \boldsymbol{X}) = \boldsymbol{y}(\boldsymbol{X}^{||}) - \boldsymbol{y}(\boldsymbol{X}) \,, \\
\boldsymbol{\Xi}^{|||} &:= \boldsymbol{X}^{|||} - \boldsymbol{X} & \text{and} \quad & \boldsymbol{\xi}^{|||} := \boldsymbol{x}^{|||} - \boldsymbol{x} & \text{where} \quad & \boldsymbol{\xi}^{|||} = \boldsymbol{\xi}(\boldsymbol{X}^{|||}; \boldsymbol{X}) = \boldsymbol{y}(\boldsymbol{X}^{|||}) - \boldsymbol{y}(\boldsymbol{X}) \,.
\end{aligned}
\tag{2}
$$

In addition, we define the conventional infinitesimal line elements, by a limit operation, as

$$\mathrm{d}\boldsymbol{X}^{|} := \lim_{\delta_o \to 0} \boldsymbol{\Xi}^{|}, \; \mathrm{d}\boldsymbol{x}^{|} := \lim_{\delta_o \to 0} \boldsymbol{\xi}^{|}, \quad \mathrm{d}\boldsymbol{X}^{||} := \lim_{\delta_o \to 0} \boldsymbol{\Xi}^{||}, \; \mathrm{d}\boldsymbol{x}^{||} := \lim_{\delta_o \to 0} \boldsymbol{\xi}^{||}, \quad \mathrm{d}\boldsymbol{X}^{|||} := \lim_{\delta_o \to 0} \boldsymbol{\Xi}^{|||}, \; \mathrm{d}\boldsymbol{x}^{|||} := \lim_{\delta_o \to 0} \boldsymbol{\xi}^{|||} \,.$$

In order to overcome the bond-based restrictions of early PD formulations, and in the spirit of classical constitutive modelling, we first recall the three local kinematic measures of relative deformation, namely the deformation gradient $\boldsymbol{F}$, its cofactor $\boldsymbol{K}$ and its determinant J, where

$$\boldsymbol{F} := \operatorname{Grad} \boldsymbol{y} \quad \text{and} \quad \boldsymbol{K} := \operatorname{Cof} \boldsymbol{F} \quad \text{and} \quad J := \operatorname{Det} \boldsymbol{F} \,. \tag{3}$$

We now introduce three non-local PD kinematic measures of relative deformation chosen to resemble the local measures (3).

(i) The first relative deformation measure $\boldsymbol{\xi}^{|}$ mimics the linear map $\boldsymbol{F}$ from the infinitesimal line element $\mathrm{d}\boldsymbol{X}^{|}$ in the material configuration to its spatial counterpart $\mathrm{d}\boldsymbol{x}^{|}$. The infinitesimal spatial line element $\mathrm{d}\boldsymbol{x}^{|}$ is related to its material counterpart $\mathrm{d}\boldsymbol{X}^{|}$ via a Taylor expansion at $\boldsymbol{X}$ as

$$
\begin{aligned}
\mathrm{d}\boldsymbol{x}^{|} &= \lim_{\delta_0 \to 0} [\boldsymbol{x}^{|} - \boldsymbol{x}] \\
&= \lim_{\delta_0 \to 0} \boldsymbol{\xi}^{|} \\
&= \lim_{\delta_0 \to 0} \left[\boldsymbol{F} \big|_{\boldsymbol{X}} \cdot \boldsymbol{\Xi}^{|} + \tfrac{1}{2} \boldsymbol{G} \big|_{\boldsymbol{X}} : \left[\boldsymbol{\Xi}^{|} \otimes \boldsymbol{\Xi}^{|} \right] + \dots \right] \\
&\approx \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{X}^{|},
\end{aligned}
$$

where $\boldsymbol{G}$ is the second gradient of the deformation map $\boldsymbol{y}$. In view of our proposed PD formalism, the relative deformation measure $\boldsymbol{x}^{|} - \boldsymbol{x}$ is the main ingredient to describe *one-neighbour interactions*, see Fig. 3.

(ii) Similar to finite line elements, we introduce finite area elements constructed from two finite line elements. For instance, the vectorial area element $\boldsymbol{A}^{|/||}$ in the material configuration corresponds to the vector product of the line elements $\boldsymbol{\Xi}^{|}$ and $\boldsymbol{\Xi}^{||}$ as $\boldsymbol{A}^{|/||} := \boldsymbol{\Xi}^{|} \times \boldsymbol{\Xi}^{||}$ with its counterpart in the spatial configuration denoted as $\boldsymbol{a}^{|/||} := \boldsymbol{\xi}^{|} \times \boldsymbol{\xi}^{||}$, i.e.

$$\boldsymbol{A}^{|/||} := \boldsymbol{\Xi}^{|} \times \boldsymbol{\Xi}^{||} \quad \text{and} \quad \boldsymbol{a}^{|/||} := \boldsymbol{\xi}^{|} \times \boldsymbol{\xi}^{||} \quad \text{where} \quad \boldsymbol{a}^{|/||} = \boldsymbol{a}(\boldsymbol{X}^{|}, \boldsymbol{X}^{||}; \boldsymbol{X}) \,. \tag{4}$$

Fig. 3. Illustration of finite line elements within the horizon in the material and spatial configurations corresponding to one-neighbour interactions. The finite line elements are the relative positions between points.
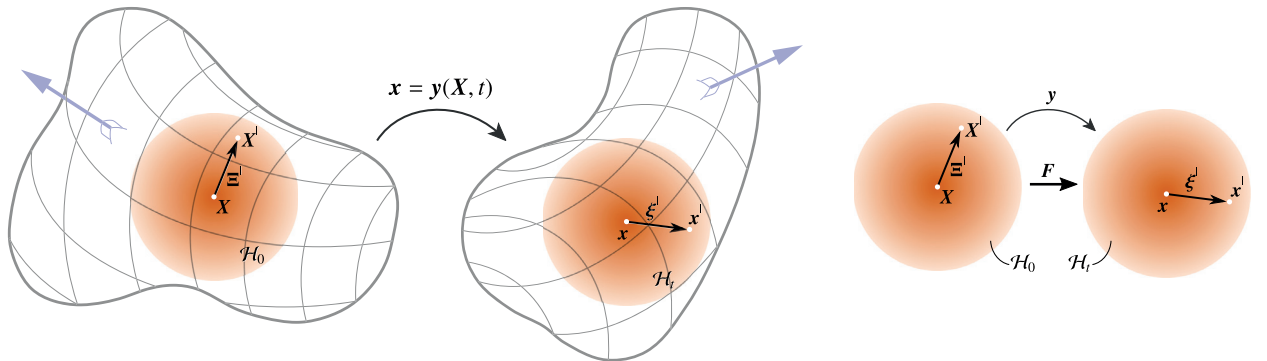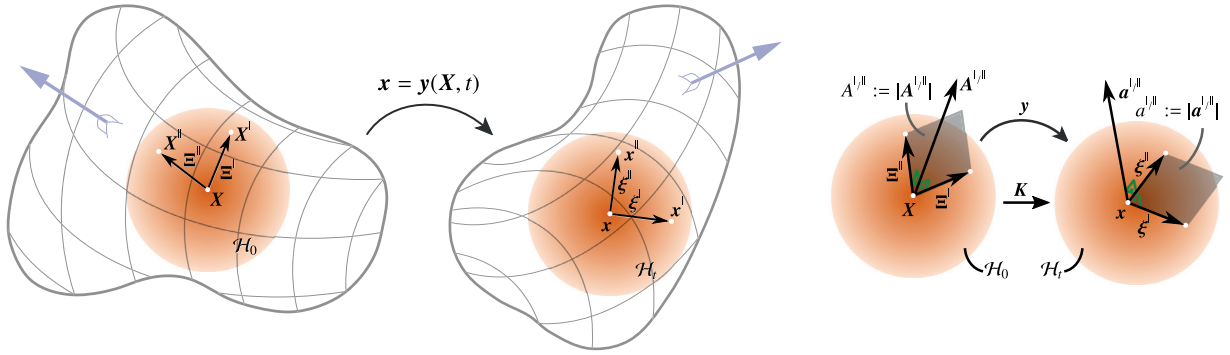
Fig. 4. Illustration of finite area elements within the horizon in the material and spatial configurations corresponding to two-neighbour interactions.

The second relative deformation measure $\boldsymbol{a}^{|/||}$ mimics the linear map from the infinitesimal (vectorial) area element $\mathrm{d}\boldsymbol{A}^{|/||}$ in the material configuration to its spatial counterpart $\mathrm{d}\boldsymbol{a}^{|/||}$. An infinitesimal area element is constructed from three points within the horizon in the limit of infinitesimal horizon measure as

$$
\begin{aligned}
\mathrm{d}\boldsymbol{a}^{|/||} = \lim_{\delta_0 \to 0} \boldsymbol{a}^{|/||} &= \lim_{\delta_0 \to 0} \left[[\boldsymbol{x}^| - \boldsymbol{x}] \times [\boldsymbol{x}^{||} - \boldsymbol{x}] \right] \\
&= \lim_{\delta_0 \to 0} \left[\boldsymbol{\xi}^| \times \boldsymbol{\xi}^{||} \right] \\
&= \left[\boldsymbol{F} \cdot \mathrm{d}\boldsymbol{X}^| \right] \times \left[\boldsymbol{F} \cdot \mathrm{d}\boldsymbol{X}^{||} \right] \\
&= \boldsymbol{K} \cdot \mathrm{d}\boldsymbol{A}^{|/||}.
\end{aligned}
$$

This is essentially the Nanson's formula frequently used in conventional continuum kinematics. In our proposed framework, the relative area measure $[\boldsymbol{x}^| - \boldsymbol{x}] \times [\boldsymbol{x}^{||} - \boldsymbol{x}]$ is the main ingredient to describe *two-neighbour interactions*, see Fig. 4. (iii) In a similar fashion to finite line elements and area elements, we define finite volume elements formed by three finite line elements. Let $V^{|/||/|||}$ denote the finite volume element in the material configuration with its spatial counterpart being $v^{|/||/|||}$. The volume elements $V^{|/||/|||}$ and $v^{|/||/|||}$ are obtained by a scalar triple product, also referred to as a mixed product, of their edges as

$$
V^{|/||/|||} := \left[\boldsymbol{\Xi}^| \times \boldsymbol{\Xi}^{||} \right] \cdot \boldsymbol{\Xi}^{|||} \qquad \text{and} \qquad v^{|/||/|||} := \left[\boldsymbol{\xi}^| \times \boldsymbol{\xi}^{||} \right] \cdot \boldsymbol{\xi}^{|||} \qquad \text{where} \qquad v^{|/||/|||} = v(\boldsymbol{X}^|, \boldsymbol{X}^{||}, \boldsymbol{X}^{|||}; \boldsymbol{X}) . \tag{5}
$$

The third and last deformation measure $v^{|/||/|||}$ mimics the linear map J from the infinitesimal volume element $\mathrm{d}V^{|/||/|||}$ in the material configuration to its spatial counterpart $\mathrm{d}v^{|/||/|||}$. However unlike J that must be strictly positive, the volume elements $v^{|/||/|||}$ and $V^{|/||/|||}$ can be positive or negative as long as they are consistent in the sense that $v^{|/||/|||}/V^{|/||/|||} > 0$ must hold. The infinitesimal volume elements are formed from four points within the horizon in the limit of infinitesimal horizon measure as

$$
\begin{aligned}
\mathrm{d}v^{|/||/|||} = \lim_{\delta_0 \to 0} v^{|/||/|||} &= \lim_{\delta_0 \to 0} \left[\left[[\boldsymbol{x}^| - \boldsymbol{x}] \times [\boldsymbol{x}^{||} - \boldsymbol{x}] \right] \cdot [\boldsymbol{x}^{|||} - \boldsymbol{x}] \right] \\
&= \lim_{\delta_0 \to 0} \left[\left[\boldsymbol{\xi}^| \times \boldsymbol{\xi}^{||} \right] \cdot \boldsymbol{\xi}^{|||} \right] \\
&= \left[\left[\boldsymbol{F} \cdot \mathrm{d}\boldsymbol{X}^| \right] \times \left[\boldsymbol{F} \cdot \mathrm{d}\boldsymbol{X}^{||} \right] \right] \cdot \left[\boldsymbol{F} \cdot \mathrm{d}\boldsymbol{X}^{|||} \right] \\
&= J \, \mathrm{d}V^{|/||/|||}.
\end{aligned}
$$

The relative volume measure $[[\boldsymbol{x}^| - \boldsymbol{x}] \times [\boldsymbol{x}^{||} - \boldsymbol{x}] \cdot [\boldsymbol{x}^{|||} - \boldsymbol{x}]]$ is the main ingredient to describe *three-neighbour interactions*, see Fig. 5.

3. Dirichlet principle setting

To gain insight into the thermodynamic balance laws before investigating the general case in Section 4, we begin with the special case of a quasi-static conservative problem. Thus, in order to set the stage and to motivate the structure of the governing equations for the important problem of a conservative system that is equipped with a total potential energy functional, we consider the Dirichlet principle. More precisely, we obtain the governing equations by minimizing the corresponding total potential energy functional via setting its first variation to zero. The total potential energy functional Π
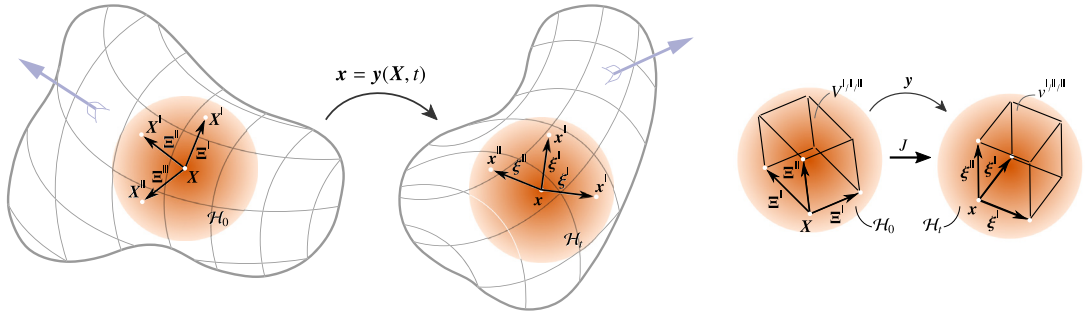
Fig. 5. Illustration of finite volume elements within the horizon in the material and spatial configurations corresponding to three-neighbour interactions.

consists of internal and external contributions, denoted as Π^{int} and Π^{ext}, respectively, and is given by

$$\Pi = \Pi^{\mathrm{int}} + \Pi^{\mathrm{ext}}. \tag{6}$$

The internal and external contributions are detailed in Sections 3.1 and 3.2, respectively. In Sections 3.3 the governing equations are derived and their connection to classical (local) Cauchy continuum mechanics is highlighted. The discussion on the variational setting in this section is entirely restricted to non-dissipative processes. As outlined by dell'Isola and Placidi (2011), however, this variational setting can be extended to more generic dissipative cases using the Hamilton–Rayleigh variational principle, as will be explored in a separate contribution.

3.1. Internal potential energy

The internal potential energy of the system Π^{int} is assumed without loss of generality to be separable, i.e. to be composed of the internal potential energy due to one-neighbour interactions Π_1^{int}, two-neighbour interactions Π_2^{int} and three-neighbour interactions Π_3^{int}, that is

$$\Pi^{\mathrm{int}} = \Pi_1^{\mathrm{int}} + \Pi_2^{\mathrm{int}} + \Pi_3^{\mathrm{int}},$$

where the number in the subscript indicates the type of interaction. These contributions to the internal potential energy are now explored.

3.1.1. One-neighbour interactions

To proceed, we define the one-neighbour interaction energy density per volume squared in the material configuration $w_1^|$ as a function of the relative position $\boldsymbol{\xi}^|$ between two points, that is

$$w_1^| := w_1(\boldsymbol{\xi}^|) = w_1(\boldsymbol{\xi}(\boldsymbol{X}^|; \boldsymbol{X})) \equiv w_1(\boldsymbol{\xi}^|; \boldsymbol{\Xi}^|, \boldsymbol{X}) \qquad \text{with} \qquad [w_1] = \mathrm{N.m/m^6}$$

where the semi-colon delineates arguments of a function from its parametrisation. Furthermore, we define the more familiar energy density per volume as half of the integral of w_1 over the horizon $\mathcal{H}_0$, that is

$$W_1 := \frac{1}{2} \int_{\mathcal{H}_0} w_1 \, \mathrm{d}V^| \qquad \text{with} \qquad [W_1] = \mathrm{N.m/m^3}$$

wherein the factor one-half is introduced to prevent double counting since we visit each point twice due to the resulting double-integration in the next step. Consequently, the internal potential energy due to one-neighbour interactions Π_1^{int} is defined by

$$\Pi_1^{\mathrm{int}} := \int_{\mathcal{B}_0} W_1 \, \mathrm{d}V = \frac{1}{2} \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} w_1(\boldsymbol{\xi}^|) \, \mathrm{d}V^| \, \mathrm{d}V \qquad \text{with} \qquad \left[\Pi_1^{\mathrm{int}}\right] = \mathrm{N.m}$$

$$\equiv \frac{1}{2} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} w_1(\boldsymbol{\xi}^|) \, \mathrm{d}V^| \, \mathrm{d}V.$$

The last step holds since at any point $\boldsymbol{X}$ one-neighbour interactions with points outside the horizon vanish. Next, the variation of Π_1^{int} can be expressed as

$$\delta \Pi_1^{\mathrm{int}} = \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \frac{\partial w_1}{\partial \boldsymbol{\xi}^|} \cdot \delta \boldsymbol{\xi}^| \, \mathrm{d}V^| \, \mathrm{d}V$$

$$= \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \frac{\partial w_1}{\partial \boldsymbol{\xi}^|} \cdot \delta \boldsymbol{\xi}^| \, \mathrm{d}V^| \, \mathrm{d}V \tag{7}$$

in which the previously introduced factor one-half disappears due to the variation rules on multiple integrals. Motivated by the structure of Eq. (7), we define the force density per volume squared due to one-neighbour interactions by

$$\boldsymbol{p}_1^{|} := \frac{\partial w_1}{\partial \boldsymbol{\xi}^{|}} \qquad \text{with} \qquad \left[\boldsymbol{p}_1^{|}\right] = \text{N/m}^6 \tag{8}$$

and therefore the variation of Π_1^{int}, using $\delta \boldsymbol{\xi}^{|} = \delta \boldsymbol{y}^{|} - \delta \boldsymbol{y}$ from Eqs. (1) and (2), reads

$$
\begin{aligned}
\delta \Pi_1^{\text{int}} &= \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{p}_1^{|} \cdot \delta \boldsymbol{\xi}^{|} \, dV^{|} \, dV \\
&= \int_{\mathcal{B}_0} \left[\int_{\mathcal{H}_0} \boldsymbol{p}_1^{|} \cdot \delta \boldsymbol{y}^{|} \, dV^{|} - \int_{\mathcal{H}_0} \boldsymbol{p}_1^{|} \, dV^{|} \cdot \delta \boldsymbol{y} \right] dV \\
&= \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \boldsymbol{p}_1^{|} \cdot \delta \boldsymbol{y}^{|} \, dV^{|} \, dV - \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{p}_1^{|} \, dV^{|} \cdot \delta \boldsymbol{y} \, dV.
\end{aligned}
\tag{9}
$$

We identify the internal force density per volume in the material configuration due to one-neighbour interactions $\boldsymbol{b}^{\text{int}}_{0\,1}$ as

$$\boldsymbol{b}_{0\,1}^{\text{int}} := \int_{\mathcal{H}_0} \boldsymbol{p}_1^{|} \, dV^{|} \qquad \text{with} \qquad \left[\boldsymbol{b}_{0\,1}^{\text{int}}\right] = \text{N/m}^3 \,. \tag{10}$$

Note, we recognize the right-hand side of Eq. (10) as an internal force density since it is the virtual power conjugated quantity to $\delta \boldsymbol{y}$ according to Eq. (9). Finally, the variation of the internal potential energy due to one-neighbour interactions Π_1^{int} reads

$$\delta \Pi_1^{\text{int}} = \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \boldsymbol{p}_1^{|} \cdot \delta \boldsymbol{y}^{|} \, dV^{|} \, dV - \int_{\mathcal{B}_0} \boldsymbol{b}_{0\,1}^{\text{int}} \cdot \delta \boldsymbol{y} \, dV \,.$$

3.1.2. Two-neighbour interactions

Next, we define the two-neighbour interaction energy density per volume cubed in the material configuration $w_2^{|/||}$ as a function of the area element $\boldsymbol{a}^{|/||}$ between three points, that is

$$w_2^{|/||} = w_2(\boldsymbol{a}^{|/||}) = w_2\Big(\boldsymbol{\xi}(\boldsymbol{X}_{\text{I}}; \boldsymbol{X}) \times \boldsymbol{\xi}(\boldsymbol{X}^{||}; \boldsymbol{X}) \Big) \equiv w_2(\boldsymbol{a}^{|/||}; \boldsymbol{A}^{|/||}, \boldsymbol{X}) \qquad \text{with} \qquad [w_2] = \text{N.m/m}^9 \,.$$

Furthermore, we define the more familiar energy density per volume as one third of the double integral of w_2 over the horizon $\mathcal{H}_0$, that is

$$W_2 := \frac{1}{3} \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} w_2 \, dV^{||} \, dV^{|} \qquad \text{with} \qquad [W_2] = \text{N.m/m}^3 \,.$$

The factor one-third is introduced to prevent triple counting due to the resulting triple-integrals that come next. Note that the sequence of integration may be exchanged. The internal potential energy due to two-neighbour interactions denoted Π_2^{int} is defined by

$$
\begin{aligned}
\Pi_2^{\text{int}} &:= \int_{\mathcal{B}_0} W_2 \, dV = \frac{1}{3} \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} w_2(\boldsymbol{a}^{|/||}) \, dV^{||} \, dV^{|} \, dV \qquad \text{with} \qquad [\Pi_2^{\text{int}}] = \text{N.m} \\
&\equiv \frac{1}{3} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} w_2(\boldsymbol{a}^{|/||}) \, dV^{||} \, dV^{|} \, dV.
\end{aligned}
$$

Again, the last step holds since at any point $\boldsymbol{X}$ two-neighbour interactions with points outside the horizon vanish. Next, the variation of Π_2^{int} can be written as

$$\delta \Pi_2^{\text{int}} = \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \frac{\partial w_2}{\partial \boldsymbol{a}^{|/||}} \cdot \delta \boldsymbol{a}^{|/||} \, dV^{||} \, dV^{|} \, dV =: \frac{1}{2} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \boldsymbol{m}^{|/||} \cdot \delta \boldsymbol{a}^{|/||} \, dV^{||} \, dV^{|} \, dV,$$

in which the previously introduced factor one-third disappears and the factor one-half is introduced for convenience. The double force density per volume cubed is defined by $\boldsymbol{m}^{|/||}$ where

$$\boldsymbol{m}^{|/||} \equiv \boldsymbol{m}\Big(\boldsymbol{\xi}^{|} \times \boldsymbol{\xi}^{||} \Big) := 2 \frac{\partial w_2}{\partial \boldsymbol{a}^{|/||}} \qquad \text{with} \qquad \left[\boldsymbol{m}^{|/||}\right] = \text{N/m}^{10} \,.$$

Importantly,[1] $\boldsymbol{m}$ is assumed to be homogeneous of degree one in $\boldsymbol{a}^{|/||}$ so that

$$\boldsymbol{m}^{||/|} = \boldsymbol{m}\Big(\boldsymbol{\xi}^{||} \times \boldsymbol{\xi}^{|} \Big) = \boldsymbol{m}\Big(-\boldsymbol{\xi}^{|} \times \boldsymbol{\xi}^{||} \Big) = -\boldsymbol{m}\Big(\boldsymbol{\xi}^{|} \times \boldsymbol{\xi}^{||} \Big) = -\boldsymbol{m}^{|/||} \,. \tag{11}$$

---

[1] This is not only a model assumption but also requirement to satisfy sufficiently the balance of angular momentum, as will be shown in the discussion after Eq. (35).

Using the relation $\delta \boldsymbol{a}^{|/||} = \delta \boldsymbol{\xi}^{|} \times \boldsymbol{\xi}^{||} + \boldsymbol{\xi}^{|} \times \delta \boldsymbol{\xi}^{||}$ from Eq. (4), the variation of Π_2^{int} reads

$$\delta \Pi_2^{\text{int}} = \frac{1}{2} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \left[\left[\boldsymbol{\xi}^{||} \times \boldsymbol{m}^{|/||} \right] \cdot \delta \boldsymbol{\xi}^{|} + \left[\boldsymbol{m}^{|/||} \times \boldsymbol{\xi}^{|} \right] \cdot \delta \boldsymbol{\xi}^{||} \right] \mathrm{d}V^{||} \, \mathrm{d}V^{|} \, \mathrm{d}V$$

$$= \frac{1}{2} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \left[\left[\boldsymbol{\xi}^{||} \times \boldsymbol{m}^{|/||} \right] \cdot \delta \boldsymbol{\xi}^{|} - \left[\boldsymbol{\xi}^{|} \times \boldsymbol{m}^{|/||} \right] \cdot \delta \boldsymbol{\xi}^{||} \right] \mathrm{d}V^{||} \, \mathrm{d}V^{|} \, \mathrm{d}V.$$

To proceed, we change the order of integration for the second term and relabel the quantities, which yields

$$\delta \Pi_2^{\text{int}} = \frac{1}{2} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \left[\left[\boldsymbol{\xi}^{||} \times \boldsymbol{m}^{|/||} \right] \cdot \delta \boldsymbol{\xi}^{|} - \left[\boldsymbol{\xi}^{||} \times \boldsymbol{m}^{||/|} \right] \cdot \delta \boldsymbol{\xi}^{|} \right] \mathrm{d}V^{||} \, \mathrm{d}V^{|} \, \mathrm{d}V$$

$$= \frac{1}{2} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \left[\left[\boldsymbol{\xi}^{||} \times \boldsymbol{m}^{|/||} \right] \cdot \delta \boldsymbol{\xi}^{|} + \left[\boldsymbol{\xi}^{||} \times \boldsymbol{m}^{|/||} \right] \cdot \delta \boldsymbol{\xi}^{|} \right] \mathrm{d}V^{||} \, \mathrm{d}V^{|} \, \mathrm{d}V$$

$$= \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \left[\boldsymbol{\xi}^{||} \times \boldsymbol{m}^{|/||} \right] \cdot \delta \boldsymbol{\xi}^{|} \, \mathrm{d}V^{||} \, \mathrm{d}V^{|} \, \mathrm{d}V$$

$$= \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \left[\boldsymbol{\xi}^{||} \times \boldsymbol{m}^{|/||} \right] \cdot \delta \boldsymbol{\xi}^{|} \, \mathrm{d}V^{||} \, \mathrm{d}V^{|} \, \mathrm{d}V. \tag{12}$$

Motivated by the structure of Eq. (12), we define the force density per volume squared due to two-neighbour interactions by

$$\boldsymbol{p}_2^{|} := \int_{\mathcal{H}_0} \boldsymbol{\xi}^{||} \times \boldsymbol{m}^{|/||} \, \mathrm{d}V^{||} \qquad \text{with} \qquad \left[\boldsymbol{p}_2^{|} \right] = \mathrm{N/m}^6. \tag{13}$$

This result should be compared with the force density per volume squared due to one-neighbour interactions (8). The variation of Π_2^{int} with $\delta \boldsymbol{\xi}_1 = \delta \boldsymbol{y}_1 - \delta \boldsymbol{y}$ reads

$$\delta \Pi_2^{\text{int}} = \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{p}_2^{|} \cdot \delta \boldsymbol{\xi}^{|} \, \mathrm{d}V^{|} \, \mathrm{d}V$$

$$= \int_{\mathcal{B}_0} \left[\int_{\mathcal{H}_0} \boldsymbol{p}_2^{|} \cdot \delta \boldsymbol{y}^{|} \, \mathrm{d}V^{|} - \int_{\mathcal{H}_0} \boldsymbol{p}_2^{|} \, \mathrm{d}V^{|} \cdot \delta \boldsymbol{y} \right] \mathrm{d}V$$

$$= \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \boldsymbol{p}_2^{|} \cdot \delta \boldsymbol{y}^{|} \, \mathrm{d}V^{|} \, \mathrm{d}V - \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{p}_2^{|} \, \mathrm{d}V^{|} \cdot \delta \boldsymbol{y} \, \mathrm{d}V, \tag{14}$$

where we identify the internal force density per volume in the material configuration due to two-neighbour interactions $\boldsymbol{b}^{\text{int}}_{02}$ as

$$\boldsymbol{b}_{0\,2}^{\text{int}} := \int_{\mathcal{H}_0} \boldsymbol{p}_2^{|} \, \mathrm{d}V^{|} \qquad \text{with} \qquad \left[\boldsymbol{b}_{0\,2}^{\text{int}} \right] = \mathrm{N/m}^3. \tag{15}$$

Again, we recognize the right-hand side of Eq. (15) as an internal force density since it is the virtual power conjugated quantity to $\delta \boldsymbol{y}$ according to Eq. (14). Finally, the variation of the internal potential energy due to two-neighbour interactions Π_2^{int} reads

$$\delta \Pi_2^{\text{int}} = \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \boldsymbol{p}_2^{|} \cdot \delta \boldsymbol{y}^{|} \, \mathrm{d}V^{|} \, \mathrm{d}V - \int_{\mathcal{B}_0} \boldsymbol{b}_{0\,2}^{\text{int}} \cdot \delta \boldsymbol{y} \, \mathrm{d}V.$$

3.1.3. Three-neighbour interactions

The three-neighbour interaction energy density per volume to the fourth power in the material configuration $w_3^{|/||/|||}$ is a function of the volume element $v^{|/||/|||}$ between four points and reads

$$w_3^{|/||/|||} = w_3(v^{|/||/|||}) = w_3 \left(\left[\boldsymbol{\xi}(\boldsymbol{X}_1; \boldsymbol{X}) \times \boldsymbol{\xi}(\boldsymbol{X}^{||}; \boldsymbol{X}) \right] \cdot \boldsymbol{\xi}(\boldsymbol{X}^{|||}; \boldsymbol{X}) \right) \equiv w_3(v^{|/||/|||}; V^{|/||/|||}, \boldsymbol{X})$$

$$\text{with} \quad \left[w_3^{|/||/|||} \right] = \mathrm{N.m/m}^{12}.$$

We define the more familiar energy density per volume as one quarter of the triple integral of w_3 over the horizon $\mathcal{H}_0$ by

$$W_3 := \frac{1}{4} \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} w_3 \, \mathrm{d}V^{|||} \, \mathrm{d}V^{||} \, \mathrm{d}V^{|} \qquad \text{with} \qquad [W_3] = \mathrm{N.m/m}^3$$

with the factor one-fourth preventing quadruple counting due to the following quadruple interchangeable integrals. Consequently the internal potential energy due to three-neighbour interactions denoted Π_3^{int} reads

$$\Pi_3^{\text{int}} := \int_{\mathcal{B}_0} W_3 \, dV = \frac{1}{4} \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} w_3(v^{|/||/|||}) \, dV^{|||} \, dV^{||} \, dV^{|} \, dV \qquad \text{with} \qquad \left[\Pi_3^{\text{int}}\right] = \text{N.m}$$

$$\equiv \frac{1}{4} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} w_3(v^{|/||/|||}) \, dV^{|||} \, dV^{||} \, dV^{|} \, dV.$$

Next, the variation of Π_3^{int} can be written as

$$\delta \Pi_3^{\text{int}} = \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \frac{\partial w_3}{\partial v^{|/||/|||}} \, \delta v^{|/||/|||} \, dV^{|||} \, dV^{||} \, dV^{|} \, dV =: \frac{1}{3} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} p^{|/||/|||} \delta v^{|/||/|||} \, dV^{|||} \, dV^{||} \, dV^{|} \, dV$$

wherein the previously introduced factor one-fourth disappears due to the variation rules on multiple integrals and the factor one-third on the last term is introduced for convenience. The triple force density per volume to the fourth power $p^{|/||/|||}$ is defined by

$$p^{|/||/|||} \equiv p\left(\left[\boldsymbol{\xi}^{|} \times \boldsymbol{\xi}^{||}\right] \cdot \boldsymbol{\xi}^{|||}\right) := 3 \frac{\partial w_3}{\partial v^{|/||/|||}} \qquad \text{with} \qquad \left[p^{|/||/|||}\right] = \text{N/m}^{14}.$$

We note that p is invariant with respect to even permutations in $\boldsymbol{\xi}^{|}$, $\boldsymbol{\xi}^{||}$ and $\boldsymbol{\xi}^{|||}$ since

$$\left[\boldsymbol{\xi}^{|} \times \boldsymbol{\xi}^{||}\right] \cdot \boldsymbol{\xi}^{|||} = \left[\boldsymbol{\xi}^{||} \times \boldsymbol{\xi}^{|||}\right] \cdot \boldsymbol{\xi}^{|} = \left[\boldsymbol{\xi}^{|||} \times \boldsymbol{\xi}^{|}\right] \cdot \boldsymbol{\xi}^{||} \quad \Rightarrow \quad v^{|/||/|||} = v^{||/|||/|} = v^{|||/|/||} \quad \Rightarrow \quad p^{|/||/|||} = p^{||/|||/|} = p^{|||/|/||}. \quad (16)$$

We emphasize that $\boldsymbol{m}$ was assumed to be homogeneous of degree one such that the property $\boldsymbol{m}^{|/||} = -\boldsymbol{m}^{||/|}$ holds. However, p is *invariant with respect to even permutations by definition*. Using the relation $\delta v^{|/||/|||} = [\boldsymbol{\xi}^{||} \times \boldsymbol{\xi}^{|||}] \cdot \delta \boldsymbol{\xi}^{|} + [\boldsymbol{\xi}^{|||} \times \boldsymbol{\xi}^{|}] \cdot \delta \boldsymbol{\xi}^{||} + [\boldsymbol{\xi}^{|} \times \boldsymbol{\xi}^{||}] \cdot \delta \boldsymbol{\xi}^{|||}$ from Eq. (5), the variation of Π_3^{int} reads

$$\delta \Pi_3^{\text{int}} = \frac{1}{3} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} p^{|/||/|||} \left[[\boldsymbol{\xi}^{||} \times \boldsymbol{\xi}^{|||}] \cdot \delta \boldsymbol{\xi}^{|} + [\boldsymbol{\xi}^{|||} \times \boldsymbol{\xi}_1] \cdot \delta \boldsymbol{\xi}^{||} + [\boldsymbol{\xi}^{|} \times \boldsymbol{\xi}^{||}] \cdot \delta \boldsymbol{\xi}^{|||}\right] dV^{|||} \, dV^{||} \, dV^{|} \, dV$$

$$= \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} p^{|/||/|||} \left[[\boldsymbol{\xi}^{||} \times \boldsymbol{\xi}^{|||}] \cdot \delta \boldsymbol{\xi}^{|}\right] dV^{|||} \, dV^{||} \, dV^{|} \, dV$$

$$= \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} p^{|/||/|||} \left[[\boldsymbol{\xi}^{||} \times \boldsymbol{\xi}^{|||}] \cdot \delta \boldsymbol{\xi}^{|}\right] dV^{|||} \, dV^{||} \, dV^{|} \, dV, \qquad (17)$$

in which in the second step we changed the order of integration and relabelled the quantities. Motivated by the structure of Eq. (17), we define the force density per volume squared due to three-neighbour interactions as

$$\boldsymbol{p}_3^{|} := \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} p^{|/||/|||} [\boldsymbol{\xi}^{||} \times \boldsymbol{\xi}^{|||}] \, dV^{|||} \, dV^{||} \qquad \text{with} \qquad \left[\boldsymbol{p}_3^{|}\right] = \text{N/m}^6.$$

This should be compared with the force density per volume squared due to one-neighbour interactions (8) and the force density per volume squared due to two-neighbour interactions (13). The variation of Π_3^{int} with $\delta \boldsymbol{\xi}^{|} = \delta \boldsymbol{y}^{|} - \delta \boldsymbol{y}$ reads

$$\delta \Pi_3^{\text{int}} = \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{p}_3^{|} \cdot \delta \boldsymbol{\xi}^{|} \, dV^{|} \, dV$$

$$= \int_{\mathcal{B}_0} \left[\int_{\mathcal{H}_0} \boldsymbol{p}_3^{|} \cdot \delta \boldsymbol{y}^{|} \, dV^{|} - \int_{\mathcal{H}_0} \boldsymbol{p}_3^{|} \, dV^{|} \cdot \delta \boldsymbol{y}\right] dV$$

$$= \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \boldsymbol{p}_3^{|} \cdot \delta \boldsymbol{y}^{|} \, dV^{|} \, dV - \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{p}_3^{|} \, dV^{|} \cdot \delta \boldsymbol{y} \, dV \qquad (18)$$

in which we identify the internal force density per volume in the material configuration due to three-neighbour interactions $\boldsymbol{b}_{03}^{\text{int}}$ as

$$\boldsymbol{b}_{03}^{\text{int}} := \int_{\mathcal{H}_0} \boldsymbol{p}_3^{|} \, dV^{|} \qquad \text{with} \qquad \left[\boldsymbol{b}_{03}^{\text{int}}\right] = \text{N/m}^3. \qquad (19)$$

The right-hand side of Eq. (19) is again an internal force density since it is the virtual power conjugated quantity to $\delta \boldsymbol{y}$ according to Eq. (18). Finally, the variation of the internal potential energy due to three-neighbour interactions Π_3^{int} reads

$$\delta \Pi_3^{\text{int}} = \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \boldsymbol{p}_3^{|} \cdot \delta \boldsymbol{y}^{|} \, dV^{|} \, dV - \int_{\mathcal{B}_0} \boldsymbol{b}_{03}^{\text{int}} \cdot \delta \boldsymbol{y} \, dV.$$

3.2. External potential energy

Let Π^{ext} be the external potential energy functional consisting of the contributions from both the externally prescribed forces within the bulk and *tractions* on the surface of the body. Note that, in contrast to Silling (2000), we allow for the externally prescribed tractions exclusively acting on the boundary of the body, i.e. they are not considered as the result of a cut-out volume within the body. We emphasize that *our assumption is in contrast to, but not necessarily in violation of the standard PD* since the tractions could be embedded within the internal force densities. The external potential energy Π^{ext} can thus be expressed as

$$\Pi^{\mathrm{ext}} = -\int_{\mathcal{B}_0} \boldsymbol{b}_0^{\mathrm{ext}} \cdot \boldsymbol{y} \, \mathrm{d}V - \int_{\partial\mathcal{B}_0} \boldsymbol{t}_0^{\mathrm{ext}} \cdot \boldsymbol{y} \, \mathrm{d}A$$

where $\boldsymbol{b}^{\mathrm{ext}}_0$ denotes the external force density per volume in the material configuration, with units N/m^3, and $\boldsymbol{t}^{\mathrm{ext}}_0$ is the external traction on the boundary in the material configuration, with units N/m^2. Note, this format of the external potential energy is a particular sub-case of a more general case applicable to higher gradient and non-local continua as elaborated by Auffray et al. (2015); Javili et al. (2013a), among others.

3.3. Governing equations

The total potential energy functional Π that we seek to minimize with respect to all admissible (spatial) variations $\delta\boldsymbol{y}$ at fixed material placement is composed of the internal and external contributions according to Eq. (6), that is

$$\delta\Pi = 0 \quad \forall\delta\boldsymbol{y} \qquad \text{with} \qquad \Pi = \Pi^{\mathrm{int}} + \Pi^{\mathrm{ext}} \qquad \text{and} \qquad \Pi^{\mathrm{int}} = \Pi_1^{\mathrm{int}} + \Pi_2^{\mathrm{int}} + \Pi_3^{\mathrm{int}},$$

and therefore

$$\delta\Pi = \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \boldsymbol{p}^{|} \cdot \delta\boldsymbol{y}^{|} \, \mathrm{d}V^{|} \, \mathrm{d}V - \int_{\mathcal{B}_0} \boldsymbol{b}_0^{\mathrm{int}} \cdot \delta\boldsymbol{y} \, \mathrm{d}V - \int_{\mathcal{B}_0} \boldsymbol{b}_0^{\mathrm{ext}} \cdot \delta\boldsymbol{y} \, \mathrm{d}V - \int_{\partial\mathcal{B}_0} \boldsymbol{t}_0^{\mathrm{ext}} \cdot \delta\boldsymbol{y} \, \mathrm{d}A \overset{!}{=} 0 \quad \forall\delta\boldsymbol{y}, \tag{20}$$

in which

$$\boldsymbol{p}^{|} := \boldsymbol{p}_1^{|} + \boldsymbol{p}_2^{|} + \boldsymbol{p}_3^{|} \qquad \text{and} \qquad \boldsymbol{b}_0^{\mathrm{int}} := \boldsymbol{b}_{0\,1}^{\mathrm{int}} + \boldsymbol{b}_{0\,2}^{\mathrm{int}} + \boldsymbol{b}_{0\,3}^{\mathrm{int}},$$

where

$$\boldsymbol{p}^{|} := \frac{\partial w_1}{\partial \boldsymbol{\xi}^{|}} + 2\int_{\mathcal{H}_0} \boldsymbol{\xi}^{||} \times \frac{\partial w_2}{\partial \boldsymbol{a}^{|/||}} \, \mathrm{d}V^{||} + 3\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \frac{\partial w_3}{\partial v^{|/||/|||}} [\boldsymbol{\xi}^{||} \times \boldsymbol{\xi}^{|||}] \, \mathrm{d}V^{|||} \, \mathrm{d}V^{||} \qquad \text{and} \qquad \boldsymbol{b}_0^{\mathrm{int}} := \int_{\mathcal{H}_0} \boldsymbol{p}^{|} \, \mathrm{d}V^{|}. \tag{21}$$

From the structure of the variational form (20) we can readily extract the governing equation as

$$\boldsymbol{b}_0^{\mathrm{int}} + \boldsymbol{b}_0^{\mathrm{ext}} = \boldsymbol{0} \quad \forall\boldsymbol{X} \in \mathcal{B}_0 \qquad \text{subject to} \qquad \int_{\mathcal{B}_0}\int_{\mathcal{B}_0} \boldsymbol{p}^{|} \cdot \delta\boldsymbol{y}^{|} \, \mathrm{d}V^{|} \, \mathrm{d}V = \int_{\partial\mathcal{B}_0} \boldsymbol{t}_0^{\mathrm{ext}} \cdot \delta\boldsymbol{y} \, \mathrm{d}A \quad \forall\delta\boldsymbol{y}. \tag{22}$$

The internal body force density here corresponds to the stress divergence in the classical continuum mechanics formalism where $\boldsymbol{b}_0^{\mathrm{int}} = \mathrm{Div}\boldsymbol{P}$ and $\boldsymbol{P}$ is the Piola stress. The variational governing Eq. (22) should be compared to its counterpart in classical continuum mechanics where

$$\boldsymbol{b}_0^{\mathrm{int}} + \boldsymbol{b}_0^{\mathrm{ext}} = \boldsymbol{0} \quad \forall\boldsymbol{X} \in \mathcal{B}_0 \qquad \text{subject to} \qquad \int_{\mathcal{B}_0} \mathrm{Div}(\delta\boldsymbol{y} \cdot \boldsymbol{P}) \, \mathrm{d}V = \int_{\partial\mathcal{B}_0} \boldsymbol{t}_0^{\mathrm{ext}} \cdot \delta\boldsymbol{y} \, \mathrm{d}A \quad \forall\delta\boldsymbol{y},$$

or in its more familiar local form

$$\mathrm{Div}\boldsymbol{P} + \boldsymbol{b}_0^{\mathrm{ext}} = \boldsymbol{0} \qquad \text{subject to} \qquad \boldsymbol{P} \cdot \boldsymbol{N} = \boldsymbol{t}_0^{\mathrm{ext}}.$$

The above should, in turn, be compared to the relation

$$\int_{\mathcal{H}_0} \boldsymbol{p}^{|} \, \mathrm{d}V^{|} + \boldsymbol{b}_0^{\mathrm{ext}} = \boldsymbol{0}, \tag{23}$$

subject to the boundary conditions that can be extracted form Eq. (22)$_2$ and will be clarified shortly. We emphasize that the requirement for the *virtual power equivalence*,

$$\int_{\mathcal{B}_0}\int_{\mathcal{B}_0} \boldsymbol{p}^{|} \cdot \delta\boldsymbol{y}^{|} \, \mathrm{d}V^{|} \, \mathrm{d}V = \int_{\partial\mathcal{B}_0} \boldsymbol{t}_0^{\mathrm{ext}} \cdot \delta\boldsymbol{y} \, \mathrm{d}A \quad \forall\delta\boldsymbol{y}, \tag{24}$$

is an underlying postulate of our framework and a key feature of this contribution. This relation allows one to introduce and prescribe external tractions on the boundary. If the external boundary is traction free or if only displacement type boundary conditions are prescribed, the right-hand side of the requirement (24) vanishes and it reduces to

$$\int_{\mathcal{B}_0}\int_{\mathcal{B}_0} \boldsymbol{p}^{|} \cdot \delta\boldsymbol{y}^{|} \, \mathrm{d}V^{|} \, \mathrm{d}V = 0.$$

This is the more familiar requirement in classical PD.

Remark. Central to the state-based PD is the notion of "correspondence" which essentially states that a peridynamic constitutive model can "correspond" to a classical constitutive continuum model for homogeneous deformations. Correspondence allows one to calibrate a PD material model such that it furnishes the same result as the corresponding classical continuum model for a given homogeneous deformation. However, the constitutive correspondence framework of PD can lead to non-physical deformation modes including material collapse, matter inter-penetration at discontinuities, and may suffer from zero-energy mode instability. These have been addressed by Tupek and Radovitzky (2014) and Silling (2017) among others. The first and most significant step in deriving a correspondence model (Silling et al., 2007) is to approximate the deformation gradient $\boldsymbol{F}$. Since the kinematics in our approach coincides with that of classical continuum mechanics, the deformation gradient need not be approximated and can be obtained exactly. Therefore, it seems reasonable that the continuum-kinematics-inspired approach can alleviate some of the aforementioned issues with the correspondence framework of PD. Nonetheless, this task is beyond the scope of the current manuscript and shall be elaborated in a separate contribution. □

Remark While one-neighbour interactions are the more familiar type in mechanics, multiple-neighbour interactions are commonly employed for atomistic modeling and molecular dynamics simulations. Such multiple-neighbour interactions are often described in terms of angles and bond-length instead of area and volume. We adopt a continuum-kinematics-inspired approach; our deformation measures are common continuum measures, namely length, area and volume. So equipped, various interaction energy densities can be proposed and their respective coefficients calculated via a suitable parameter identification procedure. The generic forms of interaction energy densities will be given in Section 4.2. To aid understanding, elastic 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. Elastic 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, elastic 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 of classical continuum mechanics in three dimensions. □

Remark Our formulation can impose both plane-strain and plane-stress assumptions via satisfying respective boundary conditions on a three-dimensional domain. Our formulation in 2D, however, corresponds to a purely two-dimensional case similar to the surface elasticity theory of Gurtin and Murdoch (1975), see also (Javili et al., 2013b). Obviously, three-neighbour interactions do not contribute in the 2D case. Note that neither "stress" nor "strain" is present in the peridynamic formulation and they can only be computed through post-processing. Therefore, the notions of "plane strain" or "plane stress" become naturally less relevant as they correspond to a local view on continuum mechanics. □

Remark Our formulation is inherently non-local and, similar to classical non-local theories, can capture a frequency-dependent wave speed. Thus, dispersion of elastic waves occurs naturally. Dispersion would certainly be a feature of our model and motivates further investigation, in a separate contribution, in the spirit of the analyses provided by Bazant et al.(2016) and Butt et al.(2017). The current model may inherit some of the pathological behaviours reported in this context and thus this potential issue shall be explored. An in-depth analysis is left for a future contribution. □

4. Thermodynamic balance laws

Equipped with the virtual power equivalence (24) for a quasi-static conservative case, we can proceed to derive the thermodynamic balance laws for more general cases. Note the virtual power equivalence (24) must hold for any arbitrary $\delta \boldsymbol{y}$. Among all admissible motions, we select *rigid translation* and *rigid rotation* in what follows. For a rigid translation of the body $\delta \boldsymbol{y} = \delta \boldsymbol{y}^{\mid} = \text{const.}$ and therefore the virtual power equivalence reduces to

$$\int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{p}^{\mid} \, \mathrm{d}V^{\mid} \, \mathrm{d}V = \int_{\partial \mathcal{B}_0} \boldsymbol{t}_0^{\text{ext}} \, \mathrm{d}A \qquad \Rightarrow \qquad \int_{\mathcal{B}_0} \boldsymbol{b}_0^{\text{int}} \, \mathrm{d}V = \int_{\partial \mathcal{B}_0} \boldsymbol{t}_0^{\text{ext}} \, \mathrm{d}A \,. \tag{25}$$

This can be understood as *traction equivalence* and serves as the boundary condition for balance Eq. (23). Its more familiar counterpart in classical continuum mechanics, obtained using the Gauss theorem, and the traction boundary conditions are given by

$$\int_{\mathcal{B}_0} \text{Div}\boldsymbol{P} \, \mathrm{d}V = \int_{\partial \mathcal{B}_0} \boldsymbol{t}_0^{\text{ext}} \, \mathrm{d}A \qquad \text{with} \qquad \boldsymbol{P} \cdot \boldsymbol{N} = \boldsymbol{t}_0^{\text{ext}} \,.$$

For a rigid rotation of the body $\delta \boldsymbol{y} = \boldsymbol{\omega}_\delta \times \boldsymbol{y}$ and $\delta \boldsymbol{y}^{\mid} = \boldsymbol{\omega}_\delta \times \boldsymbol{y}^{\mid}$ with $\boldsymbol{\omega}_\delta = \text{const.}$ being the variational analogue to the angular velocity vector and the virtual power equivalence reduces to

$$\int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{y}^{\mid} \times \boldsymbol{p}^{\mid} \, \mathrm{d}V^{\mid} \, \mathrm{d}V = \int_{\partial \mathcal{B}_0} \boldsymbol{y} \times \boldsymbol{t}_0^{\text{ext}} \, \mathrm{d}A \,, \tag{26}$$

which can be understood as *torque equivalence*. This should be compared with its more familiar counterpart in classical continuum mechanics given by

$$\int_{\mathcal{B}_0} \text{Div}(\boldsymbol{y} \times \boldsymbol{P}) \, \mathrm{d}V = \int_{\partial \mathcal{B}_0} \boldsymbol{y} \times \boldsymbol{t}_0^{\text{ext}} \, \mathrm{d}A \qquad \text{with} \qquad \boldsymbol{P} \cdot \boldsymbol{N} = \boldsymbol{t}_0^{\text{ext}} \,.$$

4.1. Momentum balances

To derive the momentum balance equations of a dynamic and possibly non-conservative problem, we follow the standard procedure of classical continuum mechanics. In doing so, we begin with the global form of the force or moment balance in their integral forms and identify terms using the traction equivalence (25) and the torque equivalence (26) relations. Obviously, this process must be carried out for both the *linear momentum balance* and the *angular momentum balance* separately. Let $\boldsymbol{v}$ denote the velocity of the material point $\boldsymbol{X}$ and ρ_0 the mass density per volume in the material configuration. The global form of the linear momentum balance reads

$$\int_{\mathcal{B}_0} \rho_0\, \dot{\boldsymbol{v}}\, \mathrm{d}V = \int_{\partial \mathcal{B}_0} \boldsymbol{t}_0^{\mathrm{ext}}\, \mathrm{d}A + \int_{\mathcal{B}_0} \boldsymbol{b}_0^{\mathrm{ext}}\, \mathrm{d}V\,.$$

The integral of external traction $\boldsymbol{t}^{\mathrm{ext}}{}_0$ is now replaced by the traction equivalence (25) and the definition of the internal body force density $(21)_2$ is employed to obtain

$$\int_{\mathcal{B}_0} \rho_0\, \dot{\boldsymbol{v}}\, \mathrm{d}V = \int_{\mathcal{B}_0} \boldsymbol{b}_0^{\mathrm{int}}\, \mathrm{d}V + \int_{\mathcal{B}_0} \boldsymbol{b}_0^{\mathrm{ext}}\, \mathrm{d}V \qquad \Rightarrow \qquad \int_{\mathcal{B}_0} \rho_0\, \dot{\boldsymbol{v}}\, \mathrm{d}V = \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{p}^|\, \mathrm{d}V^|\, \mathrm{d}V + \int_{\mathcal{B}_0} \boldsymbol{b}_0^{\mathrm{ext}}\, \mathrm{d}V\,,$$

which yields the non-local form of the linear momentum balance via localization as

$$\rho_0\, \dot{\boldsymbol{v}} = \boldsymbol{b}_0^{\mathrm{int}} + \boldsymbol{b}_0^{\mathrm{ext}} \qquad \Rightarrow \qquad \rho_0\, \dot{\boldsymbol{v}} = \int_{\mathcal{H}_0} \boldsymbol{p}^|\, \mathrm{d}V^| + \boldsymbol{b}_0^{\mathrm{ext}}\,. \tag{27}$$

Its counterpart in classical continuum mechanics is given by

$$\rho_0\, \dot{\boldsymbol{v}} = \boldsymbol{b}_0^{\mathrm{int}} + \boldsymbol{b}_0^{\mathrm{ext}} \qquad \Rightarrow \qquad \rho_0\, \dot{\boldsymbol{v}} = \mathrm{Div}\boldsymbol{P} + \boldsymbol{b}_0^{\mathrm{ext}}\,.$$

To derive the angular momentum balance, we start from the global form of the moment balance

$$\int_{\mathcal{B}_0} \boldsymbol{y} \times [\rho_0\, \dot{\boldsymbol{v}}]\, \mathrm{d}V = \int_{\partial \mathcal{B}_0} \boldsymbol{y} \times \boldsymbol{t}_0^{\mathrm{ext}}\, \mathrm{d}A + \int_{\mathcal{B}_0} \boldsymbol{y} \times \boldsymbol{b}_0^{\mathrm{ext}}\, \mathrm{d}V\,.$$

The integral of external traction moment $\boldsymbol{y} \times \boldsymbol{t}^{\mathrm{ext}}{}_0$ is now replaced by the torque equivalence (26) to yield

$$\begin{aligned}
\int_{\mathcal{B}_0} \boldsymbol{y} \times [\rho_0\, \dot{\boldsymbol{v}}]\, \mathrm{d}V &= \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{y}^| \times \boldsymbol{p}^|\, \mathrm{d}V^|\, \mathrm{d}V + \int_{\mathcal{B}_0} \boldsymbol{y} \times \boldsymbol{b}_0^{\mathrm{ext}}\, \mathrm{d}V \\
&= \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} [\boldsymbol{\xi}_1 + \boldsymbol{y}] \times \boldsymbol{p}^|\, \mathrm{d}V^|\, \mathrm{d}V + \int_{\mathcal{B}_0} \boldsymbol{y} \times \boldsymbol{b}_0^{\mathrm{ext}}\, \mathrm{d}V \\
&= \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{\xi}^| \times \boldsymbol{p}^|\, \mathrm{d}V^|\, \mathrm{d}V + \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{y} \times \boldsymbol{p}^|\, \mathrm{d}V^|\, \mathrm{d}V + \int_{\mathcal{B}_0} \boldsymbol{y} \times \boldsymbol{b}_0^{\mathrm{ext}}\, \mathrm{d}V \\
&= \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{\xi}^| \times \boldsymbol{p}^|\, \mathrm{d}V^|\, \mathrm{d}V + \int_{\mathcal{B}_0} \boldsymbol{y} \times [\boldsymbol{b}_0^{\mathrm{int}} + \boldsymbol{b}_0^{\mathrm{ext}}]\, \mathrm{d}V\,.
\end{aligned}$$

Using the linear momentum balance (27), this reduces to the global form of the angular momentum balance

$$\int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{\xi}^| \times \boldsymbol{p}^|\, \mathrm{d}V^|\, \mathrm{d}V = \boldsymbol{0},$$

and upon localization yields the non-local form of the angular momentum balance

$$\int_{\mathcal{H}_0} \boldsymbol{\xi}^| \times \boldsymbol{p}^|\, \mathrm{d}V^| = \boldsymbol{0}\,. \tag{28}$$

Its counterpart in classical continuum mechanics is given by

$$\boldsymbol{\varepsilon} : [\boldsymbol{F} \cdot \boldsymbol{P}^{\mathrm{t}}] = \boldsymbol{0} \qquad \text{with} \qquad \boldsymbol{\varepsilon} \text{ the third-order permutation tensor}\,.$$

4.2. Consequences of balance of angular momentum on elastic interaction forces

Next, we explore the consequences of the angular momentum balance (28) on the interactions and the possible restrictions it imposes on interaction potentials. In particular, we investigate the conditions required for the nature of interactions such that the angular momentum balance is a priori fulfilled. The force density per volume squared $\boldsymbol{p}_1$ is additively composed of force densities per volume squared due to one-neighbour, two-neighbour and three-neighbour interactions. Thus, the expanded version of the angular momentum balance reads

$$\int_{\mathcal{H}_0} \boldsymbol{\xi}^| \times \boldsymbol{p}^|\, \mathrm{d}V^| \overset{!}{=} \boldsymbol{0} \quad \forall \boldsymbol{X} \qquad \Rightarrow \qquad \int_{\mathcal{H}_0} \boldsymbol{\xi}^| \times \boldsymbol{p}_1^|\, \mathrm{d}V^| + \int_{\mathcal{H}_0} \boldsymbol{\xi}^| \times \boldsymbol{p}_2^|\, \mathrm{d}V^| + \int_{\mathcal{H}_0} \boldsymbol{\xi}^| \times \boldsymbol{p}_3^|\, \mathrm{d}V^| \overset{!}{=} \boldsymbol{0} \quad \forall \boldsymbol{X}\,.$$

Each of the three integrals must vanish identically in order to *sufficiently* satisfy the angular momentum balance. Accordingly, we require

$$\int_{\mathcal{H}_0} \boldsymbol{\xi}^| \times \boldsymbol{p}_1^|\, \mathrm{d}V^| \overset{!}{=} \boldsymbol{0} \qquad , \qquad \int_{\mathcal{H}_0} \boldsymbol{\xi}^| \times \boldsymbol{p}_2^|\, \mathrm{d}V^| \overset{!}{=} \boldsymbol{0} \qquad , \qquad \int_{\mathcal{H}_0} \boldsymbol{\xi}^| \times \boldsymbol{p}_3^|\, \mathrm{d}V^| \overset{!}{=} \boldsymbol{0}\,. \tag{29}$$

Therefore, we next investigate separately the one-neighbour, two-neighbour and three-neighbour interactions.

4.2.1. One-neighbour interactions

Recall the one-neighbour interaction energy density per volume squared in the material configuration w_1 in its most generic form is a function of the relative position $\boldsymbol{\xi}^|$, i.e. the finite line element, between two points with the force density per volume squared denoted as $\boldsymbol{p}_1^|$, that is

$$w_1^| = w_1(\boldsymbol{\xi}^|) \qquad \Rightarrow \qquad \boldsymbol{p}_1^| := \frac{\partial w_1}{\partial \boldsymbol{\xi}^|} . \tag{30}$$

Inserting $\boldsymbol{p}_1^|$ from Eq. (30) into Eq. (29)$_1$ yields the condition

$$\int_{\mathcal{H}_0} \boldsymbol{\xi}^| \times \boldsymbol{p}_1^| \, dV^| \overset{!}{=} \boldsymbol{0} \qquad \Rightarrow \qquad \boldsymbol{p}_1^| \overset{!}{=} \zeta_1 \, \boldsymbol{\xi}^| \qquad \text{or} \qquad \frac{\partial w_1}{\partial \boldsymbol{\xi}^|} \propto \boldsymbol{\xi}^| , \tag{31}$$

required to satisfy the angular momentum balance due to one-neighbour interactions with $\zeta_1 = \zeta_1(\boldsymbol{\xi}^|)$ being an arbitrary function of $\boldsymbol{\xi}^|$.

Example If the one-neighbour interaction energy density w_1 takes the form $w_1^| = w_1(\imath)$ with $\imath$ being a square function $\imath := |\boldsymbol{\xi}^||^2/2$, it sufficiently fulfils the angular momentum balance condition (31). That is

$$w_1^| = w_1(\imath) \qquad \text{with} \qquad \imath := \frac{1}{2} |\boldsymbol{\xi}^||^2 = \frac{1}{2} [\xi^|]^2 \qquad \text{and} \qquad \xi^| := |\boldsymbol{\xi}^|| ,$$

resulting in

$$\boldsymbol{p}_1^| = \frac{\partial w_1}{\partial \boldsymbol{\xi}^|} = \frac{\partial w_1}{\partial \imath} \frac{\partial \imath}{\partial \xi^|} \frac{\partial \xi^|}{\partial \boldsymbol{\xi}^|} = \frac{\partial w_1}{\partial \imath} \xi^| \frac{\boldsymbol{\xi}^|}{\xi^|} = \frac{\partial w_1}{\partial \imath} \boldsymbol{\xi}^| = \zeta_1 \boldsymbol{\xi}^| \propto \boldsymbol{\xi}^| ,$$

with the function $\zeta_1 = \zeta_1(\boldsymbol{\xi}^|)$ defined as

$$\zeta_1 := \frac{\partial w_1}{\partial \imath} .$$

This is a generic example of central interaction forces corresponding to the original bond-based model of Silling (2000).

4.2.2. Two-neighbour interactions

The two-neighbour interaction energy density per volume cubed in the material configuration w_2 in its most generic form is a function of the finite vectorial area element $\boldsymbol{a}^{|/\|}$ among three points with the force density per volume squared denoted as $\boldsymbol{p}_2^|$, that is

$$w_2^| = w_2(\boldsymbol{a}^{|/\|}) \qquad \Rightarrow \qquad \boldsymbol{p}_2^| := \int_{\mathcal{H}_0} \boldsymbol{\xi}^\| \times \boldsymbol{m}^{|/\|} \, dV^\| \qquad \text{with} \qquad \boldsymbol{m}^{|/\|} := 2 \frac{\partial w_2}{\partial \boldsymbol{a}^{|/\|}} . \tag{32}$$

Inserting $\boldsymbol{p}_2^|$ from Eq. (32) into Eq. (29)$_2$ yields the condition

$$\int_{\mathcal{H}_0} \boldsymbol{\xi}^| \times \boldsymbol{p}_2^| \, dV^| \overset{!}{=} \boldsymbol{0} \qquad \Rightarrow \qquad \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \boldsymbol{\xi}^| \times [\boldsymbol{\xi}^\| \times \boldsymbol{m}^{|/\|}] \, dV^\| \, dV^| \overset{!}{=} \boldsymbol{0} . \tag{33}$$

Using the identity $\boldsymbol{a} \times [\boldsymbol{b} \times \boldsymbol{c}] = \boldsymbol{b}[\boldsymbol{a} \cdot \boldsymbol{c}] - \boldsymbol{c}[\boldsymbol{a} \cdot \boldsymbol{b}]$ for arbitrary vectors $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$, the condition (33) can be rewritten as

$$\int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \boldsymbol{\xi}^| \times [\boldsymbol{\xi}^\| \times \boldsymbol{m}^{|/\|}] \, dV^\| \, dV^| = \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} -\boldsymbol{m}^{|/\|} [\boldsymbol{\xi}^| \cdot \boldsymbol{\xi}^\|] \, dV^\| \, dV^| + \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \boldsymbol{\xi}^\| [\boldsymbol{\xi}^| \cdot \boldsymbol{m}^{|/\|}] \, dV^\| \, dV^| \overset{!}{=} \boldsymbol{0} . \tag{34}$$

The first double-integral on the right-hand side can be expressed equivalently by changing the labels as

$$\int_{\mathcal{H}_0} \int_{\mathcal{H}_0} -\boldsymbol{m}^{|/\|} [\boldsymbol{\xi}^| \cdot \boldsymbol{\xi}^\|] \, dV^\| \, dV^| \equiv \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} -\boldsymbol{m}^{\|/|} [\boldsymbol{\xi}^\| \cdot \boldsymbol{\xi}^|] \, dV^\| \, dV^| = \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \boldsymbol{m}^{|/\|} [\boldsymbol{\xi}^| \cdot \boldsymbol{\xi}^\|] \, dV^\| \, dV^| \tag{35}$$

in which the last step holds since $\boldsymbol{m}^{\|/|} = -\boldsymbol{m}^{|/\|}$ according to assumption (11). The relation (35) indicates that the first double-integral on the right-hand side of Eq. (34) is equal to its negative and thus, it can only be zero. In order to guarantee that the second term on the right-hand side of Eq. (34) vanishes, we further require $\boldsymbol{m}^{|/\|} \propto [\boldsymbol{\xi}^| \times \boldsymbol{\xi}^\|]$, or alternatively $\boldsymbol{m}^{|/\|} = \zeta_2 [\boldsymbol{\xi}^| \times \boldsymbol{\xi}^\|]$ with ζ_2 being an arbitrary function of $\boldsymbol{a}^{|/\|}$ holding the property $\zeta_2(\boldsymbol{a}^{|/\|}) = \zeta_2(\boldsymbol{a}^{\|/|})$ so that $\boldsymbol{m}^{|/\|} = -\boldsymbol{m}^{\|/|}$ according to assumption (11). This requirement enforces $\boldsymbol{\xi}^|$ to be orthogonal to $\boldsymbol{m}^{|/\|}$ and therefore, $\boldsymbol{\xi}^| \cdot \boldsymbol{m}^{|/\|}$ vanishes identically and thus the condition (34) is fulfilled a priori.

Example If the two-neighbour interaction energy density w_2 takes the form $w_2^| = w_2(a)$, with a being a square function such as $a := |\boldsymbol{a}^{|/\|}|^2/2$, it sufficiently fulfils the angular momentum balance condition (33). That is

$$w_2^| = w_2(a) \qquad \text{with} \qquad a := \frac{1}{2} |\boldsymbol{a}^{|/\|}|^2 = \frac{1}{2} [a^{|/\|}]^2 \qquad \text{and} \qquad a^{|/\|} := |\boldsymbol{a}^{|/\|}|$$

resulting in

$$\boldsymbol{m}^{|/||} = 2\frac{\partial w_2}{\partial \boldsymbol{a}^{|/||}} = 2\frac{\partial w_2}{\partial a}\frac{\partial a}{\partial a^{|/||}}\frac{\partial a^{|/||}}{\partial \boldsymbol{a}^{|/||}} = 2\frac{\partial w_2}{\partial a}a^{|/||}\frac{\boldsymbol{a}^{|/||}}{a^{|/||}} = 2\frac{\partial w_2}{\partial a}\boldsymbol{a}^{|/||} = 2\frac{\partial w_2}{\partial a}\boldsymbol{\xi}^| \times \boldsymbol{\xi}^{||} = \zeta_2\,\boldsymbol{\xi}^| \times \boldsymbol{\xi}^{||} \propto \boldsymbol{\xi}^| \times \boldsymbol{\xi}^{||},$$

with the function $\zeta_2 = \zeta_2(\boldsymbol{a}^{|/||})$ defined as

$$\zeta_2 := 2\frac{\partial w_2}{\partial a}$$

which satisfies the property $\zeta_2(\boldsymbol{a}^{|/||}) = \zeta_2(\boldsymbol{a}^{||/|})$ so that $\boldsymbol{m}^{|/||} = -\boldsymbol{m}^{|/||}$ and finally

$$\boldsymbol{p}_2^{\,|} = \int_{\mathcal{H}_0}\boldsymbol{\xi}^{||}\times\boldsymbol{m}^{|/||}\,\mathrm{d}V^{||} = \int_{\mathcal{H}_0}\boldsymbol{\xi}^{||}\times[\zeta_2\,\boldsymbol{\xi}^|\times\boldsymbol{\xi}^{||}]\,\mathrm{d}V^{||} = \int_{\mathcal{H}_0}\zeta_2\Big[\boldsymbol{\xi}^|[\boldsymbol{\xi}^{||}\cdot\boldsymbol{\xi}^{||}] - \boldsymbol{\xi}^{||}[\boldsymbol{\xi}^{||}\cdot\boldsymbol{\xi}^|]\Big]\,\mathrm{d}V^{||}.$$

This is an example of interaction forces that do not fall in the class of the bond-based models, however, it is also an alternative to the state-based approach due to Silling et al. (2007).

4.2.3. Three-neighbour interactions

The three-neighbour interaction energy density per volume to the fourth power in the material configuration w_3 in its most generic form is a function of the finite volume element $v^{|/||/|||}$ constructed by four points with the force density per volume squared denoted as $\boldsymbol{p}_3^{\,|}$, that is

$$w_3^{\,|} = w_3(v^{|/||/|||}) \qquad \Rightarrow \qquad \boldsymbol{p}_3^{\,|} := \int_{\mathcal{H}_0}\int_{\mathcal{H}_0} p^{|/||/|||}[\boldsymbol{\xi}^{||}\times\boldsymbol{\xi}^{|||}]\,\mathrm{d}V^{|||}\,\mathrm{d}V^{||} \qquad \text{with} \qquad p^{|/||/|||} := 3\frac{\partial w_3}{\partial v^{|/||/|||}}. \tag{36}$$

Inserting $\boldsymbol{p}_3^{\,|}$ from Eq. (36) into Eq. (29)$_3$ yields the condition

$$\int_{\mathcal{H}_0}\boldsymbol{\xi}^|\times\boldsymbol{p}_3^{\,|}\,\mathrm{d}V^| \overset{!}{=} \boldsymbol{0} \qquad \Rightarrow \qquad \int_{\mathcal{H}_0}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0}\boldsymbol{\xi}^|\times\Big[p^{|/||/|||}[\boldsymbol{\xi}^{||}\times\boldsymbol{\xi}^{|||}]\Big]\,\mathrm{d}V^{|||}\,\mathrm{d}V^{||}\,\mathrm{d}V^| \overset{!}{=} \boldsymbol{0}. \tag{37}$$

Relabelling the condition (37) furnishes

$$\int_{\mathcal{H}_0}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} p^{|/||/|||}\Big[\boldsymbol{\xi}^|\times[\boldsymbol{\xi}^{||}\times\boldsymbol{\xi}^{|||}]\Big]\,\mathrm{d}V^{|||}\,\mathrm{d}V^{||}\,\mathrm{d}V^| = \int_{\mathcal{H}_0}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} p^{|||/|/||}\Big[\boldsymbol{\xi}^{|||}\times[\boldsymbol{\xi}^|\times\boldsymbol{\xi}^{||}]\Big]\,\mathrm{d}V^{||}\,\mathrm{d}V^|\,\mathrm{d}V^{|||}$$

$$= \int_{\mathcal{H}_0}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} p^{||/|||/|}\Big[\boldsymbol{\xi}^{||}\times[\boldsymbol{\xi}^{|||}\times\boldsymbol{\xi}_I]\Big]\,\mathrm{d}V^|\,\mathrm{d}V^{|||}\,\mathrm{d}V^{||} \overset{!}{=} \boldsymbol{0}.$$

After adding up the arguments of the integrals considering that $p^{|/||/|||}$ is by definition invariant with respect to even permutations (16), the condition (37) reduces to

$$\frac{1}{3}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} p^{|/||/|||}\Big[\boldsymbol{\xi}^|\times[\boldsymbol{\xi}^{||}\times\boldsymbol{\xi}^{|||}] + \boldsymbol{\xi}^{|||}\times[\boldsymbol{\xi}^|\times\boldsymbol{\xi}^{||}] + \boldsymbol{\xi}^{||}\times[\boldsymbol{\xi}^{|||}\times\boldsymbol{\xi}_I]\Big]\,\mathrm{d}V^{|||}\,\mathrm{d}V^{||}\,\mathrm{d}V^| \overset{!}{=} \boldsymbol{0},$$

which is a priori satisfied due to the Jacobi identity

$$\boldsymbol{\xi}^|\times[\boldsymbol{\xi}^{||}\times\boldsymbol{\xi}^{|||}] + \boldsymbol{\xi}^{|||}\times[\boldsymbol{\xi}^|\times\boldsymbol{\xi}^{||}] + \boldsymbol{\xi}^{||}\times[\boldsymbol{\xi}^{|||}\times\boldsymbol{\xi}_I] = \boldsymbol{0}.$$

Thus, the condition (37) is fulfilled a priori with no further restriction on $p^{|/||/|||}$.

Example If the three-neighbour interaction energy density w_3 takes the form $w_3^{\,|} = w_3(v)$, with v being a square function as $v := [v^{|/||/|||}]^2/2$, it sufficiently fulfils the angular momentum balance condition (37). That is

$$w_3^{\,|} = w_3(v) \qquad \text{with} \qquad v := \frac{1}{2}[v^{|/||/|||}]^2$$

resulting in

$$p^{|/||/|||} = 3\frac{\partial w_3}{\partial v^{|/||/|||}} = 3\frac{\partial w_3}{\partial v}\frac{\partial v}{\partial v^{|/||/|||}} = 3\frac{\partial w_3}{\partial v}v^{|/||/|||} = \zeta_3\,v^{|/||/|||} \propto v^{|/||/|||}$$

with the function $\zeta_3 = \zeta_3(v^{|/||/|||})$ defined as

$$\zeta_3 := 3\frac{\partial w_3}{\partial v}$$

holding the property $\zeta_3(v^{|/||/|||}) = \zeta_3(v^{|||/|/||}) = \zeta_3(v^{||/|||/|})$ so that $p^{|/||/|||}$ would be invariant with respect to even permutations. Finally the force density per volume squared $\boldsymbol{p}_3^{\,|}$ due to three-neighbour interactions reads

$$\boldsymbol{p}_3^{\,|} := \int_{\mathcal{H}_0}\int_{\mathcal{H}_0} p^{|/||/|||}[\boldsymbol{\xi}^{||}\times\boldsymbol{\xi}^{|||}]\,\mathrm{d}V^{|||}\,\mathrm{d}V^{||} = \int_{\mathcal{H}_0}\int_{\mathcal{H}_0}\zeta_3\,v^{|/||/|||}[\boldsymbol{\xi}^{||}\times\boldsymbol{\xi}^{|||}]\,\mathrm{d}V^{|||}\,\mathrm{d}V^{||}.$$

This is another example of an interaction force that do not fall in the class of bond-based models. It is also an alternative to the state-based approach due to Silling et al. (2007). Table 2 summarizes our methodology, unifies the main observations and gathers the consequences of the angular momentum balance (28) on the interactions.

Table 2
Unification of concepts and consequences of angular momentum balance (28) on elastic interactions.

One-neighbour interactions	Two-neighbour interactions	Three-neighbour interactions
$w_1^{\mid} = w_1(\boldsymbol{\xi}^{\mid})$	$w_2^{\mid} = w_2(\boldsymbol{a}^{\mid/\mid\mid})$	$w_3^{\mid} = w_3(v^{\mid/\mid\mid/\mid\mid\mid})$
	$\boldsymbol{m}^{\mid/\mid\mid} := 2\,\dfrac{\partial w_2}{\partial \boldsymbol{a}^{\mid/\mid\mid}}$	$\boldsymbol{p}^{\mid/\mid\mid/\mid\mid\mid} := 3\,\dfrac{\partial w_3}{\partial v^{\mid/\mid\mid/\mid\mid\mid}}$
Properties		
	$\boldsymbol{m}^{\mid/\mid\mid} \overset{!}{=} -\boldsymbol{m}^{\mid\mid/\mid}$	$p^{\mid/\mid\mid/\mid\mid\mid} = p^{\mid\mid\mid/\mid/\mid\mid} = p^{\mid\mid/\mid\mid\mid/\mid}$
Force density per volume squared in the material configuration with dimension N/m⁶		
$\boldsymbol{p}_1^{\mid} := \dfrac{\partial w_1}{\partial \boldsymbol{\xi}^{\mid}}$	$\boldsymbol{p}_2^{\mid} := \displaystyle\int_{\mathcal{H}_0} \boldsymbol{\xi}^{\mid\mid} \times \boldsymbol{m}^{\mid/\mid\mid}\, dV^{\mid\mid}$	$\boldsymbol{p}_3^{\mid} := \displaystyle\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} p^{\mid/\mid\mid/\mid\mid\mid}\,[\boldsymbol{\xi}^{\mid\mid} \times \boldsymbol{\xi}^{\mid\mid\mid}]\, dV^{\mid\mid\mid}\, dV^{\mid\mid}$
Angular momentum balance		
$\displaystyle\int_{\mathcal{H}_0} \boldsymbol{\xi}^{\mid} \times \boldsymbol{p}_1^{\mid}\, dV^{\mid} \overset{!}{=} \mathbf{0}$	$\displaystyle\int_{\mathcal{H}_0} \boldsymbol{\xi}^{\mid} \times \boldsymbol{p}_2^{\mid}\, dV^{\mid} \overset{!}{=} \mathbf{0}$	$\displaystyle\int_{\mathcal{H}_0} \boldsymbol{\xi}^{\mid} \times \boldsymbol{p}_3^{\mid}\, dV^{\mid} \overset{!}{=} \mathbf{0}$
Further restrictions due to angular momentum balance		
$\dfrac{\partial w_1}{\partial \boldsymbol{\xi}^{\mid}} \overset{!}{=} \zeta_1\,\boldsymbol{\xi}^{\mid}$	$\dfrac{\partial w_2}{\partial \boldsymbol{a}^{\mid/\mid\mid}} \overset{!}{=} \dfrac{1}{2}\,\zeta_2\,[\boldsymbol{\xi}^{\mid} \times \boldsymbol{\xi}^{\mid\mid}]$	$\dfrac{\partial w_3}{\partial v^{\mid/\mid\mid/\mid\mid\mid}} \overset{!}{=} \dfrac{1}{3}\,\zeta_3\,\boldsymbol{\xi}^{\mid} \cdot [\boldsymbol{\xi}^{\mid\mid} \times \boldsymbol{\xi}^{\mid\mid\mid}]\,\mid$
$\zeta_1 = \zeta_1(\boldsymbol{\xi}^{\mid})$	$\zeta_2 = \zeta_2(\boldsymbol{a}^{\mid/\mid\mid}) \overset{!}{=} \zeta_2(\boldsymbol{a}^{\mid\mid/\mid})$	$\zeta_3 = \zeta_3(v^{\mid/\mid\mid/\mid\mid\mid}) \overset{!}{=} \zeta_3(v^{\mid\mid\mid/\mid/\mid\mid}) \overset{!}{=} \zeta_3(v^{\mid\mid/\mid\mid\mid/\mid})$
Generic examples of interaction energy densities		
$w_1^{\mid} = w_1(\iota)\ ,\quad \iota := \frac{1}{2}\,\|\boldsymbol{\xi}^{\mid}\|^2$	$w_2^{\mid} = w_2(a)\ ,\quad a := \frac{1}{2}\,\|\boldsymbol{a}^{\mid/\mid\mid}\|^2$	$w_3^{\mid} = w_3(v)\ ,\quad v := \frac{1}{2}\,[v^{\mid/\mid\mid/\mid\mid\mid}]^2$
$\zeta_1 := \dfrac{\partial w_1}{\partial \iota}$	$\zeta_2 := 2\,\dfrac{\partial w_2}{\partial a}$	$\zeta_3 := 3\,\dfrac{\partial w_3}{\partial v}$
$\boldsymbol{p}_1^{\mid} = \zeta_1\,\boldsymbol{\xi}^{\mid}$	$\boldsymbol{p}_2^{\mid} = \displaystyle\int_{\mathcal{H}_0} \zeta_2 \Big[\boldsymbol{\xi}^{\mid}[\boldsymbol{\xi}^{\mid\mid} \cdot \boldsymbol{\xi}^{\mid\mid}] - \boldsymbol{\xi}^{\mid\mid}[\boldsymbol{\xi}^{\mid\mid} \cdot \boldsymbol{\xi}^{\mid}]\Big]\, dV^{\mid\mid}$	$\boldsymbol{p}_3^{\mid} = \displaystyle\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \zeta_3\, v^{\mid/\mid\mid/\mid\mid\mid}\,[\boldsymbol{\xi}^{\mid\mid} \times \boldsymbol{\xi}^{\mid\mid\mid}]\, dV^{\mid\mid\mid}\, dV^{\mid\mid}$

4.3. Kinetic energy balance

Equipped with the balance of momentum derived in Section 4.1, we now consider energy relations. We begin with the kinetic energy and then proceed to energy, entropy and dissipation. Note that the kinetic energy balance is *not* an additional equation but is rather a consequence of the balance of linear momentum (27). Let K denote the global kinetic energy in the material configuration with its rate denoted by

$$\mathcal{K} := \dot{K} \qquad \text{with} \qquad K := \frac{1}{2}\int_{\mathcal{B}_0} \rho_0\,\boldsymbol{v} \cdot \boldsymbol{v}\, dV \qquad \Rightarrow \qquad \mathcal{K} = \int_{\mathcal{B}_0} \boldsymbol{v} \cdot [\,\rho_0\,\dot{\boldsymbol{v}}\,]\, dV ,$$

Expressing the term $\rho_0\,\dot{\boldsymbol{v}}$ via the linear momentum balance (27) yields

$$\begin{aligned}
\mathcal{K} = \int_{\mathcal{B}_0} \boldsymbol{v} \cdot [\,\rho_0\,\dot{\boldsymbol{v}}\,]\, dV &= \int_{\mathcal{B}_0} \boldsymbol{v} \cdot [\,\boldsymbol{b}_0^{\text{int}} + \boldsymbol{b}_0^{\text{ext}}\,]\, dV \\
&= \int_{\mathcal{B}_0} \boldsymbol{v} \cdot \int_{\mathcal{H}_0} \boldsymbol{p}^{\mid}\, dV^{\mid}\, dV + \int_{\mathcal{B}_0} \boldsymbol{v} \cdot \boldsymbol{b}_0^{\text{ext}}\, dV ,
\end{aligned}$$

in which $\boldsymbol{b}^{\text{int}}{}_0$ is replaced using Eq. (21)$_2$. Using the relation $\boldsymbol{v} = \boldsymbol{v}^{\mid} - \dot{\boldsymbol{\xi}}^{\mid}$, the rate of the global kinetic energy $\mathcal{K}$ reads

$$\begin{aligned}
\mathcal{K} &= \int_{\mathcal{B}_0}\int_{\mathcal{H}_0} [\boldsymbol{v}^{\mid} - \dot{\boldsymbol{\xi}}^{\mid}] \cdot \boldsymbol{p}^{\mid}\, dV^{\mid}\, dV + \int_{\mathcal{B}_0} \boldsymbol{v} \cdot \boldsymbol{b}_0^{\text{ext}}\, dV \\
&= \int_{\mathcal{B}_0}\int_{\mathcal{H}_0} \boldsymbol{v}^{\mid} \cdot \boldsymbol{p}^{\mid}\, dV^{\mid}\, dV + \int_{\mathcal{B}_0} \boldsymbol{v} \cdot \boldsymbol{b}_0^{\text{ext}}\, dV - \int_{\mathcal{B}_0}\int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{\mid} \cdot \boldsymbol{p}^{\mid}\, dV^{\mid}\, dV ,
\end{aligned} \tag{38}$$

in which the first term can be expressed via the virtual power equivalence (24) particularized to $\delta\boldsymbol{y} = \boldsymbol{v}$ as the power equivalence given by

$$\int_{\mathcal{B}_0}\int_{\mathcal{H}_0} \boldsymbol{v}^{\mid} \cdot \boldsymbol{p}^{\mid}\, dV^{\mid}\, dV = \int_{\partial\mathcal{B}_0} \boldsymbol{v} \cdot \boldsymbol{t}_0^{\text{ext}}\, dA . \tag{39}$$

Inserting Eq. (39) into Eq. (38) yields

$$\mathcal{K} = \int_{\partial\mathcal{B}_0} \boldsymbol{v} \cdot \boldsymbol{t}_0^{\text{ext}}\, dA + \int_{\mathcal{B}_0} \boldsymbol{v} \cdot \boldsymbol{b}_0^{\text{ext}}\, dV - \int_{\mathcal{B}_0}\int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{\mid} \cdot \boldsymbol{p}^{\mid}\, dV^{\mid}\, dV$$

or alternatively

$$\mathcal{K} = \mathcal{P}^{\text{ext}} - \mathcal{P}^{\text{int}} , \tag{40}$$

with

$$\mathcal{P}^{\text{ext}} := \int_{\partial\mathcal{B}_0} \boldsymbol{v} \cdot \boldsymbol{t}_0^{\text{ext}}\, dA + \int_{\mathcal{B}_0} \boldsymbol{v} \cdot \boldsymbol{b}_0^{\text{ext}}\, dV \qquad \text{and} \qquad \mathcal{P}^{\text{int}} := \int_{\mathcal{B}_0}\int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{\mid} \cdot \boldsymbol{p}^{\mid}\, dV^{\mid}\, dV . \tag{41}$$

Here, $\mathcal{P}^{\text{int}}$ denotes the internal mechanical power due to the interaction forces and $\mathcal{P}^{\text{ext}}$ the external mechanical power due to the externally prescribed forces and tractions.

4.4. Balance of energy

Let u_0 denote the internal energy density in the material configuration. The integral of u_0 over $\mathcal{B}_0$ renders the global internal energy U with its rate denoted $\mathcal{U}$, that is

$$\mathcal{U} := \dot{U} \qquad \text{with} \qquad U := \int_{\mathcal{B}_0} u_0 \, dV \qquad \Rightarrow \qquad \mathcal{U} = \int_{\mathcal{B}_0} \dot{u}_0 \, dV \, .$$

We also allow for (external) thermal power denoted by $\mathcal{Q}^{\text{ext}}$. Note that $\mathcal{Q}^{\text{ext}}$ is the thermal power due to the externally prescribed heat within the continuum body and externally prescribed heat flux on its boundary. Thus, the sum of the external mechanical power $\mathcal{P}^{\text{ext}}$ and the thermal power $\mathcal{Q}^{\text{ext}}$ equals the sum of the rate of internal energy $\mathcal{U}$ and the rate of the kinetic energy $\mathcal{K}$ as

$$\mathcal{K} + \mathcal{U} = \mathcal{P}^{\text{ext}} + \mathcal{Q}^{\text{ext}} \, .$$

Alternatively, by substituting $\mathcal{K}$ from Eq. (40), the sum of the internal mechanical power $\mathcal{P}^{\text{int}}$ and the thermal power $\mathcal{Q}^{\text{ext}}$ equals the rate of internal energy $\mathcal{U}$, that is

$$\mathcal{U} = \mathcal{P}^{\text{int}} + \mathcal{Q}^{\text{ext}} \, . \tag{42}$$

In other words, the internal energy balance states that the internal mechanical power and (external) thermal power cause a change in the internal energy. The thermal power $\mathcal{Q}^{\text{ext}}$ is composed of thermal power $\mathcal{Q}_{\mathcal{B}}^{\text{ext}}$ within the body and thermal power $\mathcal{Q}_{\partial\mathcal{B}}^{\text{ext}}$ on the boundary as

$$\mathcal{Q}^{\text{ext}} = \mathcal{Q}_{\mathcal{B}}^{\text{ext}} + \mathcal{Q}_{\partial\mathcal{B}}^{\text{ext}} \tag{43}$$

where

$$\mathcal{Q}_{\mathcal{B}}^{\text{ext}} := \int_{\mathcal{B}_0} \mathscr{R}_0^{\text{ext}} \, dV \qquad \text{and} \qquad \mathcal{Q}_{\partial\mathcal{B}}^{\text{ext}} := -\int_{\partial\mathcal{B}_0} \mathscr{Q}_0^{\text{ext}} \, dA \, . \tag{44}$$

The external thermal power term $\mathcal{Q}_{\mathcal{B}}^{\text{ext}}$ is the integral of the heat source density $\mathscr{R}_0^{\text{ext}}$ in the material configuration. The (external) heat source density $\mathscr{R}_0^{\text{ext}}$ should be compared with the externally prescribed body force density $\boldsymbol{b}^{\text{ext}}_0$ for the mechanical problem. In a similar fashion, the external heat flux density $\mathscr{Q}_0^{\text{ext}}$ is reminiscent of the externally prescribed traction $\boldsymbol{t}^{\text{ext}}_0$ for the mechanical problem. Similar to the virtual power equivalence (24), or its direct consequence (23)$_2$ for the mechanical problem, a thermal power equivalence can be established as

$$\int_{\mathcal{B}_0} \int_{\mathcal{H}_0} q^| \, dV^| \, dV = \int_{\partial\mathcal{B}_0} \mathscr{Q}_0^{\text{ext}} \, dA \tag{45}$$

with $q^|$ being the heat flux density per volume squared in the material configuration with units N.m/s.m^6. The thermal power equivalence (45) should be compared with its more familiar counterpart in classical continuum mechanics, obtained via the Gauss theorem and the flux boundary condition, and given by

$$\int_{\mathcal{B}_0} \text{Div}\boldsymbol{Q} \, dV = \int_{\partial\mathcal{B}_0} \mathscr{Q}_0^{\text{ext}} \, dA \qquad \text{subject to} \qquad \boldsymbol{Q} \cdot \boldsymbol{N} = \mathscr{Q}_0^{\text{ext}}$$

with $\boldsymbol{Q}$ being the heat flux vector in the material configuration. Inserting the thermal power equivalence (45) and the definition (44) into the thermal power (43) results in

$$\mathcal{Q}^{\text{ext}} = \int_{\mathcal{B}_0} \mathscr{R}_0^{\text{ext}} \, dV - \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} q^| \, dV^| \, dV = \int_{\mathcal{B}_0} \left[\mathscr{R}_0^{\text{ext}} - \int_{\mathcal{H}_0} q^| \, dV^| \right] dV \, . \tag{46}$$

To proceed, we substitute the thermal power $\mathcal{Q}^{\text{ext}}$ from Eq. (46) and the internal (mechanical) power $\mathcal{P}^{\text{int}}$ from Eq. (41)$_2$ into the internal energy balance (42) which yields the important global relation

$$\mathcal{U} = \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^| \cdot \boldsymbol{p}^| \, dV^| \, dV + \int_{\mathcal{B}_0} \left[\mathscr{R}_0^{\text{ext}} - \int_{\mathcal{H}_0} q^| \, dV^| \right] dV$$

or alternatively

$$\int_{\mathcal{B}_0} \dot{u}_0 \, dV = \int_{\mathcal{B}_0} \left[\int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^| \cdot \boldsymbol{p}^| \, dV^| + \mathscr{R}_0^{\text{ext}} \, dV - \int_{\mathcal{H}_0} q^| \, dV^| \right] dV \, .$$

The non-local form of the energy balance follows via localization of the global form as

$$\dot{u}_0 = \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^| \cdot \boldsymbol{p}^| \, dV^| + \mathscr{R}_0^{\text{ext}} - \int_{\mathcal{H}_0} q^| \, dV^| \, . \tag{47}$$

This is also referred to the first law of thermodynamics. The non-local form of the energy balance (47) should be compared with its local form in classical continuum mechanics

$$\dot{u}_0 = \boldsymbol{P} : \dot{\boldsymbol{F}} + \mathscr{R}_0^{\text{ext}} - \text{Div}\boldsymbol{Q} \, .$$

4.5. Balance of entropy

Let s_0 denote the entropy density in the material configuration with its rate denoted $\dot{s}_0$. The integral of s_0 over $\mathcal{B}_0$ renders the global entropy S with its rate denoted $\mathcal{S}$ as

$$\mathcal{S} := \dot{S} \quad \text{with} \quad S := \int_{\mathcal{B}_0} s_0 \, \mathrm{d}V \quad \Rightarrow \quad \mathcal{S} = \int_{\mathcal{B}_0} \dot{s}_0 \, \mathrm{d}V \,. \tag{48}$$

The balance of entropy states that the rate of the entropy $\mathcal{S}$ equals the entropy input as

$$\mathcal{S} = \mathcal{H}^{\mathrm{ext}} + \mathcal{H}^{\mathrm{prd}} \quad \text{with} \quad \mathcal{H}^{\mathrm{prd}} \geq 0 \tag{49}$$

where the global entropy input is decomposed into external contributions $\mathcal{H}^{\mathrm{ext}}$ and the positive entropy production $\mathcal{H}^{\mathrm{prd}}$. We further decompose the external entropy input $\mathcal{H}^{\mathrm{ext}}$ into a source part within the body and a flux part on the boundary of the body, that is

$$\mathcal{H}^{\mathrm{ext}} = \mathcal{H}_{\mathcal{B}}^{\mathrm{ext}} + \mathcal{H}_{\partial \mathcal{B}}^{\mathrm{ext}} \,. \tag{50}$$

To proceed, we adopt the widely adopted Clausius–Duhem assumptions to express $\mathcal{H}_{\mathcal{B}}^{\mathrm{ext}}$ and $\mathcal{H}_{\partial \mathcal{B}}^{\mathrm{ext}}$ in terms of the heat source density $\mathscr{R}_0^{\mathrm{ext}}$ and heat flux density $\mathscr{Q}_0^{\mathrm{ext}}$, respectively, as

$$\mathcal{H}_{\mathcal{B}}^{\mathrm{ext}} = \int_{\mathcal{B}_0} \frac{\mathscr{R}_0^{\mathrm{ext}}}{T} \, \mathrm{d}V \quad \text{and} \quad \mathcal{H}_{\partial \mathcal{B}}^{\mathrm{ext}} = - \int_{\partial \mathcal{B}_0} \frac{\mathscr{Q}_0^{\mathrm{ext}}}{T} \, \mathrm{d}A \tag{51}$$

with $T > 0$ denoting the absolute temperature. Furthermore, we define $\mathscr{D}_0$ as the dissipation power density in the material configuration resulting in the entropy production rate $\mathcal{H}^{\mathrm{prd}}$ as

$$\mathcal{H}^{\mathrm{prd}} = \int_{\mathcal{B}_0} \frac{\mathscr{D}_0}{T} \, \mathrm{d}V \quad \text{with} \quad \mathscr{D}_0 \geq 0 \,.$$

Next, Eq. (51) is inserted into the external entropy input (50) and then using the thermal power equivalence (45), in accordance with the virtual power equivalence (24) or its direct consequence $(23)_2$ for the mechanical problem, an entropic power equivalence is established as

$$\int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \frac{q^|}{T^|} \, \mathrm{d}V^| \, \mathrm{d}V = \int_{\partial \mathcal{B}_0} \frac{\mathscr{Q}_0^{\mathrm{ext}}}{T} \, \mathrm{d}A \quad \text{or} \quad \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \frac{q^|}{T^|} \, \mathrm{d}V^| \, \mathrm{d}V = \int_{\mathcal{B}_0} \frac{\mathscr{R}_0^{\mathrm{ext}}}{T} \, \mathrm{d}V - \mathcal{H}^{\mathrm{ext}} \tag{52}$$

with $T^|$ the temperature of the neighbouring point $\boldsymbol{X}^|$ within the horizon. Inserting the relations (52) and $(48)_3$ into the entropic power equivalence (49) results in the global balance of entropy

$$\int_{\mathcal{B}_0} \dot{s}_0 \, \mathrm{d}V = \int_{\mathcal{B}_0} \frac{\mathscr{R}_0^{\mathrm{ext}}}{T} \, \mathrm{d}V - \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \frac{q^|}{T^|} \, \mathrm{d}V^| \, \mathrm{d}V + \int_{\mathcal{B}_0} \frac{\mathscr{D}_0}{T} \, \mathrm{d}V$$

which after localization reads

$$\dot{s}_0 \, T = \mathscr{R}_0^{\mathrm{ext}} - T \int_{\mathcal{H}_0} \frac{q^|}{T^|} \, \mathrm{d}V^| + \mathscr{D}_0 \,. \tag{53}$$

The non-local form of the entropy balance (53) should be compared with its local form in classical continuum mechanics

$$\dot{s}_0 \, T = \mathscr{R}_0^{\mathrm{ext}} - T \operatorname{Div} \left(\frac{\boldsymbol{Q}}{T} \right) + \mathscr{D}_0 \,.$$

4.6. Dissipation inequality and coleman–Noll procedure

Motivated by the format of the entropy balance (53), we proceed with the dissipation inequality and derive the constitutive relations via a Coleman–Noll-like procedure. Henceforth, we limit our study to isothermal (mechanical) problems for the sake of brevity. Further discussions on the implication of temperature shall be postponed to a separate contribution. Employing the energy balance (47), the non-local form of the entropy balance (53) for isothermal processes can be re-written as

$$\dot{s}_0 \, T = \dot{u}_0 - \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^| \cdot \boldsymbol{p}^| \, \mathrm{d}V^| + \mathscr{D}_0 \quad \text{with} \quad \mathscr{D}_0 \geq 0 \,. \tag{54}$$

Next, we introduce the Helmholtz energy density and exploit the dissipation inequality via a Coleman–Noll-like procedure to obtain constitutive equations. The Helmholtz energy density Ψ_0 in the material configuration is introduced as a Legendre transformation of the internal energy density in terms of entropy and temperature as

$$\Psi_0 := u_0 - T s_0 \quad \Rightarrow \quad \dot{\Psi}_0 = \dot{u}_0 - s_0 \dot{T} - \dot{s}_0 T \quad \Rightarrow \quad \dot{\Psi}_0 = \dot{u}_0 - \dot{s}_0 T \,, \tag{55}$$

in which the last relation holds since for isothermal problems of interest here $\dot{T}$ vanishes identically. Replacing the internal energy density (55) into the entropy balance (54) results in the non-local form of the dissipation inequality

$$\mathscr{D}_0 = \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^| \cdot \boldsymbol{p}^| \, \mathrm{d}V^| - \dot{\Psi}_0 \geq 0 \,. \tag{56}$$

Table 3
Governing equations of classical continuum mechanics (CCM) and continuum-kinematics-inspired peridynamics (CPD).

Linear momentum balance	CCM	$\rho_0 \dot{\boldsymbol{v}} = \text{Div}\boldsymbol{P} + \boldsymbol{b}_0^{\text{ext}}$ subject to $\boldsymbol{P} \cdot \boldsymbol{N} = \boldsymbol{t}_0^{\text{ext}}$
	CPD	$\rho_0 \dot{\boldsymbol{v}} = \int_{\mathcal{H}_0} \boldsymbol{p}^{|} \, dV^{|} + \boldsymbol{b}_0^{\text{ext}}$ subject to $\int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \boldsymbol{p}^{|} \, dV^{|} \, dV = \int_{\partial \mathcal{B}_0} \boldsymbol{t}_0^{\text{ext}} \, dA$
Angular momentum balance	CCM	$\boldsymbol{\varepsilon} : [\boldsymbol{F} \cdot \boldsymbol{P}^{\text{t}}] = \boldsymbol{0}$
	CPD	$\int_{\mathcal{H}_0} \boldsymbol{\xi}^{|} \times \boldsymbol{p}^{|} \, dV^{|} = \boldsymbol{0}$
Energy balance	CCM	$\dot{u}_0 = \boldsymbol{P} : \dot{\boldsymbol{F}} + \mathscr{R}_0^{\text{ext}} - \text{Div}\boldsymbol{Q}$ subject to $\boldsymbol{Q} \cdot \boldsymbol{N} = \mathscr{Q}_0^{\text{ext}}$
	CPD	$\dot{u}_0 = \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{|} \cdot \boldsymbol{p}^{|} \, dV^{|} + \mathscr{R}_0^{\text{ext}} - \int_{\mathcal{H}_0} q^{|} \, dV^{|}$ subject to $\int_{\mathcal{B}_0} \int_{\mathcal{B}_0} q^{|} \, dV^{|} \, dV = \int_{\partial \mathcal{B}_0} \mathscr{Q}_0^{\text{ext}} \, dA$
Entropy balance	CCM	$\dot{s}_0 \, T = \mathscr{R}_0^{\text{ext}} - T \, \text{Div}\left(\dfrac{\boldsymbol{Q}}{T}\right) + \mathscr{D}_0$ subject to $\dfrac{\boldsymbol{Q}}{T} \cdot \boldsymbol{N} = \dfrac{\mathscr{Q}_0^{\text{ext}}}{T}$
	CPD	$\dot{s}_0 \, T = \mathscr{R}_0^{\text{ext}} - T \int_{\mathcal{H}_0} \dfrac{q^{|}}{T^{|}} \, dV^{|} + \mathscr{D}_0$ subject to $\int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \dfrac{q^{|}}{T^{|}} \, dV^{|} \, dV = \int_{\partial \mathcal{B}_0} \dfrac{\mathscr{Q}_0^{\text{ext}}}{T} \, dA$
Dissipation inequality	CCM	$\boldsymbol{P} : \dot{\boldsymbol{F}} - \dot{\Psi}_0 \geq 0$
	CPD	$\int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{|} \cdot \boldsymbol{p}^{|} \, dV^{|} - \int_{\mathcal{H}_0} \dot{\psi}_0^{|} \, dV^{|} \geq 0$

Table 3 gathers the key governing equations of continua for both classical continuum mechanics and the current continuum-kinematics-inspired peridynamics approach and highlights their similarities and differences.

Before we proceed to the Coleman–Noll-like exploitation, we further localize the non-local form of the dissipation inequality (56) within the horizon to obtain the neighbour-wise form. To do so, we define the Helmholtz energy density per volume squared in the material configuration $\psi_0^{|}$ with units N.m/m^6 and the dissipation density per volume squared in the material configuration $d_0^{|}$ as

$$\Psi_0 = \int_{\mathcal{H}_0} \psi_0^{|} \, dV^{|} \qquad \text{and} \qquad \mathscr{D}_0 = \int_{\mathcal{H}_0} d_0^{|} \, dV^{|} \, . \tag{57}$$

Inserting the densities (57) into the non-local form of the dissipation inequality (56) yields

$$\int_{\mathcal{H}_0} d_0^{|} \, dV^{|} = \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{|} \cdot \boldsymbol{p}^{|} \, dV^{|} - \int_{\mathcal{H}_0} \dot{\psi}_0^{|} \, dV^{|} \geq 0 \, . \tag{58}$$

Consequently, the neighbour-wise form of the dissipation inequality (58) reads

$$d_0^{|} = \dot{\boldsymbol{\xi}}^{|} \cdot \boldsymbol{p}^{|} - \dot{\psi}_0^{|} \geq 0 \, . \tag{59}$$

Note, the more restrictive condition $d_0^{|} \geq 0$ on the neighbour-wise form of the dissipation implies but is not implied by its non-local form $\mathscr{D}_0 \geq 0$ or more precisely

$$d_0^{|} \geq 0 \; \Rightarrow \; \mathscr{D}_0 \geq 0 \qquad \text{but} \qquad \mathscr{D}_0 \geq 0 \; \nRightarrow \; d_0^{|} \geq 0 \, .$$

Therefore, in the exploitation process that follows next we begin with the non-local form (56) first and thereafter elaborate on the implications due to the neighbour-wise form of the dissipation inequality (59).

To exploit the non-local form of the dissipation inequality (56) using a Coleman–Noll-like procedure and to derive the associated constitutive laws, we particularize the Helmholtz energy density for the case of elasticity and specify its arguments as

$$\Psi_0 = \int_{\mathcal{H}_0} \psi_0^{|} \, dV^{|} \qquad \text{with} \qquad \psi_0^{|} = \psi_0(\boldsymbol{\xi}^{|}, \boldsymbol{a}^{|/||}, v^{|/||/|||}) \, . \tag{60}$$

Remark Motivated by the discussion in Section 4.2 on the consequences of angular momentum balance, one can argue that a more precise representation of the Helmholtz energy density per volume squared in the material configuration to sufficiently fulfil the angular momentum balance (28) would be in terms of $\imath$, a and v instead of $\boldsymbol{\xi}^{|}$, $\boldsymbol{a}^{|/||}$ and $v^{|/||/|||}$, respectively.   □

Following the classical Coleman–Noll procedure, we (i) calculate the rate of the Helmholtz energy density Ψ_0 from its density integral over the horizon (60), (ii) replace $\dot{\Psi}_0$ in the non-local form of the dissipation inequality (56) and (iii) analyse its consequences to sufficiently satisfy the second law of thermodynamics. To calculate the rate of the Helmholtz energy density Ψ_0, consider that ψ_0 includes $\boldsymbol{a}^{|/||}$ and $v^{|/||/|||}$ resulting in a double-integral and a triple-integral, respectively. The
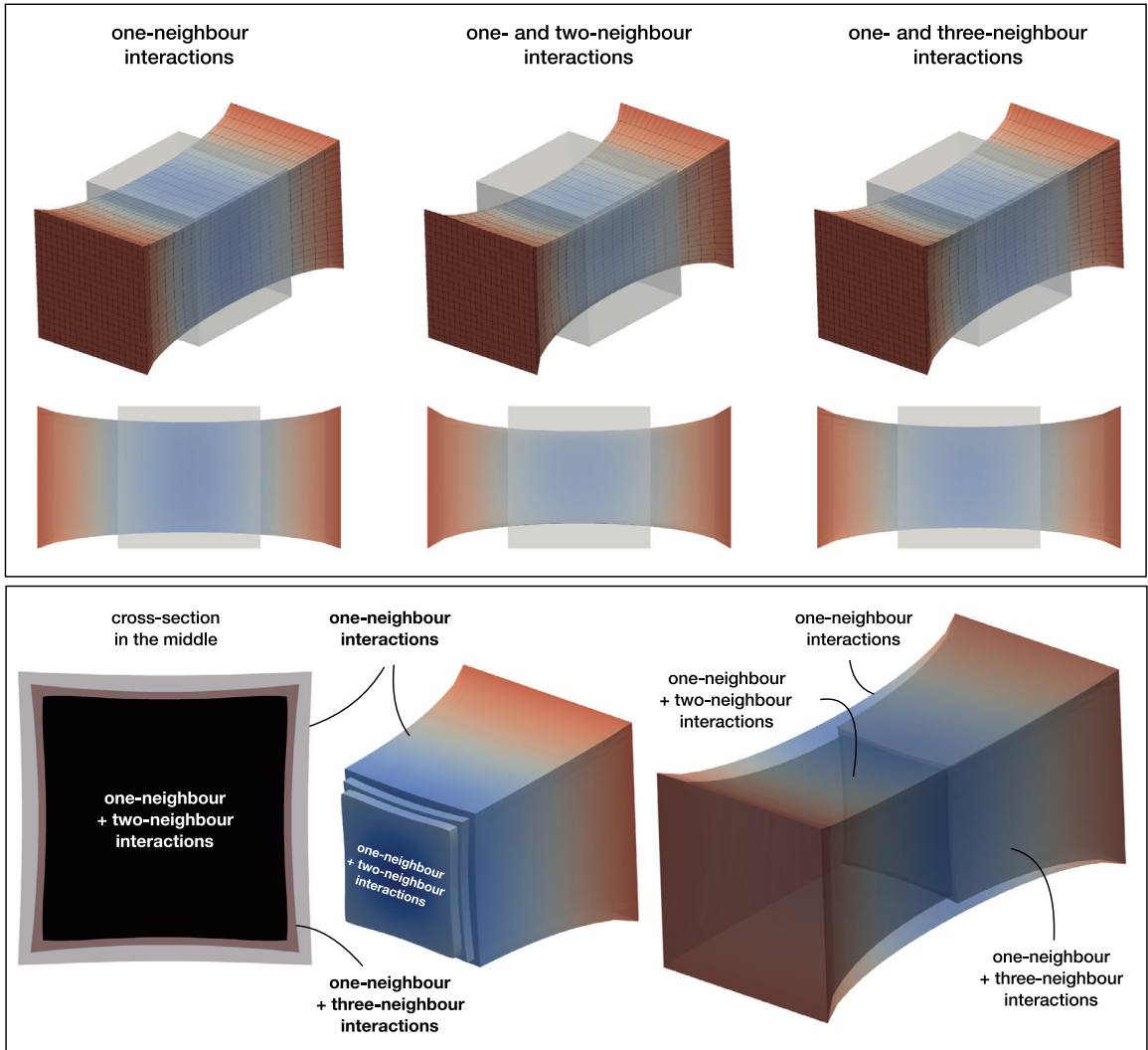
Fig. 6. Computational illustration of the proposed theory. A cube under large deformations whose constitutive behaviour is defined by our continuum-kinematics-inspired theory. Further details on computational aspects of the proposed theory shall be provided in a separate contribution.

rate of the Helmholtz energy density reads

$$\dot{\Psi}_0 = \int_{\mathcal{H}_0} \dot{\psi}_0^{|} \, dV^{|} = \int_{\mathcal{H}_0} \dot{\psi}_0(\boldsymbol{\xi}_{1}, \boldsymbol{a}^{|/||}, v^{|/||/|||}) \, dV^{|} = \int_{\mathcal{H}_0} \frac{\delta \psi_0}{\delta \boldsymbol{\xi}^{|}} \cdot \dot{\boldsymbol{\xi}}^{|} \, dV^{|}, \tag{61}$$

in which the term $\delta \psi_0 / \delta \boldsymbol{\xi}^{|}$ denotes a variational derivative defined as

$$\frac{\delta \psi_0}{\delta \boldsymbol{\xi}^{|}} := \frac{\partial \psi_0}{\partial \boldsymbol{\xi}^{|}} + \int_{\mathcal{H}_0} 2\,\boldsymbol{\xi}^{||} \times \frac{\partial \psi_0}{\partial \boldsymbol{a}^{|/||}} \, dV^{||} + \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} 3\,[\boldsymbol{\xi}^{||} \times \boldsymbol{\xi}^{|||}] \frac{\partial \psi_0}{\partial v^{|/||/|||}} \, dV^{|||} \, dV^{||}, \tag{62}$$

the derivation of which is omitted for the sake of brevity. To obtain the relation (62), we have assumed the properties

$$\frac{\partial \psi_0}{\partial \boldsymbol{a}^{|/||}} = -\frac{\partial \psi_0}{\partial \boldsymbol{a}^{||/|}} \qquad \text{and} \qquad \frac{\partial \psi_0}{\partial v^{|/||/|||}} = \frac{\partial \psi_0}{\partial v^{||/|||/|}} = \frac{\partial \psi_0}{\partial v^{|||/|/||}},$$

consistent with our earlier assumptions. Replacing Eq. (61) into the non-local form of the dissipation inequality (56) yields

$$\mathscr{D}_0 = \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{|} \cdot \boldsymbol{p}^{|} \, dV^{|} - \int_{\mathcal{H}_0} \frac{\delta \psi_0}{\delta \boldsymbol{\xi}^{|}} \cdot \dot{\boldsymbol{\xi}}^{|} \, dV^{|} \geq 0 \quad \Rightarrow \quad \mathscr{D}_0 = \int_{\mathcal{H}_0} \left[\boldsymbol{p}^{|} - \frac{\delta \psi_0}{\delta \boldsymbol{\xi}^{|}} \right] \cdot \dot{\boldsymbol{\xi}}^{|} \, dV^{|} \geq 0. \tag{63}$$

The sufficient condition to fulfil Eq. (63), in the case of equality, yields the constitutive relation

$$\boldsymbol{p}^{|} = \frac{\delta \psi_0}{\delta \boldsymbol{\xi}^{|}} \,.$$

Next, we discuss the more restrictive neighbour-wise form of the dissipation inequality (59). The neighbour-wise form of the dissipation inequality for the case of $\psi_0^{|} = \psi_0(\boldsymbol{\xi}^{|}, \boldsymbol{a}^{|/||}, v^{|/||/|||})$ reads

$$d_0^{|} = \dot{\boldsymbol{\xi}}^{|} \cdot \boldsymbol{p}^{|} - \dot{\psi}_0 \geq 0 \,. \tag{64}$$

Using the relation (61), it can be readily seen that

$$\dot{\Psi}_0 = \int_{\mathcal{H}_0} \frac{\delta \psi_0}{\delta \boldsymbol{\xi}^{|}} \cdot \dot{\boldsymbol{\xi}}^{|} \, \mathrm{d}V^{|} \qquad \Rightarrow \qquad \dot{\psi}_0 = \frac{\delta \psi_0}{\delta \boldsymbol{\xi}^{|}} \cdot \dot{\boldsymbol{\xi}}^{|} \,. \tag{65}$$

Replacing $\dot{\psi}_0$ from Eq. (65) into the dissipation inequality (64) yields

$$d_0^{|} = \dot{\boldsymbol{\xi}}^{|} \cdot \boldsymbol{p}^{|} - \frac{\delta \psi_0}{\delta \boldsymbol{\xi}^{|}} \cdot \dot{\boldsymbol{\xi}}^{|} \geq 0 \,, \tag{66}$$

The sufficient condition to fulfil Eq. (66), in the case of equality, yields the constitutive relation

$$\boldsymbol{p}^{|} = \frac{\delta \psi_0}{\delta \boldsymbol{\xi}^{|}} \,.$$

Summarizing, the outcome of the Coleman–Noll procedure imposed on the neighbour-wise form of the dissipation inequality (59) is identical to that obtained from the non-local form of the dissipation inequality (56).

5. Concluding remarks

Peridynamics is an alternative approach to formulate continuum mechanics that inherently allows for geometrical discontinuities thanks to the integro-differential nature of its governing equations. This contribution critically revisits the kinematic foundations of peridynamics and provides a continuum-kinematics-inspired alternative. To do so, we define one-neighbour, two-neighbour and three-neighbour interactions. While our one-neighbour interactions are essentially identical to bond-based interactions, two- and three-neighbour interactions are alternative to and fundamentally different from state-based interactions. Thermodynamic restrictions on the interaction energies have been discussed and thermodynamically-consistent constitutive laws are provided.

In order to demonstrate the potential of our proposed framework, a numerical example is shown in Fig. 6. The results show the deformation of a cube under extension governed by the proposed theory. The deformation due to one-neighbour interactions is identical to that of a bond-based PD. The contribution of two- and three-neighbour interactions is clearly observed by comparing the resulting deformations to one another and with the one-neighbour interactions. In summary, this manuscript presents a continuum-kinematics-inspired formulation of peridynamics in a thermodynamically consistent framework. We believe that this generic approach is broadly applicable to enhance understanding of material behaviour for a large variety of applications in multi-field problems accounting for geometrical discontinuities.

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References

Aguiar, A.R., Fosdick, R., 2014. A constitutive model for a linearly elastic peridynamic body. Math. Mech. Solids 19 (5), 502–523.

Agwai, A., Guven, I., Madenci, E., 2011. Predicting crack propagation with peridynamics: a comparative study. Int. J. Fract. 171 (1), 65–78.

Auffray, N., Dell'Isola, F., Eremeyev, V.A., Madeo, A., Rosi, G., 2015. Analytical continuum mechanics á la hamilton-Piola least action principle for second gradient continua and capillary fluids. Math. Mech. Solids 20 (4), 375–417.

Bazant, Z.P., Luo, W., Chau, V.T., Bessa, M.A., 2016. Wave dispersion and basic concepts of peridynamics compared to classical nonlocal damage models. J. Appl. Mech. 83 (11). doi:10.1115/1.4034319.

Bobaru, F., Duangpanya, M., 2010. The peridynamic formulation for transient heat conduction. Int. J. Heat Mass Transf. 53 (19–20), 4047–4059.

Bobaru, F., Yang, M., Alves, L.F., Silling, S.A., Askari, E., Xu, J., 2009. Convergence, adaptive refinement, and scaling in 1D peridynamics. Int. J. Numer. Method.Eng. 77 (6), 852–877.

Breitenfeld, M.S., Geubelle, P.H., Weckner, O., Silling, S.A., 2014. Non-ordinary state-based peridynamic analysis of stationary crack problems. Comput. Method. Appl. Mech.Eng. 272, 233–250.

Butt, S.N., Timothy, J.J., Meschke, G., 2017. Wave dispersion and propagation in state-based peridynamics. Comput. Mech. 60 (5), 1–14. doi:10.1007/s00466-017-1439-7.

Chen, Z., Bobaru, F., 2015. Peridynamic modeling of pitting corrosion damage. J. Mech. Phys. Solids 78, 352–381.

Chowdhury, S.R., Roy, P., Roy, D., Reddy, J.N., 2016. A peridynamic theory for linear elastic shells. Int. J. Solid Struct. 84, 110–132.

Dayal, K., Bhattacharya, K., 2006. Kinetics of phase transformations in the peridynamic formulation of continuum mechanics. J. Mech. Phys. Solids 54 (9), 1811–1842.

De Meo, D., Zhu, N., Oterkus, E., 2016. Peridynamic modeling of granular fracture in polycrystalline materials. J. Eng. Mater. Technol. 138 (4).

dell'Isola, F., Andreaus, U., Placidi, L., 2015. At the origins and in the vanguard of peridynamics, non-local and higher-gradient continuum mechanics: an underestimated and still topical contribution of Gabrio Piola. Math. Mech. Solids 20 (8), 887–928.

dell'Isola, F., Corte, A.D., Esposito, R., Russo, L., 2016. Some cases of unrecognized transmission of scientific knowledge : from antiquity to Gabrio Piola's peridynamics and generalized continuum theories. Adv. Struct. Mater. 42, 77–128.

dell'Isola, F., Della Corte, A., Giorgio, I., 2017. Higher-gradient continua: the legacy of Piola, Mindlin, Sedov and Toupin and some future research perspectives. Math. Mech. Solid. 22 (4), 1–21.

dell'Isola, F., Placidi, L., 2011. Variational Principles are a Powerful Tool also for Formulating Field Theories. Springer Vienna, Vienna, pp. 1–15. Doi: 10.1007/978-3-7091-0983-0_1

Dipasquale, D., Zaccariotto, M., Galvanetto, U., 2014. Crack propagation with adaptive grid refinement in 2D peridynamics. Int. J. Fract. 190 (1–2), 1–22.

Diyaroglu, C., Oterkus, E., Madenci, E., Rabczuk, T., Siddiq, A., 2016. Peridynamic modeling of composite laminates under explosive loading. Compos. Struct. 144, 14–23.

Ebrahimi, S., Steigmann, D., Komvopoulos, K., 2015. Peridynamics analysis of the nanoscale friction and wear properties of amorphous carbon thin films. J. Mech. Mater. Struct. 10 (5), 559–572.

Emmrich, E., Puhst, D., 2016. A short note on modeling damage in peridynamics. J. Elast. 123 (2), 245–252.

Eringen, A.C., 2002. Nonlocal Continuum Field Theories. Springer.

Fosdick, R., 2013. A causality approach to particle dynamics for systems. Arch. Ration. Mech. Anal. 207, 247–302.

Foster, J., Silling, S.A., Chen, W., 2011. An energy based failure criterion for use with peridynamic states. Int. J. Multiscale Comput.Eng. 9 (6), 675–688.

Fried, E., 2010. New insights into the classical mechanics of particle systems. Discrete Contin. Dyn. Syst. 28 (4), 1469–1504. doi:10.3934/dcds.2010.28.1469.

Gerstle, W., Silling, S., Read, D., Tewary, V., Lehoucq, R., 2008. Peridynamic simulation of electromigration. Comput. Mater. Continua 8 (2), 75–92.

Gurtin, M.E., Murdoch, A.I., 1975. A continuum theory of elastic material surfaces. Arch. Ration. Mech. Anal. 57 (4), 291–323.

Han, F., Lubineau, G., Azdoud, Y., 2016. Adaptive coupling between damage mechanics and peridynamics: a route for objective simulation of material degradation up to complete failure. J. Mech. Phys. Solids 94, 453–472.

Huang, D., Lu, G., Qiao, P., 2015. An improved peridynamic approach for quasi-static elastic deformation and brittle fracture analysis. Int. J. Mech. Sci. 94–95, 111–122.

Javili, A., Dell'Isola, F., Steinmann, P., 2013a. Geometrically nonlinear higher-gradient elasticity with energetic boundaries. J. Mech. Phys. Solid 61 (12), 2381–2401.

Javili, A., Mcbride, A., Steinmann, P., 2013b. Thermomechanics of solids with lower-dimensional energetics: on the importance of surface, interface, and curve structures at the nanoscale. a unifying review. Appl. Mech. Rev. 65 (1), 010802.

Javili, A., Morasata, R., Oterkus, E., Oterkus, S., 2018. Peridynamics review. Math. Mech. Solid. doi:10.1177/1081286518803411.

Kilic, B., Madenci, E., 2009. Prediction of crack paths in a quenched glass plate by using peridynamic theory. Int. J. Fract. 156 (2), 165–177.

Lejeune, E., Linder, C., 2017a. Modeling tumor growth with peridynamics. Biomech. Model. Mechanobiol. 16 (4), 1141–1157.

Lejeune, E., Linder, C., 2017b. Quantifying the relationship between cell division angle and morphogenesis through computational modeling. J. Theor. Biol. 418, 1–7.

Lejeune, E., Linder, C., 2018a. Modeling mechanical inhomogeneities in small populations of proliferating monolayers and spheroids. Biomech. Model. Mech. 17 (3), 727–743.

Lejeune, E., Linder, C., 2018b. Understanding the relationship between cell death and tissue shrinkage via a stochastic agent-based model. J. Biomech. 73, 9–17.

Li, H., Zhang, H., Zheng, Y., Zhang, L., 2016. A peridynamic model for the nonlinear static analysis of truss and tensegrity structures. Comput. Mech. 57 (5), 843–858.

Madenci, E., Oterkus, E., 2014. Peridynamic theory and its applications.

Madenci, E., Oterkus, S., 2016. Ordinary state-based peridynamics for plastic deformation according to von mises yield criteria with isotropic hardening. J. Mech. Phys. Solids 86, 192–219.

Madenci, E., Oterkus, S., 2017. Ordinary state-based peridynamics for thermoviscoelastic deformation. Eng. Fract. Mech. 175, 31–45.

Mikata, Y., 2012. Analytical solutions of peristatic and peridynamic problems for a 1D infinite rod. Int. J. Solid. Struct. 49 (21), 2887–2897.

Murdoch, A., 2012. Physical Foundations of Continuum Mechanics. Cambridge University Press.

Nishawala, V.V., Ostoja-Starzewski, M., Leamy, M.J., Demmie, P.N., 2016. Simulation of elastic wave propagation using cellular automata and peridynamics, and comparison with experiments. Wave Motion 60, 73–83.

O'Grady, J., Foster, J., 2014. Peridynamic beams: a non-ordinary, state-based model. Int. J. Solid. Struct. 51 (18), 3177–3183.

Ostoja-Starzewski, M., Demmie, P.N., Zubelewicz, a., 2013. On thermodynamic restrictions in peridynamics. J. Appl. Mech. 80 (1), 014502. doi:10.1115/1. 4006945.

Oterkus, S., Madenci, E., Agwai, A., 2014a. Fully coupled peridynamic thermomechanics. J. Mech. Phys. Solid 64 (1), 1–23.

Oterkus, S., Madenci, E., Agwai, A., 2014b. Peridynamic thermal diffusion. J. Comput. Phys. 265, 71–96.

Oterkus, S., Madenci, E., Oterkus, E., 2017. Fully coupled poroelastic peridynamic formulation for fluid-filled fractures. Eng. Geol. 225, 19–28.

Podio-Guidugli, P., 2017. On the modeling of transport phenomena in continuum and statistical mechanics. Discrete Contin. Dyn. Syst. - Ser.S 10 (6), 1393–1411.

Rahman, R., Foster, J.T., 2014. Bridging the length scales through nonlocal hierarchical multiscale modeling scheme. Comput. Mater. Sci. 92, 401–415.

Shelke, A., Banerjee, S., Kundu, T., Amjad, U., Grill, W., 2011. Multi-scale damage state estimation in composites using nonlocal elastic kernel: an experimental validation. Int. J. Solid Struct. 48 (7–8), 1219–1228.

Silhavý, M., 2017. Higher gradient expansion for linear isotropic peridynamic materials. Math. Mech. Solid. 22 (6), 1483–1493.

Silling, S.A., 2000. Reformulation of elasticity theory for discontinuities and long-range forces. J. Mech. Phys. Solid. 48 (1), 175–209.

Silling, S.A., 2016. Solitary waves in a peridynamic elastic solid. J. Mech. Phys. Solid. 96, 121–132.

Silling, S.A., 2017. Stability of peridynamic correspondence material models and their particle discretizations. Comput. Method. Appl. Mech. Eng. 322, 42–57.

Silling, S.A., Bobaru, F., 2005. Peridynamic modeling of membranes and fibers. Int. J. Non-Linear Mech. 40 (2–3), 395–409.

Silling, S.A., Epton, M., Weckner, O., Xu, J., Askari, E., 2007. Peridynamic states and constitutive modeling. J. Elast. 88 (2), 151–184.

Silling, S.A., Lehoucq, R.B., 2010. Peridynamic theory of solid mechanics. Adv. Appl. Mech. 44, 73–168.

Silling, S.A., Weckner, O., Askari, E., Bobaru, F., 2010. Crack nucleation in a peridynamic solid. Int. J. Fract. 162 (1–2), 219–227.

Sun, C., Huang, Z., 2016. Peridynamic simulation to impacting damage in composite laminate. Compos. Struct. 138, 335–341.

Sun, S., Sundararaghavan, V., 2014. A peridynamic implementation of crystal plasticity. Int. J. Solid. Struct. 51 (19), 3350–3360.

Talebi, H., Silani, M., Bordas, S.P.A., Kerfriden, P., Rabczuk, T., 2014. A computational library for multiscale modeling of material failure. Comput. Mech. 53 (5), 1047–1071. doi:10.1007/s00466-013-0948-2.

Taylor, M., Gözen, I., Patel, S., Jesorka, A., Bertoldi, K., 2016. Peridynamic modeling of ruptures in biomembranes. PLoS ONE 11 (11). doi:10.1371/journal.pone. 0165947.

Taylor, M., Steigmann, D.J., 2015. A two-dimensional peridynamic model for thin plates. Math. Mech. Solids 20 (8), 998–1010.

Tong, Q., Li, S., 2016. Multiscale coupling of molecular dynamics and peridynamics. J. Mech. Phys. Solid 95, 169–187.

Tupek, M.R., Radovitzky, R., 2014. An extended constitutive correspondence formulation of peridynamics based on nonlinear bond-strain measures. J. Mech. Phys. Solid 65 (1), 82–92.

Vogler, T.J., Borg, J.P., Grady, D.E., 2012. On the scaling of steady structured waves in heterogeneous materials. J. Appl. Phys. 112 (12). doi:10.1063/1.4768705.

Wildman, R.A., Gazonas, G.A., 2014. A finite difference-augmented peridynamics method for reducing wave dispersion. Int. J. Fract. 190 (1–2), 39–52.

Xu, F., Gunzburger, M., Burkardt, J., 2016. A multiscale method for nonlocal mechanics and diffusion and for the approximation of discontinuous functions. Comput. Method. Appl. Mech.Eng. 307, 117–143.

Zingales, M., 2011. Wave propagation in 1D elastic solids in presence of long-range central interactions. J. Sound Vib. 330 (16), 3973–3989.