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ORIGINAL ARTICLE

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Continuum-kinematics-inspired peridynamics: Thermo-mechanical problems

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Abstract The recently proposed continuum-kinematics-inspired peridynamics (CPD) is extended to account for thermo-mechanical coupling at large deformations. The key features of CPD are that it is geometrically exact and is built upon multi-neighbour interactions. The bond-based interactions of the original PD formalism are equivalent to one-neighbour interactions of CPD. Two- and three-neighbour interactions, however, are fundamentally different from state-based PD in that the basic elements of continuum kinematics are preserved exactly. We elaborate on thermodynamic restrictions on the interaction energies and derive thermodynamically consistent constitutive laws through a Coleman–Noll-like procedure. Notably, we show that various choices for temperature, or coldness, satisfy the dissipation inequality and provide meaningful temperature, or coldness, evolution equations together with Fourier-like conduction relations.

Keywords Thermo-mechanical CPD · Peridynamics · Continuum kinematics · Thermodynamic consistency

1 Introduction

Peridynamics (PD) is an alternative approach to formulate continuum mechanics [1]. The fundamental aspects of peridynamics had already been outlined by Piola in the nineteenth century according to dell'Isola et al. [2–4]. PD is a non-local continuum formulation wherein the concepts of stress and strain are absent. As a non-local theory, the behaviour of each material point is dictated by its interactions with other material points in its vicinity. The governing equations of PD are integro-differential and thus appropriate for problems involving discontinuities such as cracks. Since PD inherently accounts for geometrical discontinuities, it is readily employed in fracture mechanics and related problems [5–17]. However, the range of PD applications is broad and not limited to fracture mechanics. For a brief description of PD together with a review of its applications and related studies in different fields, see the review [18]. As a continuum formulation, PD can account for non-mechanical fields and their evolution.

The original PD theory of Silling [1] was restricted to bond-based interactions. Bond-based PD is geometrically exact. The bond-based assumption of PD, however, limited its applicability for material modelling,

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including the inability to account for the Poisson effect correctly. This shortcoming was addressed in state-based PD [19], but the kinematics were not accurately preserved. The recently proposed [20] continuum-kinematics-inspired peridynamics (CPD) approach does not suffer from such issues. CPD is a geometrically exact PD formulation suitable for large deformations whose underlying kinematics are reminiscent of classical continuum mechanics. The interaction potential of CPD is composed of three parts corresponding to one-neighbour, two-neighbour and three-neighbour interactions. The novel contribution of this work is the extension of CPD [20–22] to account for thermo-mechanical behaviour at finite deformation. The treatment of thermoelasticity within the framework of PD has been addressed in [23,24]. A state-based approach is adopted in [23] allowing for the recovery of familiar measures of stress and strain from the underlying non-local PD formulation. Temperature evolution is thus treated in a near-classical fashion [see [25], among others]. The current contribution directly accounts for thermo-mechanical coupling within the non-local CPD formulation and therefore crucially does not require the notion of stress or strain. The temperature evolution relations resemble those of classical thermomechanics but follow directly from the thermodynamics restrictions imposed on CPD. The main features of this contribution are:

- To extend the CPD formalism to account for thermo-mechanical problems at large deformations,
- To establish a geometrically exact thermo-mechanical formulation of PD, for the first time,
- To develop a thermodynamically consistent CPD formalism for thermoelasticity,
- To elaborate on thermodynamic restrictions on the interaction energies and derive thermodynamically consistent constitutive laws through a Coleman–Noll-like procedure,
- To identify various options for temperature, or coldness, to satisfy the dissipation inequality,
- To provide meaningful temperature, or coldness, evolution equations together with Fourier-like conduction relations,
- To elucidate the proposed theory via a series of numerical examples.

The manuscript is organised as follows. Section 2 introduces the notation and definitions and elaborates on the kinematics of the problem. Multi-neighbour interactions are presented in accordance with CPD and thus the basic elements of classical continuum kinematics are preserved. Thereafter, the thermodynamic balance laws are discussed in Sect. 3. In particular, we briefly review the balance of mechanical, thermal and entropic power. Afterwards, we detail the dissipation inequality and its consequences. Through a Coleman–Noll-like procedure, we provide thermodynamically consistent constitutive laws and carefully analyse the notion of temperature and coldness. Temperature and coldness evolution equations are provided accounting for Fourier-like conduction and Gough–Joule-like effects. The proposed theory is elucidated via numerical examples in Sect. 4. Section 5 concludes the work and provides further outlook.

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 (CCM). 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 $\boldsymbol{X}$ that are not integrals and thus are local. On the contrary, point-wise equations at each $\boldsymbol{X}$ 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 $\boldsymbol{X}^{|}$. 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. This is illustrated in Fig. 1 for the dissipation inequality. □

2 Kinematics

Central to CPD [20] is the geometrically exact description inspired by CCM. Consider a continuum body that occupies the material configuration $\mathcal{B}_0 \subset \mathbb{R}^3$ at time $t = 0$ and that is mapped to the spatial configuration $\mathcal{B}_t \subset \mathbb{R}^3$ via the nonlinear deformation map $\boldsymbol{y}$ as $\boldsymbol{x} = \boldsymbol{y}(\boldsymbol{X}, t) : \mathcal{B}_0 \times \mathbb{R}_+ \to \mathcal{B}_t$ with $\boldsymbol{X}$ and $\boldsymbol{x}$ identifying points in the material and spatial configurations, respectively, as illustrated in Fig. 2. A key characteristic of CPD that distinguishes it from CCM is the non-locality assumption that any point $\boldsymbol{X}$ in the material configuration can interact with other points within its finite neighbourhood $\mathcal{H}_0(\boldsymbol{X})$. The neighbourhood $\mathcal{H}_0$ is referred

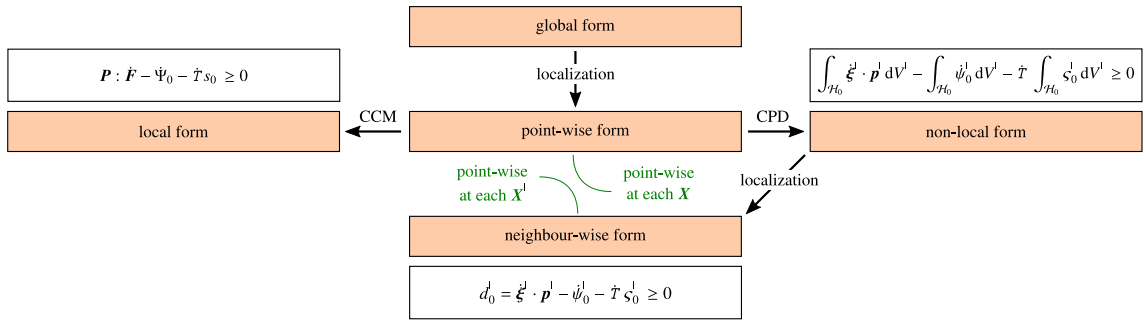

Fig. 1 Schematic of the notions localization procedure, point-wise equations and neighbour-wise equations. The equations in the white boxes are the dissipation inequalities corresponding to each form

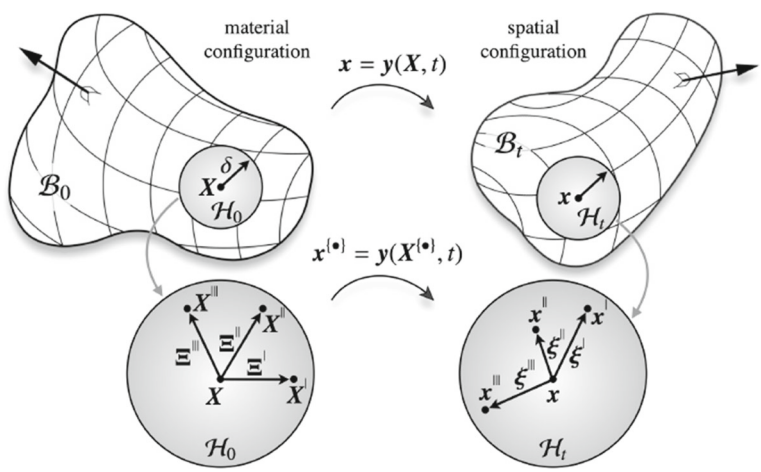

Fig. 2 Motion of a continuum body within the CPD formulation. The continuum body that occupies the material configuration $\mathcal{B}_0 \subset \mathbb{R}^3$ at time $t = 0$ is mapped to the spatial configuration $\mathcal{B}_t \subset \mathbb{R}^3$ via the nonlinear deformation map $\boldsymbol{y}$. The neighbourhood of $\boldsymbol{X}$ is mapped onto the neighbourhood of $\boldsymbol{x}$. That is, the neighbour set $\{\boldsymbol{X}^{\mathrm{I}}, \boldsymbol{X}^{\mathrm{II}}, \boldsymbol{X}^{\mathrm{III}}\}$ is mapped onto $\{\boldsymbol{x}^{\mathrm{I}}, \boldsymbol{x}^{\mathrm{II}}, \boldsymbol{x}^{\mathrm{III}}\}$, respectively

to as the *horizon* in the material configuration. The *measure* of the horizon in the material configuration is denoted $\delta_0 := \mathrm{meas}(\mathcal{H}_0)$ and is generally the radius of a spherical neighbourhood at $\boldsymbol{X}$. The spatial horizon $\mathcal{H}_t = \boldsymbol{y}(\mathcal{H}_0, t)$ is the image of the material horizon $\mathcal{H}_0$ under the deformation map $\boldsymbol{y}$.

We identify the neighbours within the horizon by a superscript. For instance, the point $\boldsymbol{X}^{\mathrm{I}} \in \mathcal{H}_0(\boldsymbol{X})$ denotes any (first) neighbour of point $\boldsymbol{X}$ in the material configuration. Similarly, the points $\boldsymbol{X}^{\mathrm{II}} \in \mathcal{H}_0(\boldsymbol{X})$ and $\boldsymbol{X}^{\mathrm{III}} \in \mathcal{H}_0(\boldsymbol{X})$ denote any second and third neighbour of point $\boldsymbol{X}$ in the material configuration, respectively. The point $\boldsymbol{x}^{\mathrm{I}}$ within the horizon of $\boldsymbol{x}$ is the spatial counterpart of the point $\boldsymbol{X}^{\mathrm{I}}$ defined via the nonlinear deformation map $\boldsymbol{y}$ as $\boldsymbol{x}^{\mathrm{I}} := \boldsymbol{y}(\boldsymbol{X}^{\mathrm{I}}, t)$. For any point $\boldsymbol{X}$ we identify the possible neighbour sets $\{\boldsymbol{X}^{\mathrm{I}}, \boldsymbol{X}^{\mathrm{II}}, \boldsymbol{X}^{\mathrm{III}}\}$ that are mapped onto $\{\boldsymbol{x}^{\mathrm{I}}, \boldsymbol{x}^{\mathrm{II}}, \boldsymbol{x}^{\mathrm{III}}\}$, respectively, as shown in Fig. 2. The relative positions, i.e. the finite line elements, in the material and spatial configurations are denoted by $\boldsymbol{\Xi}^{\{\bullet\}}$ and $\boldsymbol{\xi}^{\{\bullet\}}$, respectively, where the superscript $\{\bullet\}$ identifies the neighbour, that is

$$\boldsymbol{\Xi}^{\mathrm{I}} := \boldsymbol{X}^{\mathrm{I}} - \boldsymbol{X} \quad , \quad \boldsymbol{\Xi}^{\mathrm{II}} := \boldsymbol{X}^{\mathrm{II}} - \boldsymbol{X} \quad , \quad \boldsymbol{\Xi}^{\mathrm{III}} := \boldsymbol{X}^{\mathrm{III}} - \boldsymbol{X} \, ,$$

in the material configuration and

$$\boldsymbol{\xi}^{\mathrm{I}} := \boldsymbol{x}^{\mathrm{I}} - \boldsymbol{x} \quad , \quad \boldsymbol{\xi}^{\mathrm{II}} := \boldsymbol{x}^{\mathrm{II}} - \boldsymbol{x} \quad , \quad \boldsymbol{\xi}^{\mathrm{III}} := \boldsymbol{x}^{\mathrm{III}} - \boldsymbol{x} \, ,$$

in the spatial configuration. Recall the three *local kinematic measures* of relative deformation, namely the deformation gradient $\boldsymbol{F} := \mathrm{Grad}\, \boldsymbol{y}$, its cofactor $\boldsymbol{K} := \mathrm{Cof}\, \boldsymbol{F}$ and its determinant $J := \mathrm{Det}\, \boldsymbol{F}$. In the spirit of these local measures, we introduce three *non-local kinematic measures* of relative deformation, namely $\boldsymbol{\xi}^{\mathrm{I}}$,

Table 1 Summary of CPD kinematics

One-neighbour interactions	Two-neighbour interaction	Three-neighbour interactions
$\boldsymbol{\Xi}^{\mathrm{I}} = \boldsymbol{X}^{\mathrm{I}} - \boldsymbol{X}$	$\boldsymbol{\Xi}^{\mathrm{II}} = \boldsymbol{X}^{\mathrm{II}} - \boldsymbol{X}$	$\boldsymbol{\Xi}^{\mathrm{III}} = \boldsymbol{X}^{\mathrm{III}} - \boldsymbol{X}$
$\boldsymbol{\xi}^{\mathrm{I}} = \boldsymbol{x}^{\mathrm{I}} - \boldsymbol{x}$	$\boldsymbol{\xi}^{\mathrm{II}} = \boldsymbol{x}^{\mathrm{II}} - \boldsymbol{x}$	$\boldsymbol{\xi}^{\mathrm{III}} = \boldsymbol{x}^{\mathrm{III}} - \boldsymbol{x}$
$\boldsymbol{\Xi}^{\mathrm{I}}$	$\boldsymbol{A}^{\mathrm{I/II}} = \boldsymbol{\Xi}^{\mathrm{I}} \times \boldsymbol{\Xi}^{\mathrm{II}}$	$V^{\mathrm{I/II/III}} = \boldsymbol{\Xi}^{\mathrm{I}} \cdot [\boldsymbol{\Xi}^{\mathrm{II}} \times \boldsymbol{\Xi}^{\mathrm{III}}]$
$\boldsymbol{\xi}^{\mathrm{I}}$	$\boldsymbol{a}^{\mathrm{I/II}} = \boldsymbol{\xi}^{\mathrm{I}} \times \boldsymbol{\xi}^{\mathrm{II}}$	$v^{\mathrm{I/II/III}} = \boldsymbol{\xi}^{\mathrm{I}} \cdot [\boldsymbol{\xi}^{\mathrm{II}} \times \boldsymbol{\xi}^{\mathrm{III}}]$

$\boldsymbol{a}^{\mathrm{I}/\mathrm{II}}$ and $v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}$ that are associated with CPD. *The first relative deformation measure* $\boldsymbol{\xi}^{\mathrm{I}}$ mimics the linear map $\boldsymbol{F}$ of the infinitesimal line element $\mathrm{d}\boldsymbol{X}$ in the material configuration to its spatial counterpart $\mathrm{d}\boldsymbol{x}$. In view of our proposed CPD formalism, the relative deformation measure

$$\boldsymbol{\xi}^{\mathrm{I}} = \boldsymbol{x}^{\mathrm{I}} - \boldsymbol{x}\,,$$

is the main ingredient to describe *one-neighbour interactions*. Note that the horizons $\mathcal{H}_0$ and $\mathcal{H}_t$ coincide with the points $\boldsymbol{X}$ and $\boldsymbol{x}$ in the limit of an infinitesimal neighbourhood. It can be shown [20] that in the infinitesimal limit the relation $\boldsymbol{\xi}^{\mathrm{I}} = \boldsymbol{F} \cdot \boldsymbol{\Xi}^{\mathrm{I}}$ holds. *The second relative deformation measure* $\boldsymbol{a}^{\mathrm{I}/\mathrm{II}}$ is reminiscent of the linear map $\boldsymbol{K}$ from the infinitesimal vectorial area element $\mathrm{d}\boldsymbol{A}$ in the material configuration to its spatial counterpart $\mathrm{d}\boldsymbol{a}$. This is essentially the Nanson's formula. In our proposed framework, the relative area measure

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

is the main ingredient to describe *two-neighbour interactions*. Again, in the infinitesimal limit, the relation $\boldsymbol{a}^{\mathrm{I}/\mathrm{II}} = \boldsymbol{K} \cdot \boldsymbol{A}^{\mathrm{I}/\mathrm{II}}$ is obtained [20]. *The third relative deformation measure* $v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}$ mimics the linear map J from the infinitesimal volume element $\mathrm{d}V$ in the material configuration to its spatial counterpart $\mathrm{d}v$. The relative volume measure

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

is the main ingredient to describe *three-neighbour interactions*. Similarly, the relation $v^{\mathrm{I}/\mathrm{II}/\mathrm{III}} = J\, V^{\mathrm{I}/\mathrm{II}/\mathrm{III}}$ is obtained [20] in the infinitesimal limit. Table 1 summarises the kinematics of CPD.

3 Thermodynamic balance laws

This section introduces the thermodynamic balance laws specific to CPD. Following a brief overview of the momentum balances, the balances of mechanical, thermal and entropic powers in Sects. 3.1, 3.2 and 3.3 are established. Various aspects of this introduction are included in our recent contribution [20], and are presented here as they are the basis of the subsequent derivations. Thereafter, temperature-based and coldness-based dissipation inequalities are provided in Sect. 3.4. Thermodynamically consistent constitutive equations are derived in Sect. 3.5 via a Coleman–Noll-like procedure. Evolution equations for temperature and coldness are given in Sect. 3.6. Table 2 gathers the key governing equations of thermo-mechanical continua for both classical continuum mechanics and the current continuum-kinematics-inspired peridynamics approach and highlights their similarities and differences. The point of departure and the underlying postulate here is the virtual power equivalence

$$\int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{p}^{\mathrm{I}} \cdot \delta \boldsymbol{y}^{\mathrm{I}}\, \mathrm{d}V^{\mathrm{I}}\, \mathrm{d}V = \int_{\delta\mathcal{B}_0} \boldsymbol{t}_0^{\mathrm{ext}} \cdot \delta \boldsymbol{y}\, \mathrm{d}A \qquad \forall \delta \boldsymbol{y}\,, \tag{1}$$

where $\boldsymbol{p}^{\mathrm{I}}$ is a force density vector and $\boldsymbol{t}_0^{\mathrm{ext}}$ is the external traction on the boundary in the material configuration. Note, this format of the external traction on the boundary is a particular sub-case of a more general case applicable to higher gradient and non-local continua as elaborated in [26–29], among others. This restriction here is only imposed for the sake of brevity and more complex boundary conditions shall be investigated separately. In general, the nature of suitable (non-local) boundary conditions of a PD formulation can be identified only through establishing a fully variational structure, which is not a trivial task for the thermo-mechanical problem at hand. For further details on higher gradient boundary conditions relevant to the discussion here, see [30–32]

Table 2 Governing equations of classical continuum mechanics (CCM) and continuum-kinematics-inspired peridynamics (CPD). Only the more familiar quantity "temperature" is presented but "coldness" is elaborated on in the manuscript

Linear momentum balance	CCM	$\rho_0 \dot{\boldsymbol{v}} = \mathrm{Div}\boldsymbol{P} + \boldsymbol{b}_0^{\mathrm{ext}}$ subject to $\boldsymbol{P}\cdot\boldsymbol{N} = \boldsymbol{t}_0^{\mathrm{ext}}$
	CPD	$\rho_0 \dot{\boldsymbol{v}} = \int_{\mathcal{H}_0} \boldsymbol{p}^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}} + \boldsymbol{b}_0^{\mathrm{ext}}$ subject to $\int_{\mathcal{B}_0}\int_{\mathcal{B}_0} \boldsymbol{p}^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}} \mathrm{d}V = \int_{\partial\mathcal{B}_0} \boldsymbol{t}_0^{\mathrm{ext}} \mathrm{d}A$
Angular momentum balance	CCM	$\boldsymbol{\varepsilon} : [\boldsymbol{F}\cdot\boldsymbol{P}^{\mathrm{t}}] = \boldsymbol{0}$
	CPD	$\int_{\mathcal{H}_0} \xi^{\mathsf{I}} \times \boldsymbol{p}^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}} = \boldsymbol{0}$
Thermal power balance	CCM	$\dot{u}_0 = \boldsymbol{P} : \dot{\boldsymbol{F}} + \mathscr{R}_0^{\mathrm{ext}} - \mathrm{Div}\boldsymbol{Q}$ subject to $\boldsymbol{Q}\cdot\boldsymbol{N} = \mathscr{Q}_0^{\mathrm{ext}}$
	CPD	$\dot{u}_0 = \int_{\mathcal{H}_0} \dot{\xi}^{\mathsf{I}} \cdot \boldsymbol{p}^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}} + \mathscr{R}_0^{\mathrm{ext}} - \int_{\mathcal{H}_0} q^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}}$ subject to $\int_{\mathcal{B}_0}\int_{\mathcal{B}_0} q^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}} \mathrm{d}V = \int_{\partial\mathcal{B}_0} \mathscr{Q}_0^{\mathrm{ext}} \mathrm{d}A$
Entropic power balance	CCM	$\dot{s}_0 T = \mathscr{R}_0^{\mathrm{ext}} - T\mathrm{Div}\left(\frac{\boldsymbol{Q}}{T}\right) + \mathscr{D}_0$ subject to $\frac{\boldsymbol{Q}}{T}\cdot\boldsymbol{N} = \frac{\mathscr{Q}_0^{\mathrm{ext}}}{T}$
	CPD	$\dot{s}_0 T = \mathscr{R}_0^{\mathrm{ext}} - T\int_{\mathcal{H}_0} \frac{q^{\mathsf{I}}}{T^{\mathsf{I}}} \mathrm{d}V^{\mathsf{I}} + \mathscr{D}_0$ subject to $\int_{\mathcal{B}_0}\int_{\mathcal{B}_0} \frac{q^{\mathsf{I}}}{T^{\mathsf{I}}} \mathrm{d}V^{\mathsf{I}} \mathrm{d}V = \int_{\partial\mathcal{B}_0} \frac{\mathscr{Q}_0^{\mathrm{ext}}}{T} \mathrm{d}A$
Fourier heat conduction	CCM	$\boldsymbol{Q} = -\mathbb{K}\cdot\mathrm{Grad}T$
	CPD	$q^{\mathsf{I}} = -K[T^{\mathsf{I}} - T]$
Dissipation inequality	CCM	$\boldsymbol{P} : \dot{\boldsymbol{F}} - \dot{\Psi}_0 - \dot{T}s_0 \geq 0$
	CPD	$\int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{\mathsf{I}} \cdot \boldsymbol{p}^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}} - \int_{\mathcal{H}_0} \dot{\psi}_0^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}} - \dot{T}\int_{\mathcal{H}_0} \varsigma_0^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}} \geq 0$
Temperature evolution equation	CCM	$c\,\dot{T} = \mathscr{R}_0^{\mathrm{ext}} - \mathrm{Div}\boldsymbol{Q} + T\frac{\partial\boldsymbol{P}}{\partial T} : \dot{\boldsymbol{F}}$
	CPD	$c^T\,\dot{T} = \mathscr{R}_0^{\mathrm{ext}} - \int_{\mathcal{H}_0} q^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}} + T\int_{\mathcal{H}_0} \frac{\partial\boldsymbol{P}^{\mathsf{I}}}{\partial T^{\mathsf{I}}} \cdot \dot{\boldsymbol{\xi}}^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}}$

among others. Utilising the virtual power equivalence (1) for a quasi-static conservative case, one can derive the thermodynamic balance laws for more general cases. Among all admissible motions for any arbitrary $\delta\boldsymbol{y}$, consider *rigid translation* and *rigid rotation*. For a rigid translation of the body, $\delta\boldsymbol{y} = \delta\boldsymbol{y}^{\mathsf{I}} = \text{const.}$, and therefore the virtual power equivalence reduces to

$$\int_{\mathcal{B}_0} \underbrace{\int_{\mathcal{H}_0} \boldsymbol{p}^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}}}_{=:\,\boldsymbol{b}_0^{\mathrm{int}}} \mathrm{d}V = \int_{\partial\mathcal{B}_0} \boldsymbol{t}_0^{\mathrm{ext}} \mathrm{d}A \qquad \Rightarrow \qquad \int_{\mathcal{B}_0} \boldsymbol{b}_0^{\mathrm{int}} \mathrm{d}V = \int_{\partial\mathcal{B}_0} \boldsymbol{t}_0^{\mathrm{ext}} \mathrm{d}A. \tag{2}$$

This can be understood as *traction equivalence*. Using the Gauss theorem and $\boldsymbol{P}\cdot\boldsymbol{N} = \boldsymbol{t}_0^{\mathrm{ext}}$, the more familiar counterpart of (2) in classical continuum mechanics is

$$\int_{\mathcal{B}_0} \underbrace{\mathrm{Div}\boldsymbol{P}}_{=:\,\boldsymbol{b}_0^{\mathrm{int}}} \mathrm{d}V = \int_{\partial\mathcal{B}_0} \boldsymbol{t}_0^{\mathrm{ext}} \mathrm{d}A \qquad \Rightarrow \qquad \int_{\mathcal{B}_0} \boldsymbol{b}_0^{\mathrm{int}} \mathrm{d}V = \int_{\partial\mathcal{B}_0} \boldsymbol{t}_0^{\mathrm{ext}} \mathrm{d}A.$$

For a rigid rotation of the body, $\delta\boldsymbol{y} = \boldsymbol{\omega}_\delta \times \boldsymbol{y}$ and $\delta\boldsymbol{y}^{\mathsf{I}} = \boldsymbol{\omega}_\delta \times \boldsymbol{y}^{\mathsf{I}}$ with a constant; otherwise arbitrary, $\boldsymbol{\omega}_\delta$ being the variational analogue to the angular velocity vector, the virtual power equivalence reduces to

$$\int_{\mathcal{B}_0}\int_{\mathcal{H}_0} \boldsymbol{y}^{\mathsf{I}} \times \boldsymbol{p}^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}} \mathrm{d}V = \int_{\partial\mathcal{B}_0} \boldsymbol{y} \times \boldsymbol{t}_0^{\mathrm{ext}} \mathrm{d}A\,, \tag{3}$$

which is the *torque equivalence*. This should be compared with the more conventional counterpart in classical continuum mechanics given by

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

The momentum balance equations of a dynamic problem are obtained by following the standard procedure of classical continuum mechanics. First, using the traction equivalence (2) and the torque equivalence (3) we identify terms of the global form of the force or moment balance in their integral forms. 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 $\boldsymbol{t}_0^{\text{ext}}$ is now replaced by the traction equivalence (2) and the definition of the internal body force density $\boldsymbol{b}_0^{\text{int}}$ is employed to obtain

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

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

$$\rho_0\, \dot{\boldsymbol{v}} = \boldsymbol{b}_0^{\text{int}} + \boldsymbol{b}_0^{\text{ext}} \qquad \Rightarrow \qquad \rho_0\, \dot{\boldsymbol{v}} = \int_{\mathcal{H}_0} \boldsymbol{p}^{|}\, \mathrm{d}V^{|} + \boldsymbol{b}_0^{\text{ext}}\,. \tag{4}$$

Its analogue in classical continuum mechanics is given by

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

To derive the angular momentum balance, one starts from the global form of the moment balance

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

The integral of external traction moment $\boldsymbol{y} \times \boldsymbol{t}_0^{\text{ext}}$ is now replaced by the torque equivalence (3) to yield

$$\int_{\mathcal{B}_0} \boldsymbol{y} \times [\rho_0\, \dot{\boldsymbol{v}}]\, \mathrm{d}V = \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{y}^{|} \times \boldsymbol{p}^{|}\, \mathrm{d}V^{|}\, \mathrm{d}V + \int_{\mathcal{B}_0} \boldsymbol{y} \times \boldsymbol{b}_0^{\text{ext}}\, \mathrm{d}V$$

which after some mathematical steps reads

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

Using the linear momentum balance (4), this reduces to the global form of the angular momentum balance

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

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

$$\int_{\mathcal{H}_0} \boldsymbol{\xi}^{|} \times \boldsymbol{p}^{|}\, \mathrm{d}V^{|} = \boldsymbol{0}\,, \tag{5}$$

with its counterpart in classical continuum mechanics given by

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

3.1 Balance of mechanical power

Equipped with the balance of linear momentum, we now consider the balance of mechanical power. Note that this is *not* an additional equation but rather a consequence of the balance of linear momentum (4). Let K denote the global kinetic energy in the material configuration, with its rate denoted by

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

Expressing the term $\rho_0\, \dot{\boldsymbol{v}}$ via the linear momentum balance (4) yields

$$\mathcal{K} = \int_{\mathcal{B}_0} \boldsymbol{v} \cdot [\, \rho_0\, \dot{\boldsymbol{v}}\,]\, \mathrm{d}V = \int_{\mathcal{B}_0} \boldsymbol{v} \cdot [\, \boldsymbol{b}_0^{\text{int}} + \boldsymbol{b}_0^{\text{ext}}\,]\, \mathrm{d}V = \int_{\mathcal{B}_0} \boldsymbol{v} \cdot \int_{\mathcal{H}_0} \boldsymbol{p}^{|}\, \mathrm{d}V^{|}\, \mathrm{d}V + \int_{\mathcal{B}_0} \boldsymbol{v} \cdot \boldsymbol{b}_0^{\text{ext}}\, \mathrm{d}V.$$

Using the relation $\boldsymbol{v} = \boldsymbol{v}^{|} - \dot{\boldsymbol{\xi}}^{|}$, the rate of the global kinetic energy $\mathcal{K}$ reads

$$\mathcal{K} = \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \boldsymbol{v}^{|} \cdot \boldsymbol{p}^{|} \, \mathrm{d}V^{|} \, \mathrm{d}V + \int_{\mathcal{B}_0} \boldsymbol{v} \cdot \boldsymbol{b}_0^{\text{ext}} \, \mathrm{d}V - \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{|} \cdot \boldsymbol{p}^{|} \, \mathrm{d}V^{|} \, \mathrm{d}V \,, \tag{6}$$

where the first term can be expressed via the virtual power equivalence (1) particularised to $\delta \boldsymbol{y} = \boldsymbol{v}$ as the *power equivalence* thus,

$$\mathcal{K} = \underbrace{\int_{\partial \mathcal{B}_0} \boldsymbol{v} \cdot \boldsymbol{t}_0^{\text{ext}} \, \mathrm{d}A + \int_{\mathcal{B}_0} \boldsymbol{v} \cdot \boldsymbol{b}_0^{\text{ext}} \, \mathrm{d}V}_{\mathcal{P}^{\text{ext}}} - \underbrace{\int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{|} \cdot \boldsymbol{p}^{|} \, \mathrm{d}V^{|} \, \mathrm{d}V}_{\mathcal{P}^{\text{int}}} \quad \Rightarrow \quad \mathcal{K} = \mathcal{P}^{\text{ext}} - \mathcal{P}^{\text{int}}. \tag{7}$$

$\mathcal{P}^{\text{int}}$ 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.

3.2 Balance of thermal power

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

$$\mathcal{U} := \dot{U} \quad \text{with} \quad U := \int_{\mathcal{B}_0} u_0 \, \mathrm{d}V \quad \Rightarrow \quad \mathcal{U} = \int_{\mathcal{B}_0} \dot{u}_0 \, \mathrm{d}V.$$

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 prescribed heat sources within the continuum body and 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. (7), 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

$$\mathcal{U} = \mathcal{P}^{\text{int}} + \mathcal{Q}^{\text{ext}}. \tag{8}$$

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 within the body $\mathcal{Q}_{\mathcal{B}}^{\text{ext}}$ and thermal power on the boundary $\mathcal{Q}_{\partial\mathcal{B}}^{\text{ext}}$ as

$$\mathcal{Q}^{\text{ext}} = \mathcal{Q}_{\mathcal{B}}^{\text{ext}} + \mathcal{Q}_{\partial\mathcal{B}}^{\text{ext}} \,, \tag{9}$$

where

$$\mathcal{Q}_{\mathcal{B}}^{\text{ext}} := \int_{\mathcal{B}_0} \mathscr{R}_0^{\text{ext}} \, \mathrm{d}V \quad \text{and} \quad \mathcal{Q}_{\partial\mathcal{B}}^{\text{ext}} := -\int_{\partial\mathcal{B}_0} \mathscr{Q}_0^{\text{ext}} \, \mathrm{d}A. \tag{10}$$

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 $\boldsymbol{b}_0^{\text{ext}}$ for the mechanical problem, e.g. in Eq. (4). In a similar fashion, the external heat flux density $\mathscr{Q}_0^{\text{ext}}$ is reminiscent of the externally prescribed traction $\boldsymbol{t}_0^{\text{ext}}$ for the mechanical problem. Similar to the virtual power equivalence (1) for the mechanical problem, a *thermal power equivalence* can be established as

$$\int_{\mathcal{B}_0} \int_{\mathcal{H}_0} q^{|} \, \mathrm{d}V^{|} \, \mathrm{d}V = \int_{\partial\mathcal{B}_0} \mathscr{Q}_0^{\text{ext}} \, \mathrm{d}A \,, \tag{11}$$

with $q^{|}$ the heat flux density per volume squared in the material configuration with units N.m/s.m^6. The thermal power equivalence (11) should be compared with its more familiar counterpart in classical continuum mechanics, obtained via the Gauss theorem and the postulate $\boldsymbol{Q} \cdot \boldsymbol{N} = \mathscr{Q}_0^{\text{ext}}$, and given by

$$\int_{\mathcal{B}_0} \operatorname{Div} \boldsymbol{Q} \, \mathrm{d}V = \int_{\partial \mathcal{B}_0} \mathscr{Q}_0^{\text{ext}} \, \mathrm{d}A \,,$$

with $\boldsymbol{Q}$ the heat flux vector in the material configuration. Inserting the thermal power equivalence (11) and the definition (10) into the thermal power expression (9) yields

$$\mathcal{Q}^{\text{ext}} = \int_{\mathcal{B}_0} \mathscr{R}_0^{\text{ext}} \, \mathrm{d}V - \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} q^{|} \, \mathrm{d}V^{|} \, \mathrm{d}V = \int_{\mathcal{B}_0} \Big[\mathscr{R}_0^{\text{ext}} - \int_{\mathcal{H}_0} q^{|} \, \mathrm{d}V^{|} \Big] \mathrm{d}V. \tag{12}$$

To proceed, we substitute the thermal power $\mathcal{Q}^{\text{ext}}$ and the internal (mechanical) power $\mathcal{P}^{\text{int}}$ into the internal energy balance (8) which yields the important global relation

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

or alternatively

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

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

$$\dot{u}_0 = \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{|} \cdot \boldsymbol{p}^{|} \, \mathrm{d}V^{|} + \mathscr{R}_0^{\text{ext}} - \int_{\mathcal{H}_0} q^{|} \, \mathrm{d}V^{|}. \tag{13}$$

This is also referred to as the balance of energy or more generally, the first law of thermodynamics. The non-local form of the thermal power balance (13) should be compared with its local form in classical continuum mechanics

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

3.3 Balance of entropic power

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 rate denoted by $\mathcal{S}$, as

$$\mathcal{S} := \dot{S} \quad \text{with} \quad S := \int_{\mathcal{B}_0} s_0 \, \mathrm{d}V \quad \Rightarrow \quad \mathcal{S} = \int_{\mathcal{B}_0} \dot{s}_0 \, \mathrm{d}V. \tag{14}$$

The balance of entropic power states that the rate of the entropy $\mathcal{S}$ equals the entropy input that is,

$$\mathcal{S} = \mathcal{H}^{\text{ext}} + \mathcal{H}^{\text{prd}} \quad \text{with} \quad \mathcal{H}^{\text{prd}} \geq 0 \,, \tag{15}$$

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

$$\mathcal{H}^{\text{ext}} = \mathcal{H}_{\mathcal{B}}^{\text{ext}} + \mathcal{H}_{\partial\mathcal{B}}^{\text{ext}}. \tag{16}$$

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

$$\mathcal{H}_{\mathcal{B}}^{\text{ext}} = \int_{\mathcal{B}_0} \frac{\mathscr{R}_0^{\text{ext}}}{T} \, \mathrm{d}V \quad \text{and} \quad \mathcal{H}_{\partial\mathcal{B}}^{\text{ext}} = - \int_{\partial\mathcal{B}_0} \frac{\mathscr{Q}_0^{\text{ext}}}{T} \, \mathrm{d}A \,, \tag{17}$$

with $\mathcal{T} > 0$ 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 $\mathcal{H}^{\text{prd}}$ as

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

Next, Eq. (17) is inserted into the external entropy input (16) and then motivated by the thermal power equivalence (11), in accordance with the virtual power equivalence (1) for the mechanical problem, an *entropic power equivalence* is postulated as

$$\int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \frac{q^{|}}{\mathcal{T}^{|}} \, \mathrm{d}V^{|} \, \mathrm{d}V = \int_{\partial\mathcal{B}_0} \frac{\mathscr{Q}_0^{\text{ext}}}{\mathcal{T}} \, \mathrm{d}A \,, \tag{18}$$

with $\mathcal{T}^{|}$ being the temperature of the neighbouring point $\boldsymbol{X}^{|}$ within the horizon. Inserting the relations (18) and $(14)_3$ into the entropic power equivalence (15) results in the global entropic power balance

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

which after localization reads

$$\dot{s}_0 \, \mathcal{T} = \mathscr{R}_0^{\text{ext}} - \mathcal{T} \int_{\mathcal{H}_0} \frac{q^{|}}{\mathcal{T}^{|}} \, \mathrm{d}V^{|} + \mathscr{D}_0. \tag{19}$$

The non-local form of the entropic power balance (19) should be compared with its local form in classical continuum mechanics

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

The non-local form of the entropic power balance can likewise be expressed in terms of coldness $\mathcal{C} := \mathcal{T}^{-1}$ as

$$\frac{\dot{s}_0}{\mathcal{C}} = \mathscr{R}_0^{\text{ext}} - \frac{1}{\mathcal{C}} \int_{\mathcal{H}_0} \mathcal{C}^{|} q^{|} \, \mathrm{d}V^{|} + \mathscr{D}_0. \tag{20}$$

3.4 Dissipation inequality

Motivated by the format of the entropic power balance Eqs. (19) and (20), we consider two representations for the relative temperature and coldness, respectively, and study their consequences. In the first representation, we utilise the relative temperature $\vartheta^{|} := \mathcal{T}^{|} - \mathcal{T}$ whereas for the second, we use the relative coldness $\kappa^{|} := \mathcal{C}^{|} - \mathcal{C}$. That is,

$$\begin{cases} \text{option } \mathtt{T}: \quad \vartheta^{|} := \mathcal{T}^{|} - \mathcal{T} \qquad \text{suitable for (19)} \qquad \dot{s}_0 \, \mathcal{T} = \mathscr{R}_0^{\text{ext}} + \mathscr{D}_0 - \mathcal{T} \displaystyle\int_{\mathcal{H}_0} \frac{q^{|}}{\mathcal{T}^{|}} \, \mathrm{d}V^{|} \,, \\ \text{option } \mathtt{C}: \quad \kappa^{|} := \mathcal{C}^{|} - \mathcal{C} \qquad \text{suitable for (20)} \qquad \dfrac{\dot{s}_0}{\mathcal{C}} = \mathscr{R}_0^{\text{ext}} + \mathscr{D}_0 - \dfrac{1}{\mathcal{C}} \displaystyle\int_{\mathcal{H}_0} \mathcal{C}^{|} q^{|} \, \mathrm{d}V^{|} \,, \end{cases}$$

and for both cases, we focus on the last terms only

$$\begin{cases} \text{option } \mathtt{T}: \quad \mathcal{T} := \mathcal{T}^{|} - \vartheta^{|} \quad \Rightarrow \quad -\mathcal{T} \displaystyle\int_{\mathcal{H}_0} \frac{q^{|}}{\mathcal{T}^{|}} \, \mathrm{d}V^{|} = -\int_{\mathcal{H}_0} q^{|} \, \mathrm{d}V^{|} + \int_{\mathcal{H}_0} \frac{\vartheta^{|}}{\mathcal{T}^{|}} q^{|} \, \mathrm{d}V^{|} \,, \\ \text{option } \mathtt{C}: \quad \mathcal{C}^{|} := \mathcal{C} + \kappa^{|} \quad \Rightarrow \quad -\dfrac{1}{\mathcal{C}} \displaystyle\int_{\mathcal{H}_0} \mathcal{C}^{|} q^{|} \, \mathrm{d}V^{|} = -\int_{\mathcal{H}_0} q^{|} \, \mathrm{d}V^{|} - \dfrac{1}{\mathcal{C}} \int_{\mathcal{H}_0} \kappa^{|} q^{|} \, \mathrm{d}V^{|}. \end{cases}$$

Thus, the non-local forms of the entropic power balance equations can be unified as

$$\left\{\begin{array}{llll} \text{option } \mathtt{T}: & \dot{s}_0\, T = \mathscr{R}_0^{\text{ext}} + \mathscr{D}_0 - \displaystyle\int_{\mathcal{H}_0} q^{|}\, \mathrm{d}V^{|} - \mathscr{D}_0^{\text{con}} & \text{with} & \mathscr{D}_0^{\text{con}} := -\displaystyle\int_{\mathcal{H}_0} \frac{\vartheta^{|}}{T^{|}}\, q^{|}\, \mathrm{d}V^{|}\,, \\ \text{option } \mathtt{C}: & \dfrac{\dot{s}_0}{C} = \mathscr{R}_0^{\text{ext}} + \mathscr{D}_0 - \displaystyle\int_{\mathcal{H}_0} q^{|}\, \mathrm{d}V^{|} - \mathscr{D}_0^{\text{con}} & \text{with} & \mathscr{D}_0^{\text{con}} := \dfrac{1}{C}\displaystyle\int_{\mathcal{H}_0} \kappa^{|}\, q^{|}\, \mathrm{d}V^{|}\,, \end{array}\right. \tag{21}$$

in which $\mathscr{D}_0^{\text{con}}$ denotes the dissipation density due to heat conduction. Note, the only place where the choice of $\mathtt{T}$ or $\mathtt{C}$ enters is the definition of the conductive dissipation power density $\mathscr{D}_0^{\text{con}}$. Thus, both options can be unified as

$$\underbrace{\dot{s}_0\, T}_{=\frac{\dot{s}_0}{C}} = \mathscr{R}_0^{\text{ext}} + \mathscr{D}_0^{\text{ncon}} - \int_{\mathcal{H}_0} q^{|}\, \mathrm{d}V^{|}\,, \tag{22}$$

In the unified entropic power balance equation (22), we decomposed the dissipation power $\mathscr{D}_0$ into its conductive and non-conductive contributions as

$$\mathscr{D}_0 = \mathscr{D}_0^{\text{con}} + \mathscr{D}_0^{\text{ncon}} \geq 0 \qquad \text{with the assumption that} \qquad \mathscr{D}_0^{\text{con}} \geq 0 \;\text{ and }\; \mathscr{D}_0^{\text{ncon}} \geq 0.$$

Employing the thermal power balance (13), the non-local form of the entropic power balance (22) can be re-written as

$$\underbrace{\dot{s}_0\, T}_{=\frac{\dot{s}_0}{C}} = \dot{u}_0 - \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{|} \cdot \boldsymbol{p}^{|}\, \mathrm{d}V^{|} + \mathscr{D}_0^{\text{ncon}}. \tag{23}$$

As we will see shortly, the point of departure to derive the temperature evolution equation for thermoelasticity is to impose $\mathscr{D}_0^{\text{ncon}} = 0$. This essentially means that dissipation occurs only due to the Fourier-like conduction.

3.5 Coleman–Noll procedure

Equipped with the dissipation inequality, we now 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/coldness as

$$\left\{\begin{array}{llll} \text{option } \mathtt{T}: & \Psi_0 := u_0 - T s_0 & \Rightarrow & \dot{\Psi}_0 := \dot{u}_0 - s_0 \dot{T} - \dot{s}_0 T\,, \\ \text{option } \mathtt{C}: & \Psi_0 := u_0 - \dfrac{s_0}{C} & \Rightarrow & \dot{\Psi}_0 := \dot{u}_0 + s_0 \dfrac{\dot{C}}{C^2} - \dfrac{\dot{s}_0}{C}. \end{array}\right. \tag{24}$$

Replacing Eq. (24) into the entropic power balance (23) results in the non-local form of the dissipation inequality

$$\left\{\begin{array}{lll} \text{option } \mathtt{T}: & \mathscr{D}_0^{\text{ncon}} = \displaystyle\int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{|} \cdot \boldsymbol{p}^{|}\, \mathrm{d}V^{|} - \dot{\Psi}_0 - s_0 \dot{T} & \geq 0\,, \\ \text{option } \mathtt{C}: & \mathscr{D}_0^{\text{ncon}} = \displaystyle\int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{|} \cdot \boldsymbol{p}^{|}\, \mathrm{d}V^{|} - \dot{\Psi}_0 + s_0 \dfrac{\dot{C}}{C^2} & \geq 0. \end{array}\right. \tag{25}$$

Furthermore, we require that not only the non-conductive dissipation density $\mathscr{D}_0^{\text{ncon}}$ but also the conductive dissipation density $\mathscr{D}_0^{\text{con}}$ must be non-negative. Using Eq. (21) one arrives at the following Fourier-like heat conduction relations

$$\left\{\begin{array}{llll} \text{option } \mathtt{T}: & \mathscr{D}_0^{\text{con}} := -\displaystyle\int_{\mathcal{H}_0} \frac{\vartheta^{|}}{T^{|}}\, q^{|}\, \mathrm{d}V^{|} & \geq 0 & \Rightarrow \quad q^{|} \propto -\vartheta^{|}\,, \\ \text{option } \mathtt{C}: & \mathscr{D}_0^{\text{con}} := \dfrac{1}{C}\displaystyle\int_{\mathcal{H}_0} \kappa^{|}\, q^{|}\, \mathrm{d}V^{|} & \geq 0 & \Rightarrow \quad q^{|} \propto \kappa^{|}. \end{array}\right.$$

Again, note the choice of option T or C only effect the heat flux within the horizon. More precisely, unlike for $\mathscr{D}_0^{\text{con}}$, the options T or C for the non-conductive dissipation density $\mathscr{D}_0^{\text{ncon}}$ in Eq. (25) are merely two representations of the same function. To satisfy the Fourier-like relations $q^{|} \propto -\vartheta^{|}$ and $q^{|} \propto \kappa^{|}$, we define the *heat conduction coefficient* in the material configuration as $K > 0$ and assume the conduction law for the temperature, and consequently coldness, according to

$$q^{|} = -K\,\vartheta^{|} \qquad \Rightarrow \qquad q^{|} = \frac{K}{CC^{|}}\,\kappa^{|}. \tag{26}$$

The Fourier-like conduction relation in terms of the temperature $(26)_1$ should be compared with its counterpart in classical continuum mechanics, where

$$\boldsymbol{Q} = -\mathbb{K}\cdot\text{Grad}\,T,$$

in which $\mathbb{K}$ is the second-order positive semi-definite conduction tensor in the material configuration.

Before proceeding to the Coleman–Noll-like exploitation, we further localize the non-local form of the dissipation inequality (25) within the horizon to obtain the neighbour-wise form. To do so, we define (i) the Helmholtz energy density per volume squared in the material configuration $\psi_0^{|}$ with units N.m/m^6, (ii) the entropy density per volume squared in the material configuration $\varsigma_0^{|}$ with units N.m/K.m^6 and (iii) the non-conductive dissipation density per volume squared in the material configuration $d_0^{|}$ as

$$\Psi_0 = \int_{\mathcal{H}_0} \psi_0^{|}\,\mathrm{d}V^{|} \qquad \text{and} \qquad s_0 = \int_{\mathcal{H}_0} \varsigma_0^{|}\,\mathrm{d}V^{|} \qquad \text{and} \qquad \mathscr{D}_0^{\text{ncon}} = \int_{\mathcal{H}_0} d_0^{|}\,\mathrm{d}V^{|}. \tag{27}$$

Inserting the densities (27) into the non-local form of the dissipation inequality (25) yields

$$\left\{\begin{array}{lll} \text{option T}: & \displaystyle\int_{\mathcal{H}_0} d_0^{|}\,\mathrm{d}V^{|} = \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{|}\cdot\boldsymbol{p}^{|}\,\mathrm{d}V^{|} - \int_{\mathcal{H}_0} \dot{\psi}_0^{|}\,\mathrm{d}V^{|} - \dot{T}\int_{\mathcal{H}_0} \varsigma_0^{|}\,\mathrm{d}V^{|} & \geq 0\,, \\ \text{option C}: & \displaystyle\int_{\mathcal{H}_0} d_0^{|}\,\mathrm{d}V^{|} = \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{|}\cdot\boldsymbol{p}^{|}\,\mathrm{d}V^{|} - \int_{\mathcal{H}_0} \dot{\psi}_0^{|}\,\mathrm{d}V^{|} + \frac{\dot{C}}{C^2}\int_{\mathcal{H}_0} \varsigma_0^{|}\,\mathrm{d}V^{|} & \geq 0. \end{array}\right. \tag{28}$$

Consequently, the neighbour-wise form of the dissipation inequality (28) reads

$$\left\{\begin{array}{lll} \text{option T}: & d_0^{|} = \dot{\boldsymbol{\xi}}^{|}\cdot\boldsymbol{p}^{|} - \dot{\psi}_0^{|} - \dot{T}\varsigma_0^{|} & \geq 0\,, \\ \text{option C}: & d_0^{|} = \dot{\boldsymbol{\xi}}^{|}\cdot\boldsymbol{p}^{|} - \dot{\psi}_0^{|} + \dfrac{\dot{C}}{C^2}\varsigma_0^{|} & \geq 0. \end{array}\right. \tag{29}$$

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 $\mathscr{D}_0^{\text{ncon}} \geq 0$, that is

$$d_0^{|} \geq 0 \;\Rightarrow\; \mathscr{D}_0^{\text{ncon}} \geq 0 \qquad \text{but} \qquad \mathscr{D}_0^{\text{ncon}} \geq 0 \;\not\Rightarrow\; d_0^{|} \geq 0.$$

Therefore, in the exploitation process that follows next we begin with the non-local form (25) first and thereafter elaborate on the implications due to the neighbour-wise form of the dissipation inequality (29).

To exploit the non-local form of the dissipation inequality (25) using a Coleman–Noll-like procedure and to derive the associated constitutive laws, we particularize the Helmholtz energy density for the case of thermoelasticity and specify its arguments for the following four cases

$$\left\{\begin{array}{lll} \text{varying temperature} & : \Psi_0 = \displaystyle\int_{\mathcal{H}_0} \psi_0^{|}\,\mathrm{d}V^{|} & \text{with} \quad \psi_0^{|} = \psi_0(\boldsymbol{\xi}^{|}, \boldsymbol{a}^{|/||}, v^{|/||/|||}, T^{|})\,, \\ \text{uniform temperature} & : \Psi_0 = \displaystyle\int_{\mathcal{H}_0} \psi_0^{|}\,\mathrm{d}V^{|} & \text{with} \quad \psi_0^{|} = \psi_0(\boldsymbol{\xi}^{|}, \boldsymbol{a}^{|/||}, v^{|/||/|||}, T)\,, \\ \text{varying coldness} & : \Psi_0 = \displaystyle\int_{\mathcal{H}_0} \psi_0^{|}\,\mathrm{d}V^{|} & \text{with} \quad \psi_0^{|} = \psi_0(\boldsymbol{\xi}^{|}, \boldsymbol{a}^{|/||}, v^{|/||/|||}, C^{|})\,, \\ \text{uniform coldness} & : \Psi_0 = \displaystyle\int_{\mathcal{H}_0} \psi_0^{|}\,\mathrm{d}V^{|} & \text{with} \quad \psi_0^{|} = \psi_0(\boldsymbol{\xi}^{|}, \boldsymbol{a}^{|/||}, v^{|/||/|||}, C). \end{array}\right. \tag{30}$$

For the sake of simplicity, different functions ψ_0 are collectively expressed by the same notation. 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 (30), (ii) replace $\dot{\Psi}_0$ in the non-local form of the dissipation inequality (25), and (iii) analyse its consequences so as to sufficiently satisfy the second law of thermodynamics. We investigate the four possibilities (30) separately in Sects. 3.5.1–3.5.4.

Remark The Helmholtz energy density per volume squared in the material configuration itself is composed of the contributions due to one-, two- and three-neighbour interactions defined by

$$\begin{array}{llll}
\textit{one-neighbour Helmholtz energy density} & : \ \psi_{0:1}^{\mathrm{I}} := \psi_{0:1}(\boldsymbol{\xi}^{\mathrm{I}}, \{\bullet\}) & \textit{with} & [\psi_{0:1}] = \mathrm{N.m/m^6}\,, \\
\textit{two-neighbour Helmholtz energy density} & : \ \psi_{0:2}^{\mathrm{I}/\mathrm{II}} := \psi_{0:2}(\boldsymbol{a}^{\mathrm{I}/\mathrm{II}}, \{\bullet\}) & \textit{with} & [\psi_{0:2}] = \mathrm{N.m/m^9}\,, \\
\textit{three-neighbour Helmholtz energy density} & : \ \psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}} := \psi_{0:3}(v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}, \{\bullet\}) & \textit{with} & [\psi_{0:3}] = \mathrm{N.m/m^{12}}\,,
\end{array} \tag{31}$$

where $\{\bullet\}$ can be T^{I}, T, C^{I} or C to represent any of the energy densities (30). That is

$$\psi_0^{\mathrm{I}} = \psi_0(\boldsymbol{\xi}^{\mathrm{I}}, \boldsymbol{a}^{\mathrm{I}/\mathrm{II}}, v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}, \{\bullet\}) = \frac{1}{2}\,\psi_{0:1}^{\mathrm{I}} + \frac{1}{3}\int_{\mathcal{H}_0} \psi_{0:2}^{\mathrm{I}/\mathrm{II}}\,\mathrm{d}V^{\mathrm{II}}$$
$$+\frac{1}{4}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}\,\mathrm{d}V^{\mathrm{III}}\mathrm{d}V^{\mathrm{II}} \qquad \textit{with} \qquad \left[\psi_0^{\mathrm{I}}\right] = \mathrm{N.m/m^6}.$$

The coefficients 1/2, 1/3 and 1/4 are introduced to avoid multiple counting of energies. Note, the energy density satisfies material-frame-indifference when expressed in terms of $|\boldsymbol{\xi}^{\mathrm{I}}|$, $|\boldsymbol{a}^{\mathrm{I}/\mathrm{II}}|$ and $|v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}|$, respectively, and thus, the angular momentum balance (5) is a priori fulfilled [20]. □

3.5.1 Coleman–Noll exploitation with varying temperature in the horizon

To calculate the rate of the Helmholtz energy density Ψ_0, one integrates over ψ_0. As ψ_0 includes also $\boldsymbol{a}^{\mathrm{I}/\mathrm{II}}$ and $v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}$, this results in a double-integral and a triple-integral, respectively. The rate of the Helmholtz energy density reads

$$\dot{\Psi}_0 = \int_{\mathcal{H}_0} \dot{\psi}_0^{\mathrm{I}}\,\mathrm{d}V^{\mathrm{I}} = \int_{\mathcal{H}_0} \dot{\psi}_0(\boldsymbol{\xi}^{\mathrm{I}}, \boldsymbol{a}^{\mathrm{I}/\mathrm{II}}, v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}, T^{\mathrm{I}})\,\mathrm{d}V^{\mathrm{I}} = \int_{\mathcal{H}_0} \left[\frac{\delta\psi_0^{\mathrm{I}}}{\delta\boldsymbol{\xi}^{\mathrm{I}}}\cdot\dot{\boldsymbol{\xi}}^{\mathrm{I}} + \frac{\partial\psi_0^{\mathrm{I}}}{\partial T^{\mathrm{I}}}\dot{T}^{\mathrm{I}}\right]\mathrm{d}V^{\mathrm{I}}\,, \tag{32}$$

in which the term $\delta\psi_0^{\mathrm{I}}/\delta\boldsymbol{\xi}^{\mathrm{I}}$ denotes the variational derivative defined by

$$\frac{\delta\psi_0^{\mathrm{I}}}{\delta\boldsymbol{\xi}^{\mathrm{I}}} := \frac{\partial\psi_{0:1}^{\mathrm{I}}}{\partial\boldsymbol{\xi}^{\mathrm{I}}} + \int_{\mathcal{H}_0} 2\,\boldsymbol{\xi}^{\mathrm{II}} \times \frac{\partial\psi_{0:2}^{\mathrm{I}/\mathrm{II}}}{\partial\boldsymbol{a}^{\mathrm{I}/\mathrm{II}}}\,\mathrm{d}V^{\mathrm{II}} + \int_{\mathcal{H}_0}\int_{\mathcal{H}_0} 3\,[\boldsymbol{\xi}^{\mathrm{II}} \times \boldsymbol{\xi}^{\mathrm{III}}]\frac{\partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}{\partial v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}\,\mathrm{d}V^{\mathrm{III}}\,\mathrm{d}V^{\mathrm{II}}\,, \tag{33}$$

the derivation of which is given in Appendix A and utilises the properties

$$\frac{\partial\psi_{0:2}^{\mathrm{I}/\mathrm{II}}}{\partial\boldsymbol{a}^{\mathrm{I}/\mathrm{II}}} = -\frac{\partial\psi_{0:2}^{\mathrm{I}/\mathrm{II}}}{\partial\boldsymbol{a}^{\mathrm{II}/\mathrm{I}}} \qquad \text{and} \qquad \frac{\partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}{\partial v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}} = \frac{\partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}{\partial v^{\mathrm{II}/\mathrm{III}/\mathrm{I}}} = \frac{\partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}{\partial v^{\mathrm{III}/\mathrm{I}/\mathrm{II}}}\,,$$

consistent with the constraints to fulfil angular momentum balance. Replacing Eq. (32) into the non-local form of the dissipation inequality $(25)_1$ yields

$$\mathscr{D}_0^{\mathrm{ncon}} = \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{\mathrm{I}}\cdot\boldsymbol{p}^{\mathrm{I}}\,\mathrm{d}V^{\mathrm{I}} - \int_{\mathcal{H}_0} \frac{\delta\psi_0^{\mathrm{I}}}{\delta\boldsymbol{\xi}^{\mathrm{I}}}\cdot\dot{\boldsymbol{\xi}}^{\mathrm{I}}\,\mathrm{d}V^{\mathrm{I}} - \int_{\mathcal{H}_0} \frac{\partial\psi_0^{\mathrm{I}}}{\partial T^{\mathrm{I}}}\dot{T}^{\mathrm{I}}\,\mathrm{d}V^{\mathrm{I}} - s_0\dot{T} \geq 0\,,$$

or alternatively,

$$\mathscr{D}_0^{\mathrm{ncon}} = \int_{\mathcal{H}_0} \left[\left[\boldsymbol{p}^{\mathrm{I}} - \frac{\delta\psi_0^{\mathrm{I}}}{\delta\boldsymbol{\xi}^{\mathrm{I}}}\right]\cdot\dot{\boldsymbol{\xi}}^{\mathrm{I}} - \frac{\partial\psi_0^{\mathrm{I}}}{\partial T^{\mathrm{I}}}\dot{T}^{\mathrm{I}} - \varsigma_0^{\mathrm{I}}\dot{T}\right]\mathrm{d}V^{\mathrm{I}} \geq 0.$$

Using the relation $\dot{T}^{|} = \dot{T} + \dot{\vartheta}^{|}$, this can be written as

$$\mathscr{D}_0^{\text{ncon}} = \int_{\mathcal{H}_0} \left[\left[\boldsymbol{p}^{|} - \frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \right] \cdot \dot{\boldsymbol{\xi}}^{|} - \left[\frac{\partial \psi_0^{|}}{\partial T^{|}} + \varsigma_0^{|} \right] \dot{T} - \frac{\partial \psi_0^{|}}{\partial T^{|}} \dot{\vartheta}^{|} \right] \mathrm{d}V^{|} \geq 0. \tag{34}$$

The sufficient conditions to fulfil Eq. (34) yield the constitutive relations

$$\boldsymbol{p}^{|} = \frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \qquad \text{and} \qquad \varsigma_0^{|} = -\frac{\partial \psi_0^{|}}{\partial T^{|}},$$

and the non-local condition

$$\int_{\mathcal{H}_0} \varsigma_0^{|} \dot{\vartheta}^{|} \, \mathrm{d}V^{|} = 0. \tag{35}$$

Condition (35) can be re-expressed as

$$\int_{\mathcal{H}_0} \varsigma_0^{|} [\, \dot{T}^{|} - \dot{T}] \, \mathrm{d}V^{|} = 0 \quad \Rightarrow \quad \int_{\mathcal{H}_0} \varsigma_0^{|} \dot{T}^{|} \, \mathrm{d}V^{|} = \int_{\mathcal{H}_0} \varsigma_0^{|} \, \mathrm{d}V^{|} \dot{T} \quad \Rightarrow \quad \int_{\mathcal{H}_0} \varsigma_0^{|} \dot{T}^{|} \, \mathrm{d}V^{|} = s_0 \, \dot{T}, \tag{36}$$

which is reminiscent of the Hill–Mandel condition in homogenization [33–35]. Note, both representations of the *integral* condition (35) and (36) are identical. Summarising, the consequence of the Coleman–Noll procedure imposed on the non-local form of the dissipation inequality $(25)_1$ is

$$\boldsymbol{p}^{|} = \frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \qquad \text{and} \qquad \varsigma_0^{|} = -\frac{\partial \psi_0^{|}}{\partial T^{|}} \qquad \text{and} \qquad s_0 \, \dot{T} = \int_{\mathcal{H}_0} \varsigma_0^{|} \dot{T}^{|} \, \mathrm{d}V^{|}. \tag{37}$$

Next, we discuss the more restrictive neighbour-wise form of the dissipation inequality $(29)_1$. The neighbour-wise form of the dissipation inequality for the case of $\psi_0^{|} = \psi_0(\boldsymbol{\xi}^{|}, \boldsymbol{a}^{|/||}, v^{|/||/|||}, T^{|})$ reads

$$d_0^{|} = \dot{\boldsymbol{\xi}}^{|} \cdot \boldsymbol{p}^{|} - \dot{\psi}_0^{|} - \varsigma_0^{|} \dot{T} \geq 0. \tag{38}$$

Using the relation (32), it can be readily seen that

$$\dot{\Psi}_0^{|} = \int_{\mathcal{H}_0} \frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \cdot \dot{\boldsymbol{\xi}}^{|} \, \mathrm{d}V^{|} + \int_{\mathcal{H}_0} \frac{\partial \psi_0^{|}}{\partial T^{|}} \dot{T}^{|} \, \mathrm{d}V^{|} \qquad \Rightarrow \qquad \dot{\psi}_0^{|} = \frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \cdot \dot{\boldsymbol{\xi}}^{|} + \frac{\partial \psi_0^{|}}{\partial T^{|}} \dot{T}^{|}. \tag{39}$$

Inserting $\dot{\psi}_0^{|}$ from Eq. (39) into the dissipation inequality (38) yields

$$d_0^{|} = \dot{\boldsymbol{\xi}}^{|} \cdot \boldsymbol{p}^{|} - \frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \cdot \dot{\boldsymbol{\xi}}^{|} - \frac{\partial \psi_0^{|}}{\partial T^{|}} \dot{T}^{|} - \varsigma_0^{|} \dot{T} \geq 0,$$

which, using the relation $\dot{T}^{|} = \dot{T} + \dot{\vartheta}^{|}$, can be written as

$$d_0^{|} = \left[\boldsymbol{p}^{|} - \frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \right] \cdot \dot{\boldsymbol{\xi}}^{|} - \left[\frac{\partial \psi_0^{|}}{\partial T^{|}} + \varsigma_0^{|} \right] \dot{T} - \frac{\partial \psi_0^{|}}{\partial T^{|}} \dot{\vartheta}^{|} \geq 0. \tag{40}$$

The sufficient conditions to fulfil Eq. (40), in the case of equality, yield the constitutive relations

$$\boldsymbol{p}^{|} = \frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \qquad \text{and} \qquad \varsigma_0^{|} = -\frac{\partial \psi_0^{|}}{\partial T^{|}},$$

and the neighbour-wise condition

$$\varsigma_0^{|} \dot{\vartheta}^{|} = 0. \tag{41}$$

This is the further restriction of the neighbour-wise form compared to its non-local form (37). Summarising, the outcome of the Coleman–Noll procedure imposed on the neighbour-wise form of the dissipation inequality $(29)_1$ is

$$\boldsymbol{p}^{|} = \frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \quad \text{and} \quad \varsigma_0^{|} = -\frac{\partial \psi_0^{|}}{\partial T^{|}} \quad \text{and} \quad \varsigma_0^{|}\, \dot{\vartheta}^{|} = 0.$$

Note, as $\varsigma_0^{|}$ is in general nonzero, the condition $(41)_3$ essentially states that $\dot{\vartheta}^{|} = 0$ or more specifically $\dot{T}^{|} = \dot{T}$. This condition implies that the temperature (rate) within the horizon is uniform. This is discussed in the next section.

3.5.2 Coleman–Noll exploitation with uniform temperature in the horizon

Equipped with the detailed analysis in Section 3.5.1 for the case of varying temperature within the horizon, we elaborate next on the case of a uniform temperature within the horizon, which aligns with the assumptions of [23,36]. Considering that the case of uniform temperature can be recovered from the varying temperature assumption by setting $T^{|} = T$, we omit the derivations for the sake of brevity and only state the most important conclusions. The results of the Coleman–Noll procedure imposed on the non-local form of the dissipation inequality $(25)_1$ is

$$\boldsymbol{p}^{|} = \frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \quad \text{and} \quad \varsigma_0^{|} = -\frac{\partial \psi_0^{|}}{\partial T}.$$

These are identical to the outcomes of the Coleman–Noll procedure imposed on the neighbour-wise form of the dissipation inequality $(29)_1$. Thus, if the horizon temperature is uniform, the neighbour-wise form of the dissipation inequality does not pose any additional restriction compared to the non-local form. This conclusion should be compared with the observations in Sect. 3.5.1 and particularly the non-local condition (35) and the neighbour-wise condition (41).

3.5.3 Coleman–Noll exploitation with varying coldness in the horizon

For the case of varying coldness within the horizon, the Helmholtz energy density per volume squared in the material configuration reads $\psi_0^{|} = \psi_0(\boldsymbol{\xi}^{|}, \boldsymbol{a}^{|/||}, v^{|/||/|||}, C^{|})$, resulting in

$$\dot{\Psi}_0^{|} = \int_{\mathcal{H}_0} \dot{\psi}_0^{|}\, \mathrm{d}V^{|} = \int_{\mathcal{H}_0} \dot{\psi}_0^{|}(\boldsymbol{\xi}^{|}, \boldsymbol{a}^{|/||}, v^{|/||/|||}, C^{|})\, \mathrm{d}V^{|} = \int_{\mathcal{H}_0} \frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \cdot \dot{\boldsymbol{\xi}}^{|}\, \mathrm{d}V^{|} + \int_{\mathcal{H}_0} \frac{\partial \psi_0^{|}}{\partial C^{|}} \dot{C}^{|}\, \mathrm{d}V^{|}. \tag{42}$$

Substituting $\dot{\Psi}_0^{|}$ from Eq. (42) into the dissipation inequality $(25)_2$ yields

$$\mathscr{D}_0^{\text{ncon}} = \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{|} \cdot \boldsymbol{p}^{|}\, \mathrm{d}V^{|} - \int_{\mathcal{H}_0} \frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \cdot \dot{\boldsymbol{\xi}}^{|}\, \mathrm{d}V^{|} - \int_{\mathcal{H}_0} \frac{\partial \psi_0^{|}}{\partial C^{|}} \dot{C}^{|}\, \mathrm{d}V^{|} + s_0 \frac{\dot{C}}{C^2} \geq 0\,,$$

which, using the relation $\dot{C}^{|} = \dot{C} + \dot{\kappa}^{|}$, can be written as

$$\mathscr{D}_0^{\text{ncon}} = \int_{\mathcal{H}_0} \left[\left[\boldsymbol{p}^{|} - \frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \right] \cdot \dot{\boldsymbol{\xi}}^{|} - \left[\frac{\partial \psi_0^{|}}{\partial C^{|}} - \frac{\varsigma_0^{|}}{C^2} \right] \dot{C} - \frac{\partial \psi_0^{|}}{\partial C^{|}} \dot{\kappa}^{|} \right] \mathrm{d}V^{|} \geq 0. \tag{43}$$

To sufficiently fulfil Eq. (43), in the case of equality, we require the constitutive relations

$$\boldsymbol{p}^{|} = \frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \quad \text{and} \quad \varsigma_0^{|} = C^2 \frac{\partial \psi_0^{|}}{\partial C^{|}}\,,$$

and the non-local condition

$$\int_{\mathcal{H}_0} \frac{1}{C^2} \varsigma_0^{|} \dot{\kappa}^{|}\, \mathrm{d}V^{|} = 0 \quad \Rightarrow \quad \int_{\mathcal{H}_0} \varsigma_0^{|} \dot{\kappa}^{|}\, \mathrm{d}V^{|} = 0. \tag{44}$$

Condition (44) can be expressed as

$$\int_{\mathcal{H}_0} \varsigma_0^{|}\,[\,\dot{C}^{|} - \dot{C}\,]\,\mathrm{d}V^{|} = 0 \quad \Rightarrow \quad \int_{\mathcal{H}_0} \varsigma_0^{|}\,\dot{C}^{|}\,\mathrm{d}V^{|} = \dot{C}\int_{\mathcal{H}_0} \varsigma_0^{|}\,\mathrm{d}V^{|} \quad \Rightarrow \quad \int_{\mathcal{H}_0} \varsigma_0^{|}\,\dot{C}^{|}\,\mathrm{d}V^{|} = s_0\,\dot{C}\,,$$

which is again reminiscent of the Hill–Mandel condition in homogenization. Summarising, the outcomes of the Coleman–Noll procedure imposed on the non-local form of the dissipation inequality $(25)_2$ are

$$\boldsymbol{p}^{|} = \frac{\delta\psi_0^{|}}{\delta\boldsymbol{\xi}^{|}} \qquad \text{and} \qquad \varsigma_0^{|} = C^2\,\frac{\partial\psi_0^{|}}{\partial C^{|}} \qquad \text{and} \qquad \int_{\mathcal{H}_0} \varsigma_0^{|}\,\dot{C}^{|}\,\mathrm{d}V^{|} = s_0\,\dot{C}.$$

Next, we detail the consequences of the more restrictive neighbour-wise form of the dissipation inequality $(29)_2$ for the case of $\psi_0^{|} = \psi_0(\boldsymbol{\xi}^{|}, \boldsymbol{a}^{|/||}, v^{|/||/|||}, C^{|})$, where

$$d_0^{|} = \dot{\boldsymbol{\xi}}^{|}\cdot\boldsymbol{p}^{|} - \dot{\psi}_0^{|} + \frac{\dot{C}}{C^2}\,\varsigma_0^{|} \geq 0. \tag{45}$$

Similar to the relation (42), it can be readily seen that

$$\dot{\Psi}_0^{|} = \int_{\mathcal{H}_0} \frac{\delta\psi_0^{|}}{\delta\boldsymbol{\xi}^{|}}\cdot\dot{\boldsymbol{\xi}}^{|}\,\mathrm{d}V^{|} + \int_{\mathcal{H}_0} \frac{\partial\psi_0^{|}}{\partial C^{|}}\,\dot{C}^{|}\,\mathrm{d}V^{|} \qquad \Rightarrow \qquad \dot{\psi}_0^{|} = \frac{\delta\psi_0^{|}}{\delta\boldsymbol{\xi}^{|}}\cdot\dot{\boldsymbol{\xi}}^{|} + \frac{\partial\psi_0^{|}}{\partial C^{|}}\,\dot{C}^{|}. \tag{46}$$

Substituting $\dot{\psi}_0^{|}$ from Eq. (46) into the dissipation inequality (45) yields

$$d_0^{|} = \dot{\boldsymbol{\xi}}^{|}\cdot\boldsymbol{p}^{|} - \frac{\delta\psi_0^{|}}{\delta\boldsymbol{\xi}^{|}}\cdot\dot{\boldsymbol{\xi}}^{|} - \frac{\partial\psi_0^{|}}{\partial C^{|}}\,\dot{C}^{|} + \frac{\dot{C}}{C^2}\,\varsigma_0^{|} \geq 0\,,$$

which using the relation $\dot{C}^{|} = \dot{C} + \dot{\kappa}^{|}$ can be written as

$$d_0^{|} = \left[\,\boldsymbol{p}^{|} - \frac{\delta\psi_0^{|}}{\delta\boldsymbol{\xi}^{|}}\,\right]\cdot\dot{\boldsymbol{\xi}}^{|} - \left[\,\frac{\partial\psi_0^{|}}{\partial C^{|}} - \frac{\varsigma_0^{|}}{C^2}\,\right]\dot{C} - \frac{\partial\psi_0^{|}}{\partial C^{|}}\,\dot{\kappa}^{|} \geq 0. \tag{47}$$

The constitutive relations

$$\boldsymbol{p}^{|} = \frac{\delta\psi_0^{|}}{\delta\boldsymbol{\xi}^{|}} \qquad \text{and} \qquad \varsigma_0^{|} = C^2\,\frac{\partial\psi_0^{|}}{\partial C^{|}}\,,$$

and the neighbour-wise condition

$$\varsigma_0^{|}\,\dot{\kappa}^{|} = 0\,, \tag{48}$$

sufficiently fulfil Eq. (47). Note, the condition (48) is the further restriction of the neighbour-wise form compared to its non-local counterpart (44). Summarising, the outcomes of the Coleman–Noll procedure imposed on the neighbour-wise form of the dissipation inequality $(29)_2$ are

$$\boldsymbol{p}^{|} = \frac{\delta\psi_0^{|}}{\delta\boldsymbol{\xi}^{|}} \qquad \text{and} \qquad \varsigma_0^{|} = C^2\,\frac{\partial\psi_0^{|}}{\partial C^{|}} \qquad \text{and} \qquad \varsigma_0^{|}\,\dot{\kappa}^{|} = 0. \tag{49}$$

Note, as $\varsigma_0^{|}$ is in general nonzero, the condition $(49)_3$ essentially states that $\dot{\kappa}^{|} = 0$ or more specifically $\dot{C}^{|} = \dot{C}$. This condition implies that the coldness (rate) within the horizon is uniform. This is expanded upon further in the next section.

3.5.4 Coleman–Noll exploitation with uniform Coldness in the horizon

For the case of uniform coldness within the horizon, the Helmholtz energy density per volume squared in the material configuration reads $\psi_0^{|} = \psi_0(\boldsymbol{\xi}^{|}, \boldsymbol{a}^{|/||}, v^{|/||/|||}, C)$. Equipped with the detailed analysis in Sect. 3.5.3 for the case of varying coldness within the horizon, we elaborate now on the case of a uniform coldness within the horizon. The case of the uniform coldness can be recovered from the varying coldness assumption by setting $C^{|} = C$. In this case, the outcomes of the Coleman–Noll procedure imposed on the non-local form of the dissipation inequality $(25)_2$ are

$$\boldsymbol{p}^{|} = \frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \qquad \text{and} \qquad \varsigma_0^{|} = C^2 \, \frac{\partial \psi_0^{|}}{\partial C}.$$

These are identical to the outcomes of the Coleman–Noll procedure imposed on the neighbour-wise form of the dissipation inequality $(29)_2$. Thus, if the horizon coldness is uniform, the neighbour-wise form of the dissipation inequality does not pose any additional restriction compared to its non-local form, unlike the case of the varying coldness. Table 3 summarises the consequences of the neighbour-wise and the non-local forms the dissipation inequality via a Coleman–Noll-like procedure for the options (30). *In particular, for uniform temperature (coldness), the neighbour-wise and non-local forms require identical conditions, unlike the varying temperature (coldness) options.* Table 3 compares the commonly adopted uniform temperature assumption to the other possibilities presented here. In particular, the non-local (homogenization-like) conditions

$$\int_{\mathcal{H}_0} \varsigma_0^{|} \, \dot{T}^{|} \, \mathrm{d}V^{|} = s_0 \, \dot{T} \qquad \text{or} \qquad \int_{\mathcal{H}_0} \varsigma_0^{|} \, \dot{C}^{|} \, \mathrm{d}V^{|} = s_0 \, \dot{C},$$

are reminiscent of the Hill–Mandel condition in homogenization for which the uniform temperature (coldness) assumption mimics the Voigt bound [35].

3.6 Temperature evolution equation

To derive the temperature evolution equation, we start from the dissipation inequality and incorporate the constitutive laws derived in Sect. 3.5 for the case of thermoelasticity corresponding to vanishing $\mathscr{D}_0^{\text{ncon}}$, where dissipation occurred only as a result of the Fourier-like conduction. Furthermore, similar to our previous discussions, we elaborate on both options $\mathtt{T}$ and $\mathtt{C}$. The dissipation inequality (22) for the case of $\mathscr{D}_0^{\text{ncon}} = 0$ reads

$$\dot{s}_0 \, T = \mathscr{R}_0^{\text{ext}} - \int_{\mathcal{H}_0} q^{|} \, \mathrm{d}V^{|}, \tag{50}$$

in which

$$s_0 = \int_{\mathcal{H}_0} \varsigma_0^{|} \, \mathrm{d}V^{|} \qquad \text{with} \qquad \varsigma_0^{|} = -\frac{\partial \psi_0^{|}}{\partial T^{|}} = C^2 \, \frac{\partial \psi_0^{|}}{\partial C^{|}}.$$

Obviously, based on the observations in Table 3, it is enough to consider only the two cases of varying temperature and coldness within the horizon since the uniform case follows from $\vartheta^{|} = 0$ and $\kappa^{|} = 0$, respectively. After several mathematical steps, the rate of the entropy density reads

$$\begin{cases} \text{option } \mathtt{T}: \quad \dot{s}_0 = \displaystyle\int_{\mathcal{H}_0} \dot{\varsigma}_0^{|} \, \mathrm{d}V^{|} = -\int_{\mathcal{H}_0} \left[\frac{\partial}{\partial T^{|}} \left(\frac{\partial \psi_0^{|}}{\partial T^{|}} \right) \dot{T}^{|} + \frac{\partial}{\partial T^{|}} \left(\frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \right) \cdot \dot{\boldsymbol{\xi}}^{|} \right] \mathrm{d}V^{|}, \\ \text{option } \mathtt{C}: \quad \dot{s}_0 = \displaystyle\int_{\mathcal{H}_0} \dot{\varsigma}_0^{|} \, \mathrm{d}V^{|} = C^2 \int_{\mathcal{H}_0} \left[\frac{\partial}{\partial C^{|}} \left(\frac{\partial \psi_0^{|}}{\partial C^{|}} \right) \dot{C}^{|} + \frac{\partial}{\partial C^{|}} \left(\frac{\delta \psi_0^{|}}{\delta \boldsymbol{\xi}^{|}} \right) \cdot \dot{\boldsymbol{\xi}}^{|} \right] \mathrm{d}V^{|}. \end{cases}$$

Table 3 Unification of concepts and consequences of the dissipation inequality as obtained via a Coleman–Noll-like procedure

Option T		Option C	
$\mathscr{D}_0^{\mathrm{ncon}} = \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{\mathsf{I}} \cdot \boldsymbol{p}^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}} - \dot{\Psi}_0 - s_0 \dot{T} \geq 0$		$\mathscr{D}_0^{\mathrm{ncon}} = \int_{\mathcal{H}_0} \dot{\boldsymbol{\xi}}^{\mathsf{I}} \cdot \boldsymbol{p}^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}} - \dot{\Psi}_0 + s_0 \frac{\dot{C}}{C^2} \geq 0$	
$d_0^{\mathsf{I}} = \dot{\boldsymbol{\xi}}^{\mathsf{I}} \cdot \boldsymbol{p}^{\mathsf{I}} - \dot{\psi}_0^{\mathsf{I}} - \dot{T} \varsigma_0^{\mathsf{I}} \geq 0$		$d_0^{\mathsf{I}} = \dot{\boldsymbol{\xi}}^{\mathsf{I}} \cdot \boldsymbol{p}^{\mathsf{I}} - \dot{\psi}_0^{\mathsf{I}} - \frac{\dot{C}}{C^2} \varsigma_0^{\mathsf{I}} \geq 0$	
Varying temperature	Uniform temperature	Varying coldness	Uniform coldness
$\psi_0^{\mathsf{I}} = \psi_0(\boldsymbol{\xi}^{\mathsf{I}}, \boldsymbol{a}^{\mathsf{I/II}}, \nu^{\mathsf{I/II/III}}, T^{\mathsf{I}})$	$\psi_0^{\mathsf{I}} = \psi_0(\boldsymbol{\xi}^{\mathsf{I}}, \boldsymbol{a}^{\mathsf{I/II}}, \nu^{\mathsf{I/II/III}}, T)$	$\psi_0^{\mathsf{I}} = \psi_0(\boldsymbol{\xi}^{\mathsf{I}}, \boldsymbol{a}^{\mathsf{I/II}}, \nu^{\mathsf{I/II/III}}, C^{\mathsf{I}})$	$\psi_0^{\mathsf{I}} = \psi_0(\boldsymbol{\xi}^{\mathsf{I}}, \boldsymbol{a}^{\mathsf{I/II}}, \nu^{\mathsf{I/II/III}}, C)$
Properties and definition			
$\frac{\delta \psi_0^{\mathsf{I}}}{\delta \boldsymbol{\xi}^{\mathsf{I}}} := \frac{\partial \psi_{0:1}^{\mathsf{I}}}{\partial \boldsymbol{\xi}^{\mathsf{I}}} + \int_{\mathcal{H}_0} 2\boldsymbol{\xi}^{\mathsf{II}} \times \frac{\partial \psi_{0:2}^{\mathsf{I/II}}}{\partial \boldsymbol{a}^{\mathsf{I/II}}} \mathrm{d}V^{\mathsf{II}} + \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} 3[\boldsymbol{\xi}^{\mathsf{II}} \times \boldsymbol{\xi}^{\mathsf{III}}] \frac{\partial \psi_{0:3}^{\mathsf{I/II/III}}}{\partial \nu^{\mathsf{I/II/III}}} \mathrm{d}V^{\mathsf{III}} \mathrm{d}V^{\mathsf{II}}$			
$\dot{\Psi}_0 = \int_{\mathcal{H}_0} \dot{\psi}_0^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}}$	$\dot{\Psi}_0 = \int_{\mathcal{H}_0} \dot{\psi}_0^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}}$	$\dot{\Psi}_0 = \int_{\mathcal{H}_0} \dot{\psi}_0^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}}$	$\dot{\Psi}_0 = \int_{\mathcal{H}_0} \dot{\psi}_0^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}}$
$\dot{\psi}_0^{\mathsf{I}} = \frac{\delta \psi_0^{\mathsf{I}}}{\delta \boldsymbol{\xi}^{\mathsf{I}}} \cdot \dot{\boldsymbol{\xi}}^{\mathsf{I}} + \frac{\partial \psi_0^{\mathsf{I}}}{\partial T^{\mathsf{I}}} \dot{T}^{\mathsf{I}}$	$\dot{\psi}_0^{\mathsf{I}} = \frac{\delta \psi_0^{\mathsf{I}}}{\delta \boldsymbol{\xi}^{\mathsf{I}}} \cdot \dot{\boldsymbol{\xi}}^{\mathsf{I}} + \frac{\partial \psi_0^{\mathsf{I}}}{\partial T} \dot{T}$	$\dot{\psi}_0^{\mathsf{I}} = \frac{\delta \psi_0^{\mathsf{I}}}{\delta \boldsymbol{\xi}^{\mathsf{I}}} \cdot \dot{\boldsymbol{\xi}}^{\mathsf{I}} + \frac{\partial \psi_0^{\mathsf{I}}}{\partial C^{\mathsf{I}}} \dot{C}^{\mathsf{I}}$	$\dot{\psi}_0^{\mathsf{I}} = \frac{\delta \psi_0^{\mathsf{I}}}{\delta \boldsymbol{\xi}^{\mathsf{I}}} \cdot \dot{\boldsymbol{\xi}}^{\mathsf{I}} + \frac{\partial \psi_0^{\mathsf{I}}}{\partial C} \dot{C}$
Constitutive laws to sufficiently fulfil $\mathscr{D}_0^{\mathrm{ncon}} \geq 0$ ($\mathscr{D}_0^{\mathrm{ncon}} = 0$)			
$\boldsymbol{p}^{\mathsf{I}} = \frac{\delta \psi_0^{\mathsf{I}}}{\delta \boldsymbol{\xi}^{\mathsf{I}}}$	$\boldsymbol{p}^{\mathsf{I}} = \frac{\delta \psi_0^{\mathsf{I}}}{\delta \boldsymbol{\xi}^{\mathsf{I}}}$	$\boldsymbol{p}^{\mathsf{I}} = \frac{\delta \psi_0^{\mathsf{I}}}{\delta \boldsymbol{\xi}^{\mathsf{I}}}$	$\boldsymbol{p}^{\mathsf{I}} = \frac{\delta \psi_0^{\mathsf{I}}}{\delta \boldsymbol{\xi}^{\mathsf{I}}}$
$\varsigma_0^{\mathsf{I}} = -\frac{\partial \psi_0^{\mathsf{I}}}{\partial T^{\mathsf{I}}}$	$\varsigma_0^{\mathsf{I}} = -\frac{\partial \psi_0^{\mathsf{I}}}{\partial T}$	$\varsigma_0^{\mathsf{I}} = C^2 \frac{\partial \psi_0^{\mathsf{I}}}{\partial C^{\mathsf{I}}}$	$\varsigma_0^{\mathsf{I}} = C^2 \frac{\partial \psi_0^{\mathsf{I}}}{\partial C}$
$\int_{\mathcal{H}_0} \varsigma_0^{\mathsf{I}} \dot{T}^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}} = s_0 \dot{T}$		$\int_{\mathcal{H}_0} \varsigma_0^{\mathsf{I}} \dot{C}^{\mathsf{I}} \mathrm{d}V^{\mathsf{I}} = s_0 \dot{C}$	
Constitutive laws to sufficiently fulfil $d_0^{\mathsf{I}} \geq 0$ ($d_0^{\mathsf{I}} = 0$)			
$\boldsymbol{p}^{\mathsf{I}} = \frac{\delta \psi_0^{\mathsf{I}}}{\delta \boldsymbol{\xi}^{\mathsf{I}}}$	$\boldsymbol{p}^{\mathsf{I}} = \frac{\delta \psi_0^{\mathsf{I}}}{\delta \boldsymbol{\xi}^{\mathsf{I}}}$	$\boldsymbol{p}^{\mathsf{I}} = \frac{\delta \psi_0^{\mathsf{I}}}{\delta \boldsymbol{\xi}^{\mathsf{I}}}$	$\boldsymbol{p}^{\mathsf{I}} = \frac{\delta \psi_0^{\mathsf{I}}}{\delta \boldsymbol{\xi}^{\mathsf{I}}}$
$\varsigma_0^{\mathsf{I}} = -\frac{\partial \psi_0^{\mathsf{I}}}{\partial T^{\mathsf{I}}}$	$\varsigma_0^{\mathsf{I}} = -\frac{\partial \psi_0^{\mathsf{I}}}{\partial T}$	$\varsigma_0^{\mathsf{I}} = C^2 \frac{\partial \psi_0^{\mathsf{I}}}{\partial C^{\mathsf{I}}}$	$\varsigma_0^{\mathsf{I}} = C^2 \frac{\partial \psi_0^{\mathsf{I}}}{\partial C}$
$\dot{T}^{\mathsf{I}} = \dot{T}$		$\dot{C}^{\mathsf{I}} = \dot{C}$	

To proceed, we impose the constitutive relations and employ the relations $T^{\mathsf{I}} = T + \vartheta^{\mathsf{I}}$ or $C^{\mathsf{I}} = C + \kappa^{\mathsf{I}}$ to obtain

$$\begin{cases} \text{option T}: \quad \dot{s}_0 = \displaystyle\int_{\mathcal{H}_0} \dot{\varsigma}_0^{\mathsf{I}} \, \mathrm{d}V^{\mathsf{I}} = -\int_{\mathcal{H}_0} \left[\frac{\partial^2 \psi_0^{\mathsf{I}}}{\partial T^{\mathsf{I}} \partial T^{\mathsf{I}}} \, \dot{T} + \frac{\partial^2 \psi_0^{\mathsf{I}}}{\partial T^{\mathsf{I}} \partial T^{\mathsf{I}}} \, \dot{\vartheta}^{\mathsf{I}} + \frac{\partial \boldsymbol{p}^{\mathsf{I}}}{\partial T^{\mathsf{I}}} \cdot \dot{\boldsymbol{\xi}}^{\mathsf{I}} \right] \mathrm{d}V^{\mathsf{I}} , \\ \text{option C}: \quad \dot{s}_0 = \displaystyle\int_{\mathcal{H}_0} \dot{\varsigma}_0^{\mathsf{I}} \, \mathrm{d}V^{\mathsf{I}} = C^2 \int_{\mathcal{H}_0} \left[\frac{\partial^2 \psi_0^{\mathsf{I}}}{\partial C^{\mathsf{I}} \partial C^{\mathsf{I}}} \, \dot{C} + \frac{\partial^2 \psi_0^{\mathsf{I}}}{\partial C^{\mathsf{I}} \partial C^{\mathsf{I}}} \, \dot{\kappa}^{\mathsf{I}} + \frac{\partial \boldsymbol{p}^{\mathsf{I}}}{\partial C^{\mathsf{I}}} \cdot \dot{\boldsymbol{\xi}}^{\mathsf{I}} \right] \mathrm{d}V^{\mathsf{I}} . \end{cases}$$

Note, the terms $\partial \boldsymbol{p}^{\mathsf{I}} / \partial T^{\mathsf{I}}$ and $\partial \boldsymbol{p}^{\mathsf{I}} / \partial C^{\mathsf{I}}$ quantify the thermal sensitivity of the interaction force densities with respect to temperature and coldness, respectively. Next, we define the heat capacity coefficients c^T and c^C as

$$c^T := -T \int_{\mathcal{H}_0} \frac{\partial^2 \psi_0^{\mathsf{I}}}{\partial T^{\mathsf{I}} \partial T^{\mathsf{I}}} \, \mathrm{d}V^{\mathsf{I}} \qquad \text{and} \qquad c^C := C \int_{\mathcal{H}_0} \frac{\partial^2 \psi_0^{\mathsf{I}}}{\partial C^{\mathsf{I}} \partial C^{\mathsf{I}}} \, \mathrm{d}V^{\mathsf{I}} , \tag{51}$$

corresponding to options T and C, respectively. The heat capacity coefficients c^T and c^C can be related to one another upon defining the Helmholtz energy density ψ_0^{I} in terms of either temperature or coldness. Furthermore, we impose the additional requirement that

$$\int_{\mathcal{H}_0} \frac{\partial^2 \psi_0^{\mathsf{I}}}{\partial T^{\mathsf{I}} \partial T^{\mathsf{I}}} \, \dot{\vartheta}^{\mathsf{I}} \, \mathrm{d}V^{\mathsf{I}} = 0 \qquad \text{and} \qquad \int_{\mathcal{H}_0} \frac{\partial^2 \psi_0^{\mathsf{I}}}{\partial C^{\mathsf{I}} \partial C^{\mathsf{I}}} \, \dot{\kappa}^{\mathsf{I}} \, \mathrm{d}V^{\mathsf{I}} = 0 , \tag{52}$$

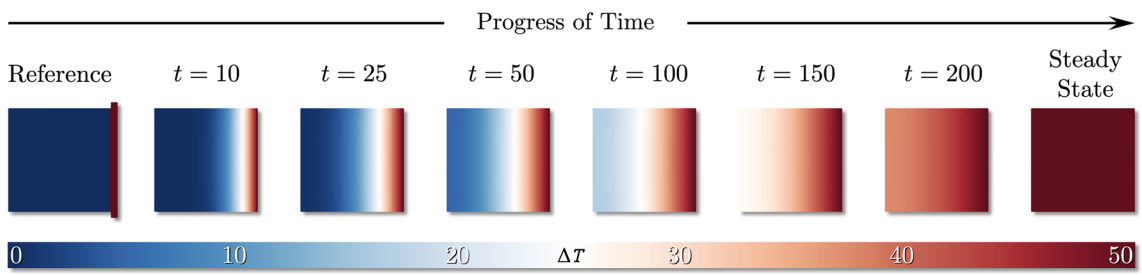

Fig. 3 The numerical example for a purely thermal, two dimensional problem, showing the temperature distribution. It demonstrates the conduction of heat in time, through a square domain. ΔT shows the temperature difference from T_0

that are for instance fulfilled a priori if the temperature or coldness is uniform within the horizon. Note that the uniform distribution is not the only possibility. Replacing $\dot{s}_0$ from Eq. (51) into Eq. (50) while employing the definitions (51) yields

$$\begin{cases} \text{option } \mathtt{T}: \quad c^T \dot{T} = \mathscr{R}_0^{\text{ext}} - \displaystyle\int_{\mathcal{H}_0} q^{\mathsf{I}} \, \mathrm{d}V^{\mathsf{I}} + T \int_{\mathcal{H}_0} \frac{\partial \boldsymbol{p}^{\mathsf{I}}}{\partial T^{\mathsf{I}}} \cdot \dot{\boldsymbol{\xi}}^{\mathsf{I}} \, \mathrm{d}V^{\mathsf{I}} , \\ \text{option } \mathtt{C}: \quad c^C \dot{C} = \mathscr{R}_0^{\text{ext}} - \displaystyle\int_{\mathcal{H}_0} q^{\mathsf{I}} \, \mathrm{d}V^{\mathsf{I}} - C \int_{\mathcal{H}_0} \frac{\partial \boldsymbol{p}^{\mathsf{I}}}{\partial C^{\mathsf{I}}} \cdot \dot{\boldsymbol{\xi}}^{\mathsf{I}} \, \mathrm{d}V^{\mathsf{I}} . \end{cases}$$

Finally, using the Fourier-like conduction Eq. (26) yields

$$\begin{cases} \text{option } \mathtt{T}: \quad c^T \dot{T} = \mathscr{R}_0^{\text{ext}} + \displaystyle\int_{\mathcal{H}_0} K \, \vartheta^{\mathsf{I}} \, \mathrm{d}V^{\mathsf{I}} + T \int_{\mathcal{H}_0} \frac{\partial \boldsymbol{p}^{\mathsf{I}}}{\partial T^{\mathsf{I}}} \cdot \dot{\boldsymbol{\xi}}^{\mathsf{I}} \, \mathrm{d}V^{\mathsf{I}} , \\ \text{option } \mathtt{C}: \quad c^C \dot{C} = \mathscr{R}_0^{\text{ext}} - \displaystyle\int_{\mathcal{H}_0} \frac{K}{C C^{\mathsf{I}}} \, \kappa^{\mathsf{I}} \, \mathrm{d}V^{\mathsf{I}} - C \int_{\mathcal{H}_0} \frac{\partial \boldsymbol{p}^{\mathsf{I}}}{\partial C^{\mathsf{I}}} \cdot \dot{\boldsymbol{\xi}}^{\mathsf{I}} \, \mathrm{d}V^{\mathsf{I}} , \end{cases}$$

in which the last terms are associated with thermo-mechanical coupling resulting from Gough–Joule-like effects [see [37], among others]. The two options $\mathtt{T}$ and $\mathtt{C}$, are introduced for the first time in the current context and require further investigations. This task is out of the scope of the current manuscript and shall be elaborated in a separate contribution.

4 Numerical illustration

The primary objective of this section is to elucidate the proposed theory via numerical examples. The theoretical framework and its computational implementation are able to resolve fully coupled thermo-mechanical problems in three dimensions. However, for the sake of illustration, a purely thermal case is considered. This is achieved by setting the thermal expansion coefficient to zero and not applying any mechanical loading. The simulations correspond to the option $\mathtt{T}$. Further details of computational implementation will be provided in a separate contribution, along with additional examples.

Consider a unit square with a uniform initial temperature of $T = T_0 = 100$ K. The domain is uniformly discretised with grid spacing $\Delta = 0.02$ and horizon size $\delta = 0.0601$. The parameters Δ and δ are chosen such that $\delta/\Delta \approx 3$. The specimen is subjected to a temperature ramp on its right edge, through the use of a "patch". The patch is visible on the reference configuration in Fig. 3 and has a thickness that corresponds to the horizon size, δ, i.e. three layers of points are generated on the patch. A constant and uniform temperature difference of 50 K is prescribed to the patch. The remainder of the domain boundaries are subject to adiabatic boundary conditions. The heat conduction coefficient K is 100 and the heat capacity c^T is 0.2. Figure 3 depicts the evolution of the temperature with time and the graph in Fig. 4 provides further details of the transient problem. Initially, the increase in temperature is localised in the vicinity of the patches but as time progresses, the specimen gradually heats up and asymptotically reaches steady state.

Next, consider the letters C, P, and D, constructed as two dimensional domains with a uniform initial temperature of $T = T_0 = 100$ K. All three domains are of size $[4 \times 5]$, with grid spacing $\Delta = 0.02$ and horizon

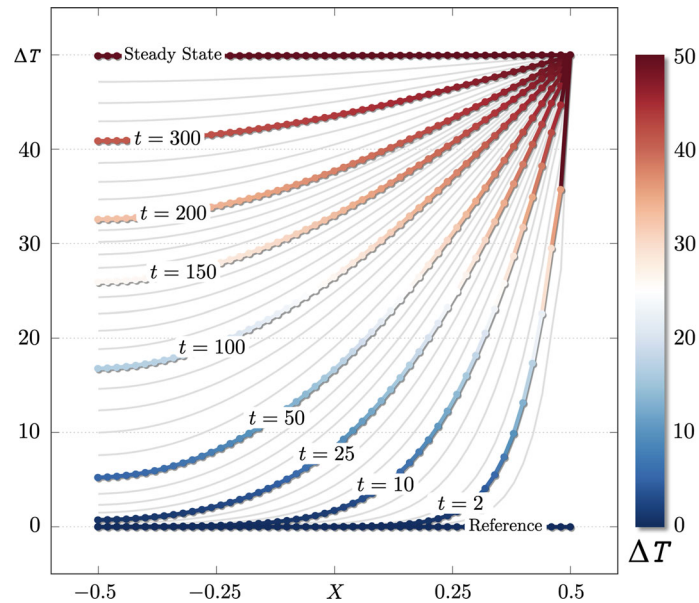

Fig. 4 The temperature distribution of the line of points taken from the centreline of the domain through time. ΔT shows the temperature difference from T_0. X corresponds to the coordinates of the points along the horizontal direction

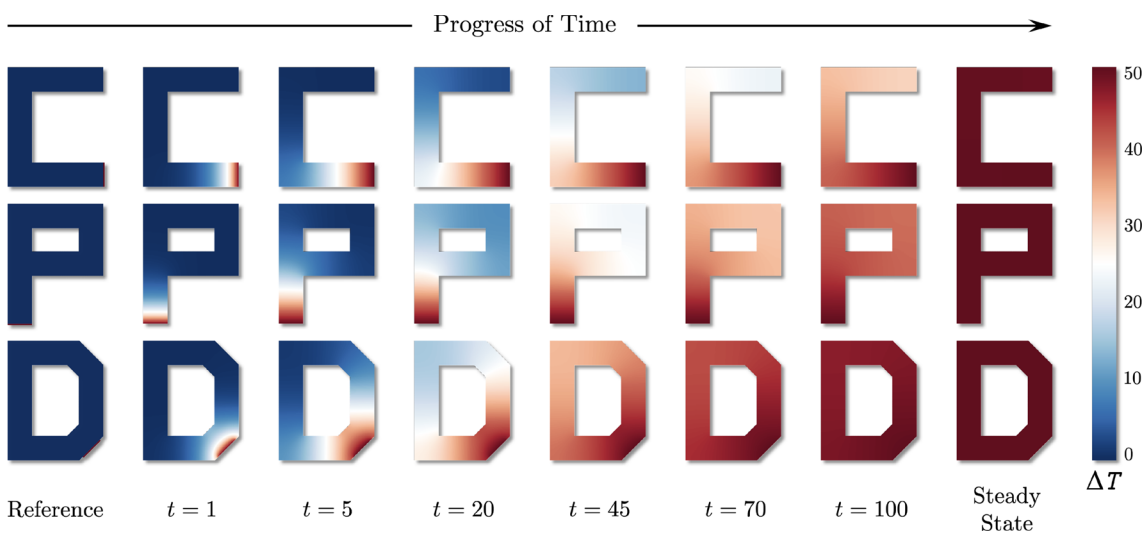

Fig. 5 The numerical example for a purely thermal, two dimensional problem, showing the temperature distribution. It demonstrates the conduction of heat in time, through domains shaped C, P and D. ΔT shows the temperature difference from T_0

size $\delta = 0.0601$. The specimens are subjected to a temperature ramp on part of their boundaries, through the use of patches that are visible on the reference configuration in Fig. 5. The patches are each in contact with the boundaries of their domains along a length of 1 unit and have the same thickness that corresponds to the horizon size, δ. The patches differ only in orientation. As a result, in the vicinity of the patch, the letter C conducts the heat in the horizontal, P in the vertical and D in the diagonal direction. A constant and uniform temperature difference of 50 K is prescribed to each patch. The remainder of the three domains' boundaries are subject to homogeneous Neumann-type conditions, also referred to as adiabatic boundary conditions. The heat conduction coefficient K is 100 and the heat capacity c^T is 0.001. Figure 5 depicts the evolution of the temperature with time. The patches are omitted from the results henceforth, as they have the same uniform temperature at all time steps. Initially, the increase of temperature is localised in the vicinity of the patches. As time progresses, the specimens gradually heat up and asymptotically reach $\Delta T = 50$ K. The letter D is the first to reach steady state, due to its geometrical features, as it has the shortest "path" between its patch and the

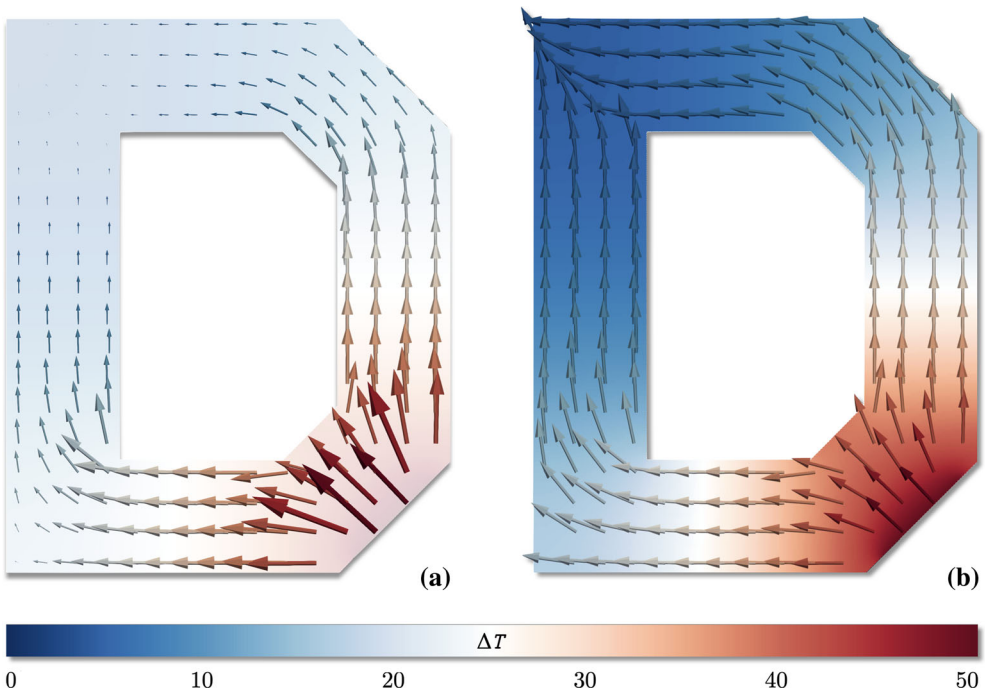

Fig. 6 Two representations of the same heat flux at time instance $t = 10$. The scale of the arrows on the left **a** show the magnitude of the heat flux at the material point that coincides with the base of each arrow, while the arrows on the right **b** are given a constant magnitude to better show the direction of the heat flux on domain D. The coloring of the arrows and the background show the temperature of the domain. ΔT shows the temperature difference from T_0. The left domain **a** is illustrated with less opacity to aid with the visibility of the arrows

furthest point from its heat source. By contrast, the letter C is the last to reach steady state. Figure 6 illustrates the heat flux at time $t = 10$. The color of the domain and the arrows show the temperature distribution. The length of the arrows in Fig. 6a correspond to the magnitude of the heat flux at the particular material points. The arrows in Fig. 6b are given a constant length to better show the direction of the heat flux in the domain. At time $t = 10$, an early stage in the process, the temperature difference between the points closer to the patch is significantly greater than that between the points in the top left section of the domain, as seen in the considerable contrast in the length of the arrows on Fig. 6a. This is expected as a sufficient amount of time for conduction to reach the steady state has not yet passed.

5 Conclusion

A significant extension of continuum kinematic-inspired peridynamics [20] to account for thermo-mechanical coupling has been presented. In doing so, the thermodynamic foundations of peridynamics have been carefully revisited. Thermodynamic restrictions on the interaction energies have been discussed and thermodynamically consistent constitutive laws together with temperature or coldness evolution equations are provided. The computational framework for thermo-mechanical CPD will be detailed in a future work, where the significance of the proposed temperature-based and coldness-based options $\mathtt{T}$ and $\mathtt{C}$, respectively, will be explored. In summary, we have presented a continuum-kinematics-inspired formulation of peridynamics suitable for thermo-mechanical problems, for the first time. This generic approach is broadly applicable to enhance the understanding of material behaviour for a large variety of applications in multi-field problems accounting for nonlocalities and geometrical discontinuities.

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Appendix A. Proof of the variational definition (33)

To prove the variational definition (33), we begin by defining the global Helmholtz energy in the material configuration Ψ_0^{GLB} as the integral of the Helmholtz energy density Ψ_0. That is

$$\Psi_0^{\text{GLB}} := \int_{\mathcal{B}_0} \Psi_0 \, \mathrm{d}V = \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \psi_0^{\mathrm{I}} \, \mathrm{d}V^{\mathrm{I}} \mathrm{d}V \,,$$

where the point-wise energy density per volume squared in the material configuration ψ_0^{I} reads

$$\psi_0^{\mathrm{I}} = \frac{1}{2} \psi_{0:1}^{\mathrm{I}} + \frac{1}{3} \int_{\mathcal{H}_0} \psi_{0:2}^{\mathrm{I}/\mathrm{II}} \, \mathrm{d}V^{\mathrm{II}} + \frac{1}{4} \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}} \, \mathrm{d}V^{\mathrm{III}} \mathrm{d}V^{\mathrm{II}} \qquad \text{with} \qquad \left[\psi_0^{\mathrm{I}}\right] = \mathrm{N.m/m^6}.$$

and thus,

$$\Psi_0^{\text{GLB}} := \underbrace{\int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \frac{1}{2} \psi_{0:1}^{\mathrm{I}} \mathrm{d}V^{\mathrm{I}} \mathrm{d}V}_{\Psi_{0:1}^{\text{GLB}}} + \underbrace{\int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \frac{1}{3} \int_{\mathcal{H}_0} \psi_{0:2}^{\mathrm{I}/\mathrm{II}} \, \mathrm{d}V^{\mathrm{II}} \mathrm{d}V^{\mathrm{I}} \mathrm{d}V}_{\Psi_{0:2}^{\text{GLB}}}$$
$$+ \underbrace{\int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \frac{1}{4} \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}} \, \mathrm{d}V^{\mathrm{III}} \mathrm{d}V^{\mathrm{II}} \mathrm{d}V^{\mathrm{I}} \mathrm{d}V}_{\Psi_{0:3}^{\text{GLB}}} .$$

The variation of Ψ_0^{GLB} reads

$$\delta \Psi_0^{\text{GLB}} = \delta \Psi_{0:1}^{\text{GLB}} + \delta \Psi_{0:2}^{\text{GLB}} + \delta \Psi_{0:3}^{\text{GLB}} \,,$$

in which

$$\begin{aligned}
\delta \Psi_{0:1}^{\text{GLB}} &= \delta \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \frac{1}{2} \psi_{0:1}^{\mathrm{I}} \mathrm{d}V^{\mathrm{I}} \mathrm{d}V \,, \\
\delta \Psi_{0:2}^{\text{GLB}} &= \delta \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \frac{1}{3} \int_{\mathcal{H}_0} \psi_{0:2}^{\mathrm{I}/\mathrm{II}} \, \mathrm{d}V^{\mathrm{II}} \mathrm{d}V^{\mathrm{I}} \mathrm{d}V \,, \\
\delta \Psi_{0:3}^{\text{GLB}} &= \delta \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \frac{1}{4} \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}} \, \mathrm{d}V^{\mathrm{III}} \mathrm{d}V^{\mathrm{II}} \mathrm{d}V^{\mathrm{I}} \mathrm{d}V \,,
\end{aligned}$$

that will be treated separately in Appendix A.1, Appendix A.2 and Appendix A.3, respectively, resulting in

$$\begin{aligned}
\delta \Psi_{0:1}^{\text{GLB}} &= \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \frac{\partial \psi_{0:1}^{\mathrm{I}}}{\partial \boldsymbol{\xi}^{\mathrm{I}}} \cdot \delta \boldsymbol{\xi}^{\mathrm{I}} \, \mathrm{d}V^{\mathrm{I}} \mathrm{d}V \,, \\
\delta \Psi_{0:2}^{\text{GLB}} &= \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \left[\int_{\mathcal{H}_0} 2 \left[\boldsymbol{\xi}^{\mathrm{II}} \times \frac{\partial \psi_{0:2}^{\mathrm{I}/\mathrm{II}}}{\partial \boldsymbol{a}^{\mathrm{I}/\mathrm{II}}} \right] \cdot \delta \boldsymbol{\xi}^{\mathrm{I}} \, \mathrm{d}V^{\mathrm{II}} \right] \cdot \delta \boldsymbol{\xi}^{\mathrm{I}} \, \mathrm{d}V^{\mathrm{I}} \mathrm{d}V \,, \\
\delta \Psi_{0:3}^{\text{GLB}} &= \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \left[\int_{\mathcal{H}_0} \int_{\mathcal{H}_0} 3 \, \frac{\partial \psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}{\partial v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}} [\boldsymbol{\xi}^{\mathrm{II}} \times \boldsymbol{\xi}^{\mathrm{III}}] \, \mathrm{d}V^{\mathrm{III}} \mathrm{d}V^{\mathrm{II}} \right] \cdot \delta \boldsymbol{\xi}^{\mathrm{I}} \, \mathrm{d}V^{\mathrm{I}} \mathrm{d}V \,,
\end{aligned} \tag{A.1}$$

that, in turn, furnishes

$$\frac{\delta \psi_0^{\mathrm{I}}}{\delta \boldsymbol{\xi}^{\mathrm{I}}} := \frac{\partial \psi_{0:1}^{\mathrm{I}}}{\partial \boldsymbol{\xi}^{\mathrm{I}}} + \int_{\mathcal{H}_0} 2 \, \boldsymbol{\xi}^{\mathrm{II}} \times \frac{\partial \psi_{0:2}^{\mathrm{I}/\mathrm{II}}}{\partial \boldsymbol{a}^{\mathrm{I}/\mathrm{II}}} \, \mathrm{d}V^{\mathrm{II}} + \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} 3 \, [\boldsymbol{\xi}^{\mathrm{II}} \times \boldsymbol{\xi}^{\mathrm{III}}] \frac{\partial \psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}{\partial v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}} \, \mathrm{d}V^{\mathrm{III}} \, \mathrm{d}V^{\mathrm{II}} .$$

Since (i) we are interested in the variation $\delta \boldsymbol{\xi}^{\mathrm{I}}$ and (ii) dealing with the contributions due to temperature or coldness is straightforward, we neglect the thermal part of the Helmholtz energy in the forthcoming derivations and assume that $\psi_{0:1}^{\mathrm{I}} := \psi_{0:1}(\boldsymbol{\xi}^{\mathrm{I}})$, $\psi_{0:2}^{\mathrm{I}/\mathrm{II}} := \psi_{0:2}(\boldsymbol{a}^{\mathrm{I}/\mathrm{II}})$ and $\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}} := \psi_{0:3}(v^{\mathrm{I}/\mathrm{II}/\mathrm{III}})$.

Appendix A.1. Variation of stored energy density per volume due to one-neighbour interactions

$$\delta\Psi_{0:1}^{\mathrm{GLB}} = \delta \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \frac{1}{2}\, \psi_{0:1}^{\mathrm{I}}\, \mathrm{d}V^{\mathrm{I}} \mathrm{d}V$$

Since the energy density $\psi_{0:1}^{\mathrm{I}}$ vanishes outside of the horizon $\mathcal{H}_0$, we can replace the integral domain as

$$= \delta \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \frac{1}{2}\, \psi_{0:1}^{\mathrm{I}}\, \mathrm{d}V^{\mathrm{I}} \mathrm{d}V$$

Due to the variation rules on multiple integrals, the previously introduced factor one-half disappears and furnishes

$$= \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \delta\psi_{0:1}^{\mathrm{I}}\, \mathrm{d}V^{\mathrm{I}} \mathrm{d}V$$

Recall that $\psi_{0:1}^{\mathrm{I}} = \psi_{0:1}(\boldsymbol{\xi}^{\mathrm{I}})$ and thus

$$= \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \frac{\partial \psi_{0:1}^{\mathrm{I}}}{\partial \boldsymbol{\xi}^{\mathrm{I}}} \cdot \delta\boldsymbol{\xi}^{\mathrm{I}}\, \mathrm{d}V^{\mathrm{I}} \mathrm{d}V$$

Transforming back the second integral domain from $\mathcal{B}_0$ to $\mathcal{H}_0$ yields

$$= \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \frac{\partial \psi_{0:1}^{\mathrm{I}}}{\partial \boldsymbol{\xi}^{\mathrm{I}}} \cdot \delta\boldsymbol{\xi}^{\mathrm{I}}\, \mathrm{d}V^{\mathrm{I}} \mathrm{d}V$$

Appendix A.2. Variation of stored energy density per volume due to two-neighbour interactions

$$\delta\Psi_{0:2}^{\mathrm{GLB}} = \delta \int_{\mathcal{B}_0} \int_{\mathcal{H}_0} \frac{1}{3} \int_{\mathcal{H}_0} \psi_{0:2}^{\mathrm{I}/\mathrm{II}}\, \mathrm{d}V^{\mathrm{II}} \mathrm{d}V^{\mathrm{I}} \mathrm{d}V$$

Since the energy density $\psi_{0:2}^{\mathrm{I}/\mathrm{II}}$ vanishes outside of the horizon $\mathcal{H}_0$, we can replace the integrals domains as

$$= \delta \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \frac{1}{3} \int_{\mathcal{B}_0} \psi_{0:2}^{\mathrm{I}/\mathrm{II}}\, \mathrm{d}V^{\mathrm{II}} \mathrm{d}V^{\mathrm{I}} \mathrm{d}V$$

Due to the variation rules on multiple integrals, the previously introduced factor one-third disappears and furnishes

$$= \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \delta\psi_{0:2}^{\mathrm{I}/\mathrm{II}}\, \mathrm{d}V^{\mathrm{II}} \mathrm{d}V^{\mathrm{I}} \mathrm{d}V$$

Recall that $\psi_{0:2}^{\mathrm{I}/\mathrm{II}} = \psi_{0:3}(\boldsymbol{a}^{\mathrm{I}/\mathrm{II}})$ and thus

$$= \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \frac{\partial \psi_{0:2}^{\mathrm{I}/\mathrm{II}}}{\partial \boldsymbol{a}^{\mathrm{I}/\mathrm{II}}} \cdot \delta\boldsymbol{a}^{\mathrm{I}/\mathrm{II}}\, \mathrm{d}V^{\mathrm{II}} \mathrm{d}V^{\mathrm{I}} \mathrm{d}V$$

Since $\boldsymbol{a}^{\mathrm{I}/\mathrm{II}} = \boldsymbol{\xi}^{\mathrm{I}} \times \boldsymbol{\xi}^{\mathrm{II}}$, its variation reads $\delta\boldsymbol{a}^{\mathrm{I}/\mathrm{II}} = \delta\boldsymbol{\xi}^{\mathrm{I}} \times \boldsymbol{\xi}^{\mathrm{II}} + \boldsymbol{\xi}^{\mathrm{I}} \times \delta\boldsymbol{\xi}^{\mathrm{II}}$ resulting in

$$= \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \frac{\partial \psi_{0:2}^{\mathrm{I}/\mathrm{II}}}{\partial \boldsymbol{a}^{\mathrm{I}/\mathrm{II}}} \cdot [\delta\boldsymbol{\xi}^{\mathrm{I}} \times \boldsymbol{\xi}^{\mathrm{II}} + \boldsymbol{\xi}^{\mathrm{I}} \times \delta\boldsymbol{\xi}^{\mathrm{II}}]\, \mathrm{d}V^{\mathrm{II}} \mathrm{d}V^{\mathrm{I}} \mathrm{d}V$$

Via changing the order of integration and relabelling the quantities accordingly, we arrive at

$$= \int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\left[\frac{\partial\psi_{0:2}^{\mathrm{I}/\mathrm{II}}}{\partial\boldsymbol{a}^{\mathrm{I}/\mathrm{II}}} - \frac{\partial\psi_{0:2}^{\mathrm{I}/\mathrm{II}}}{\partial\boldsymbol{a}^{\mathrm{II}/\mathrm{I}}}\right]\cdot[\delta\boldsymbol{\xi}^{\mathrm{I}}\times\boldsymbol{\xi}^{\mathrm{II}}]\,\mathrm{d}V^{\mathrm{II}}\mathrm{d}V^{\mathrm{I}}\mathrm{d}V$$

Next, we impose the condition $\partial\psi_{0:2}^{\mathrm{I}/\mathrm{II}}/\partial\boldsymbol{a}^{\mathrm{I}/\mathrm{II}} = -\partial\psi_{0:2}^{\mathrm{I}/\mathrm{II}}/\partial\boldsymbol{a}^{\mathrm{II}/\mathrm{I}}$. More precisely, we require $\partial\psi_{0:2}^{\mathrm{I}/\mathrm{II}}/\partial\boldsymbol{a}^{\mathrm{I}/\mathrm{II}}$ to be homogenous of degree one with respect to $\boldsymbol{a}^{\mathrm{I}/\mathrm{II}}$ which yields

$$\begin{aligned}
&= \int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\int_{\mathcal{B}_0} 2\,\frac{\partial\psi_{0:2}^{\mathrm{I}/\mathrm{II}}}{\partial\boldsymbol{a}^{\mathrm{I}/\mathrm{II}}}\cdot[\delta\boldsymbol{\xi}^{\mathrm{I}}\times\boldsymbol{\xi}^{\mathrm{II}}]\,\mathrm{d}V^{\mathrm{II}}\mathrm{d}V^{\mathrm{I}}\mathrm{d}V\\
&= \int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\int_{\mathcal{B}_0} 2\left[\boldsymbol{\xi}^{\mathrm{II}}\times\frac{\partial\psi_{0:2}^{\mathrm{I}/\mathrm{II}}}{\partial\boldsymbol{a}^{\mathrm{I}/\mathrm{II}}}\right]\cdot\delta\boldsymbol{\xi}^{\mathrm{I}}\,\mathrm{d}V^{\mathrm{II}}\mathrm{d}V^{\mathrm{I}}\mathrm{d}V
\end{aligned}$$

Transforming back the integral domains from $\mathcal{B}_0$ to $\mathcal{H}_0$ yields

$$\begin{aligned}
&= \int_{\mathcal{B}_0}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} 2\left[\boldsymbol{\xi}^{\mathrm{II}}\times\frac{\partial\psi_{0:2}^{\mathrm{I}/\mathrm{II}}}{\partial\boldsymbol{a}^{\mathrm{I}/\mathrm{II}}}\right]\cdot\delta\boldsymbol{\xi}^{\mathrm{I}}\,\mathrm{d}V^{\mathrm{II}}\mathrm{d}V^{\mathrm{I}}\mathrm{d}V\\
&= \int_{\mathcal{B}_0}\int_{\mathcal{H}_0}\left[\int_{\mathcal{H}_0} 2\left[\boldsymbol{\xi}^{\mathrm{II}}\times\frac{\partial\psi_{0:2}^{\mathrm{I}/\mathrm{II}}}{\partial\boldsymbol{a}^{\mathrm{I}/\mathrm{II}}}\right]\cdot\delta\boldsymbol{\xi}^{\mathrm{I}}\,\mathrm{d}V^{\mathrm{II}}\right]\cdot\,\delta\boldsymbol{\xi}^{\mathrm{I}}\,\mathrm{d}V^{\mathrm{I}}\mathrm{d}V.
\end{aligned}$$

Appendix A.3. Variation of stored energy density per volume due to three-neighbour interactions

$$\delta\int_{\mathcal{B}_0}\Psi_{0:3}\,\mathrm{d}V = \delta\int_{\mathcal{B}_0}\int_{\mathcal{H}_0}\frac{1}{4}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0}\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}\,\mathrm{d}V^{\mathrm{III}}\mathrm{d}V^{\mathrm{II}}\mathrm{d}V^{\mathrm{I}}\mathrm{d}V$$

Since the energy density $\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}$ vanishes outside of the horizon $\mathcal{H}_0$, we can replace the integrals domains as

$$= \delta\int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\frac{1}{4}\int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}\,\mathrm{d}V^{\mathrm{III}}\mathrm{d}V^{\mathrm{II}}\mathrm{d}V^{\mathrm{I}}\mathrm{d}V$$

Due to the variation rules on multiple integrals, the previously introduced factor one-fourth disappears and furnishes

$$= \int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\delta\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}\,\mathrm{d}V^{\mathrm{III}}\mathrm{d}V^{\mathrm{II}}\mathrm{d}V^{\mathrm{I}}\mathrm{d}V$$

Recall that $\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}} = \psi_{0:3}(v^{\mathrm{I}/\mathrm{II}/\mathrm{III}})$ and thus

$$= \int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\frac{\partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}{\partial v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}\delta v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}\,\mathrm{d}V^{\mathrm{III}}\mathrm{d}V^{\mathrm{II}}\mathrm{d}V^{\mathrm{I}}\mathrm{d}V$$

Since $v^{\mathrm{I}/\mathrm{II}/\mathrm{III}} = [\boldsymbol{\xi}^{\mathrm{I}}\times\boldsymbol{\xi}^{\mathrm{II}}]\cdot\boldsymbol{\xi}^{\mathrm{III}}$, its variation reads $\delta v^{\mathrm{I}/\mathrm{II}/\mathrm{III}} = [\boldsymbol{\xi}^{\mathrm{II}}\times\boldsymbol{\xi}^{\mathrm{III}}]\cdot\delta\boldsymbol{\xi}^{\mathrm{I}} + [\boldsymbol{\xi}^{\mathrm{III}}\times\boldsymbol{\xi}^{\mathrm{I}}]\cdot\delta\boldsymbol{\xi}^{\mathrm{II}} + [\boldsymbol{\xi}^{\mathrm{I}}\times\boldsymbol{\xi}^{\mathrm{II}}]\cdot\delta\boldsymbol{\xi}^{\mathrm{III}}$ resulting in

$$= \int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\frac{\partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}{\partial v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}\left[[\boldsymbol{\xi}^{\mathrm{II}}\times\boldsymbol{\xi}^{\mathrm{III}}]\cdot\delta\boldsymbol{\xi}^{\mathrm{I}} + [\boldsymbol{\xi}^{\mathrm{III}}\times\boldsymbol{\xi}^{\mathrm{I}}]\cdot\delta\boldsymbol{\xi}^{\mathrm{II}} + [\boldsymbol{\xi}^{\mathrm{I}}\times\boldsymbol{\xi}^{\mathrm{II}}]\cdot\delta\boldsymbol{\xi}^{\mathrm{III}}\right]\,\mathrm{d}V^{\mathrm{III}}\mathrm{d}V^{\mathrm{II}}\mathrm{d}V^{\mathrm{I}}\mathrm{d}V$$

Via changing the order of integration and relabelling the quantities accordingly, we arrive at

$$= \int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\left[\frac{\partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}{\partial v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}} + \frac{\partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}{\partial v^{\mathrm{II}/\mathrm{III}/\mathrm{I}}} + \frac{\partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}{\partial v^{\mathrm{III}/\mathrm{I}/\mathrm{II}}}\right][\boldsymbol{\xi}^{\mathrm{II}}\times\boldsymbol{\xi}^{\mathrm{III}}]\cdot\delta\boldsymbol{\xi}^{\mathrm{I}}\,\mathrm{d}V^{\mathrm{III}}\mathrm{d}V^{\mathrm{II}}\mathrm{d}V^{\mathrm{I}}\mathrm{d}V$$

Next, we investigate the condition $\partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}/\partial v^{\mathrm{I}/\mathrm{II}/\mathrm{III}} = \partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}/\partial v^{\mathrm{II}/\mathrm{III}/\mathrm{I}} = \partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}/\partial v^{\mathrm{III}/\mathrm{I}/\mathrm{II}}$. More precisely, we require $\partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}/\partial v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}$ to be invariant with respect to even premutations of $\boldsymbol{\xi}^{\mathrm{I}}$, $\boldsymbol{\xi}^{\mathrm{II}}$ and $\boldsymbol{\xi}^{\mathrm{III}}$. However, this property holds by definition, since $v^{\mathrm{I}/\mathrm{II}/\mathrm{III}} = v^{\mathrm{II}/\mathrm{III}/\mathrm{I}} = v^{\mathrm{III}/\mathrm{I}/\mathrm{II}}$ and need not be imposed additionally, which yields

$$
\begin{aligned}
&= \int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\int_{\mathcal{B}_0} 3\,\frac{\partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}{\partial v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}[\boldsymbol{\xi}^{\mathrm{II}}\times\boldsymbol{\xi}^{\mathrm{III}}]\cdot\delta\boldsymbol{\xi}^{\mathrm{I}}\,\mathrm{d}V^{\mathrm{III}}\mathrm{d}V^{\mathrm{II}}\mathrm{d}V^{\mathrm{I}}\mathrm{d}V\\
&= \int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\int_{\mathcal{B}_0}\int_{\mathcal{B}_0} 3\left[\frac{\partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}{\partial v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}[\boldsymbol{\xi}^{\mathrm{II}}\times\boldsymbol{\xi}^{\mathrm{III}}]\right]\cdot\delta\boldsymbol{\xi}^{\mathrm{I}}\,\mathrm{d}V^{\mathrm{III}}\mathrm{d}V^{\mathrm{II}}\mathrm{d}V^{\mathrm{I}}\mathrm{d}V
\end{aligned}
$$

Transforming back the integral domains from $\mathcal{B}_0$ to $\mathcal{H}_0$ yields

$$
\begin{aligned}
&= \int_{\mathcal{B}_0}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} 3\left[\frac{\partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}{\partial v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}[\boldsymbol{\xi}^{\mathrm{II}}\times\boldsymbol{\xi}^{\mathrm{III}}]\right]\cdot\delta\boldsymbol{\xi}^{\mathrm{I}}\,\mathrm{d}V^{\mathrm{III}}\mathrm{d}V^{\mathrm{II}}\mathrm{d}V^{\mathrm{I}}\mathrm{d}V\\
&= \int_{\mathcal{B}_0}\int_{\mathcal{H}_0}\left[\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} 3\,\frac{\partial\psi_{0:3}^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}{\partial v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}[\boldsymbol{\xi}^{\mathrm{II}}\times\boldsymbol{\xi}^{\mathrm{III}}]\,\mathrm{d}V^{\mathrm{III}}\mathrm{d}V^{\mathrm{II}}\right]\cdot\delta\boldsymbol{\xi}^{\mathrm{I}}\,\mathrm{d}V^{\mathrm{I}}\mathrm{d}V.
\end{aligned}
$$

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