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ORIGINAL ARTICLE

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Variational Formulation of the First Principle of Continuum Thermodynamics

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Abstract The First Principle of Continuum Thermodynamics is formulated as a variational condition whose test fields are piecewise constant virtual temperatures. Lagrange multipliers theorem is applied to relax the constraint of piecewise constancy of test fields. This provides the existence of square summable vector fields of heat flow through the body fulfilling a virtual thermal work principle, analogous to the virtual work principle in Mechanics. The issue of compatibility of thermal gradients is dealt with and expressed by the complementary variational condition. Primal, complementary and mixed variational inequalities leading to computational methods in heat-conduction boundary-value problems are briefly discussed.

Keywords Continuum Thermodynamics · Lagrange multipliers · Virtual temperatures · Heat flow

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1 Introduction

Duality is a basic concept in Mathematical Physics, and the master dual objects in Continuum Mechanics are velocity fields and force systems which interplay in the axiomatic formulation of dynamical equilibrium. The notion of a stress field in a continuous body in equilibrium was introduced in celebrated papers by Cauchy [1–3] and, starting with the pioneering contributions in [4,5], many valuable advancements have been made to provide the existence result under milder regularity assumptions, as outlined in the recent article [6] and references therein. According to Truesdell and Toupin [7], it was Piola [8] who first applied Lagrange's multiplier method to introduce the notion of stress field in a continuous body. His brilliant intuition was however not properly evaluated and the more *easy-to-follow* geometrical method by Cauchy has been reproduced almost without exceptions in mechanics textbooks, and in research articles, although, with the improvements and generalizations quoted above. The classical Cauchy method has been also adopted in [9] to propose a unified format for thermomechanics based on the notion of thermal displacement. To the best of our knowledge, the supremacy of Piola's approach has not been fully claimed until quite recently [10,11]. The motivation for this supremacy is twofold. On one hand, duality plays a basic role in Lagrange's method so that the players coming into the scene are properly defined and detected. The resulting variational scheme is most fruitful and leads directly to basic theoretical results and to most efficient computational methods. On the other hand, Lagrange's method for continuous problems is now a theorem. The existence of Lagrange's multipliers may indeed be formally motivated by the orthogonality relation between the kernel of a linear operator and the image of the dual operator, when the involved linear spaces are finite dimensional. In the infinite dimensional context of Continuum Mechanics, the topological properties of the involved linear functional spaces and operators must be properly specified and then the existence proof for the multipliers can be given by relying on standard tools

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of functional analysis [12]. More precisely, dual players must range in dual Banach spaces (or, more in general, in dual Banach vector bundles) and the linear differential operator, providing the implicit representation of the constraint, has to be such that the image of any closed linear subspace is closed. The existence result is then provided by Banach's closed range theorem. In Continuum Mechanics, the constraint dealt with by Lagrange's method is the requirement of infinitesimal isometry of virtual displacement fields, which according to Euler [13], is expressed by a vanishing symmetric part of the covariant derivative of virtual velocity vector fields, which in turn is equal to onehalf the Lie derivative of the metric tensor along the virtual flow (see e.g. [14]). When virtual velocity vector fields are assumed to belong to a Sobolev space, the closure of the image by Euler's operator of any closed linear subspace is implied by Korn's inequality [15,16], and Lagrange's method is called the theorem of virtual work [11]. A main task in Mathematical Physics is to pursue the recognition of formal analogies between theories dealing with seemingly different physical contexts, in order to apply to them the same mathematical methods and results. It is then natural to ask oneself if the powerful, modern treatment of the basics of Continuum Mechanics be shared with other fields of continuum physics. The answer is positive, even if not completely straightforward since a somewhat tricky reformulation of classical statements of balance laws is required. The reason is that, in the standard formulation of balance laws, no constraint is explicitly involved and Lagrange's method seems, at a first sight, to be inapplicable. The key observation is that balance laws are required to hold for any part of a given continuous body and this fact may be equivalently formulated in variational terms by means of piecewise constant scalar test fields. These fields play the role of virtual displacements in mechanics, with Euler's operator being replaced by the gradient operator. Lagrange's method can be applied since the closure of the image, by the gradient operator, of any closed linear subspace in a Sobolev space is a well-known result following from Poincaré inequality (see e.g. [12,17]). In this way balance laws, expressing general principles for continuous bodies in Mathematical Physics are shown to be susceptible of being treated by Lagrange's method, and this leads directly to establish the existence and the basic properties of the field interplaying with the implicit constraint. The topic is explicitly treated here with reference to the balance law expressing the First Principle of Thermodynamics, which is shown to be equivalent to a virtual thermal work theorem providing the existence and the basic properties of square integrable heat flow vector fields in the body. A complementary formulation provides the variational condition of compatibility for square integrable vector fields of thermal gradients. Finally, primary, complementary and mixed variational principles, governing a general boundary-value problem of heat conduction, are derived as direct outcomes of the variational theory.

2 The First Principle of Thermodynamics

The First Principle of Thermodynamics is a balance law prescribing an energy conservation rule to be fulfilled by any body undergoing any thermodynamical process. The principle states that given a body $\mathcal{B}$ at a placement $\mathbf{\Omega} = \boldsymbol{\varphi}(\mathcal{B})$ the time rate of change of the internal energy $\dot{\mathcal{E}}(\mathcal{P})$ of any sub-body $\mathcal{P} \subseteq \mathbf{\Omega}$ is equal to the mechanical power $\mathcal{M}(\mathcal{P})$ plus the heat power $\mathcal{Q}(\mathcal{P})$ supplied to the sub-body (see e.g. [18–20]):

$$\dot{\mathcal{E}}(\mathcal{P}) = \mathcal{M}(\mathcal{P}) + \mathcal{Q}(\mathcal{P}).$$

It is convenient to define the energy-rate gap $\mathcal{G}(\mathcal{P}) := \mathcal{M}(\mathcal{P}) + \mathcal{Q}(\mathcal{P}) - \dot{\mathcal{E}}(\mathcal{P})$ and to rewrite the first principle as $\mathcal{G}(\mathcal{P}) = 0$. To formulate the First Principle of Thermodynamics as a variational principle, the space of temperature fields and the definition of linear thermal constraints are preliminarily introduced.

2.1 Temperature fields

In the sequel $\text{PAT}(\mathbf{\Omega})$ denotes a patchwork of $\mathbf{\Omega}$ that is a finite family of open connected, non-overlapping subsets of $\mathbf{\Omega}$, say $\mathcal{P} \in \text{PAT}(\mathbf{\Omega})$ called parts or elements, such that the union of their closures is a covering for $\mathbf{\Omega}$. The set of all patchworks of $\mathbf{\Omega}$ is a directed set with the partial order relation *finer than*; the coarsest patchwork finer than $\text{PAT}_1(\mathbf{\Omega})$ and $\text{PAT}_2(\mathbf{\Omega})$ is the *grid*: $\text{PAT}_1(\mathbf{\Omega}) \wedge \text{PAT}_2(\mathbf{\Omega})$ whose elements are non-empty pairwise intersections of their elements. We denote by V, the linear space of translations in the Euclidean space; and by $L(V; V)$, the space of linear operators on V. The Hilbert spaces of square integrable scalar fields (functions), vector fields and tensor fields on $\mathcal{P}$ are denoted by $\mathcal{L}^2(\mathcal{P}; \mathcal{R})$, $\mathcal{L}^2(\mathcal{P}; V)$ and $\mathcal{L}^2(\mathcal{P}; L(V; V))$, respectively. Moreover, $BL(\mathcal{H}_1; \mathcal{H}_2)$ is the space of bounded linear transformations between the HILBERT spaces $\mathcal{H}_1, \mathcal{H}_2$. The linear space TEMP of temperature fields is composed by Green-regular scalar fields, i.e. square integrabile fields $\theta \in \mathcal{L}^2(\mathbf{\Omega}; \mathcal{R})$ whose distributional derivatives $\nabla\theta$ are piecewise square integrable in $\mathbf{\Omega}$ according to a regularity patchwork $\mathrm{PAT}_\theta(\mathbf{\Omega})$. TEMP is a pre-HILBERT space when endowed with the inner product and norm given by

$$(\theta_1, \theta_2)_{\mathrm{TEMP}} := \int_{\mathbf{\Omega}} \theta_1\theta_2\boldsymbol{\mu} + \int_{\mathrm{PAT}_{\theta_{12}}(\mathbf{\Omega})} \mathbf{g}(\nabla\theta_1, \nabla\theta_2)\boldsymbol{\mu},$$

$$\|\theta\|^2_{\mathrm{TEMP}} := \int_{\mathbf{\Omega}} \theta^2\boldsymbol{\mu} + \int_{\mathrm{PAT}_{\theta}(\mathbf{\Omega})} \|\nabla\theta\|^2\boldsymbol{\mu},$$

where $\mathrm{PAT}_{\theta_{12}}(\mathbf{\Omega}) := \mathrm{PAT}_{\theta_1}(\mathbf{\Omega}) \wedge \mathrm{PAT}_{\theta_2}(\mathbf{\Omega})$ is the grid of the involved patchworks, $\mathbf{g} \in L(V^2; \mathcal{R})$ is the Euclidean metric tensor and $\boldsymbol{\mu} \in L(V^3; \mathcal{R})$ is the associated volume form. In each element $\mathcal{P}$ of the regulatity patchwork, the distributional gradient fulfills the equivalence:

$$\|\nabla\theta\|_0 + \|\theta\|_0 \simeq \|\theta\|_1, \quad \forall\theta \in H^1(\mathcal{P}; \mathcal{R}), \quad \mathcal{P} \in \mathrm{PAT}(\mathbf{\Omega}),$$

where $\|\cdot\|_k$ is the mean square norm on $\mathcal{P}$ of the field and of all its derivatives up to the order k and $H^1(\mathcal{P}; \mathcal{R}) = W^{1,2}(\mathcal{P}; \mathcal{R})$ is a Sobolev space [21]. Indeed, the trivial norm equivalence holds:

$$\|\theta\|_1^2 := \|\nabla\theta\|_0^2 + \|\theta\|_0^2 \leq (\|\nabla\theta\|_0 + \|\theta\|_0)^2 \leq 2(\|\nabla\theta\|_0^2 + \|\theta\|_0^2).$$

Since boundary values are well defined in the Sobolev space $H^1(\mathcal{P}; \mathcal{R})$, the same is true in the pre-HILBERT space TEMP. The regular part of the distributional gradient of a temperature field is the cartesian product of the distributional gradients evaluated on the restrictions to elements of a regularity patchwork. The bounded linear operator so defined, $\nabla \in BL(\mathrm{TEMP}; \mathcal{L}^2(\mathbf{\Omega}; V))$, fulfils the condition: $\|\nabla\theta\|_0 + \|\theta\|_0 \simeq \|\theta\|_1$, for all $\theta \in \mathrm{SOB}^1_\theta$, where SOB^1_θ is the product of the Sobolev spaces $H^1(\mathcal{P}; \mathcal{R})$ for $\mathcal{P} \in \mathrm{PAT}_\theta(\mathbf{\Omega})$. We denote by $\mathrm{CONF} \subset \mathrm{TEMP}$ the space of conforming temperature fields, which is a closed linear subspace of temperature fields sharing a common regularity patchwork PAT and fulfilling continuous linear constraints on the boundary of the patchwork. The space $\mathrm{CONF} \subset \mathrm{TEMP}$ is a Hilbert space for the topology inherited by TEMP. The restriction $\nabla_{\mathrm{CONF}} \in BL(\mathrm{CONF}; \mathcal{L}^2(\mathbf{\Omega}; V))$ of $\nabla \in BL(\mathrm{TEMP}; \mathcal{L}^2(\mathbf{\Omega}; V))$ is a bounded linear operator between the Hilbert spaces. The fulfillment of the condition $\|\nabla\theta\|_0 + \|\theta\|_0 \simeq \|\theta\|_1$ for all $\theta \in \mathrm{CONF}$ ensures that the range $\nabla(\mathrm{CONF}) \subset \mathcal{L}^2(\mathbf{\Omega}; V)$ is closed and that the kernel $\ker \nabla_{\mathrm{CONF}} = \ker \nabla \cap \mathrm{CONF}$ is finite dimensional (see [22–24]). The fields $\theta \in \ker \nabla \subset \mathrm{TEMP}$ are characterized by the property that the regular part $\nabla\theta$ of their distributional gradient vanishes on each element of the regularity patchwork $\mathrm{PAT}_\theta(\mathbf{\Omega})$. It follows that they are piecewise constant temperature fields (see e.g. [17], Proposition II.5.3).

By relying on the Riesz-Fréchet representation theorem, the linear space $\mathcal{L}^2(\mathbf{\Omega}; V)$ is assumed, as usual, to be a self-dual pivot space (see e.g. [25]). Then, denoting by an exponent $*$ the dual topological vector space and by $\langle\, , \rangle$ the duality pairing, the adjoint operator $\nabla^* \in BL(\mathcal{L}^2(\mathbf{\Omega}; V); \mathrm{TEMP}^*)$ is defined by the identity

$$\langle \nabla^*\mathbf{q}, \theta\rangle = \langle \mathbf{q}, \nabla\theta\rangle = \int_{\mathrm{PAT}_\theta(\mathbf{\Omega})} \mathbf{g}(\mathbf{q}, \nabla\theta)\boldsymbol{\mu}, \qquad \forall\mathbf{q} \in \mathcal{L}^2(\mathbf{\Omega}; V), \quad \forall\theta \in \mathrm{TEMP}.$$

and the adjoint operator $\nabla^*_{\mathrm{CONF}} \in BL(\mathcal{L}^2(\mathbf{\Omega}; V); \mathrm{CONF}^*)$ by the identity

$$\langle \nabla^*_{\mathrm{CONF}}\mathbf{q}, \theta\rangle = \langle \mathbf{q}, \nabla\theta\rangle = \int_{\mathrm{PAT}(\mathbf{\Omega})} \mathbf{g}(\mathbf{q}, \nabla\theta)\boldsymbol{\mu}, \qquad \forall\mathbf{q} \in \mathcal{L}^2(\mathbf{\Omega}; V), \quad \forall\theta \in \mathrm{CONF}.$$

Let us denote by $\mathcal{S}^\circ := \{\mathbf{f} \in \mathcal{H}^* : \langle \mathbf{f}, \mathbf{v}\rangle = 0 \quad \forall\, \mathbf{v} \in \mathcal{S}\}$ the annihilator of a subset $\mathcal{S}$ of a HILBERT space $\mathcal{H}$. The following relations are then simple consequences of the definition of adjoint operator

$$\begin{cases} (\nabla^*_{\mathrm{CONF}}(\mathcal{L}^2(\mathbf{\Omega}; V)))^\circ = \ker \nabla_{\mathrm{CONF}}, \\ (\nabla(\mathrm{CONF}))^\circ = \ker \nabla^*_{\mathrm{CONF}}. \end{cases}$$

In finite dimensions we have that $\mathcal{S}^{\circ\circ} = \mathcal{S}$, but in infinite dimensions the existence result, implicit in the converse relations

$$\begin{cases} \nabla^*_{\text{CONF}}(\mathcal{L}^2(\mathbf{\Omega}; V)) = (\ker \nabla_{\text{CONF}})^{\circ}, \\ \nabla(\text{CONF}) = (\ker \nabla^*_{\text{CONF}})^{\circ}, \end{cases}$$

is provided by Banach's closed range theorem [26] under the assumption that $\nabla(\text{CONF}) \subset \mathcal{L}^2(\mathbf{\Omega}; V)$ is closed. Non-homogeneous constraints on temperature fields are formulated by considering a prescribed Green-regular temperature field $\bar{\theta} \in \text{TEMP}$ and temperature fields belonging to the affine manifold $\text{ADM} := \bar{\theta} + \text{CONF}$ are said to be *admissible*. Variations of admissible temperature fields are conforming.

2.2 Variational formulation of the First Principle

We will call *virtual temperatures* the scalar fields $\delta\theta \in \text{TEMP}$, which play the role of test fields for the variational conditions. For any patchwork $\text{PAT}(\mathbf{\Omega})$, we consider the characteristic function of the element $\mathcal{P} \in \text{PAT}(\mathbf{\Omega})$, given by:

$$1_{\mathcal{P}}(\mathbf{x}) = \begin{cases} 1 & \mathbf{x} \in \mathcal{P}, \\ 0 & \mathbf{x} \in \mathbf{\Omega} \setminus \mathcal{P}, \end{cases}$$

and define the functionals:

$$\mathcal{F}_{\dot{\mathcal{E}}}(1_{\mathcal{P}}) := \dot{\mathcal{E}}(\mathcal{P}),$$
$$\mathcal{F}_{\mathcal{M}}(1_{\mathcal{P}}) := \mathcal{M}(\mathcal{P}),$$
$$\mathcal{F}_{\mathcal{Q}}(1_{\mathcal{P}}) := \mathcal{Q}(\mathcal{P}),$$

which acting on the characteristic function $1_{\mathcal{P}}$ provide, respectively, the time rate of increase of the internal energy, the mechanical power and the heat power supplied to the sub-body $\mathcal{P}$. Performing an extension by linearity, we may define the linear functionals $\mathcal{F}_{\dot{\mathcal{E}}}$, $\mathcal{F}_{\mathcal{M}}$ and $\mathcal{F}_{\mathcal{Q}}$ on the linear subspace $\ker \nabla \subseteq \text{TEMP}$ of piecewise constant virtual temperature fields. By HAHN's extension theorem these bounded linear functionals can be extended (non-univocally) to bounded linear functionals on TEMP without increasing their norm (see e.g. [26]). The First Principle of Thermodynamics can then be formulated in variational terms as:

$$\langle \mathcal{F}_{\dot{\mathcal{E}}}, \delta\theta \rangle = \langle \mathcal{F}_{\mathcal{M}}, \delta\theta \rangle + \langle \mathcal{F}_{\mathcal{Q}}, \delta\theta \rangle, \quad \forall \delta\theta \in \ker \nabla.$$

Recalling the definition of the energy-rate gap $\mathcal{G} := \mathcal{M} + \mathcal{Q} - \dot{\mathcal{E}}$, and introducing the thermal force $\mathcal{F}_{\mathcal{G}} \in \text{TEMP}^*$ as the bounded linear functional given by:

$$\mathcal{F}_{\mathcal{G}} := \mathcal{F}_{\mathcal{M}} + \mathcal{F}_{\mathcal{Q}} - \mathcal{F}_{\dot{\mathcal{E}}},$$

the energy conservation law $\mathcal{G} = 0$ takes the variational form

$$\langle \mathcal{F}_{\mathcal{G}}, \delta\theta \rangle = 0, \quad \forall \delta\theta \in \ker \nabla \quad \Longleftrightarrow \quad \mathcal{F}_{\mathcal{G}} \in (\ker \nabla)^{\circ}.$$

This condition, which is analogous to the axiom of dynamical equilibrium in Mechanics [11], is called the axiom of thermal equilibrium and can be stated by saying that the virtual thermal work of the *thermal force* $\mathcal{F}_{\mathcal{G}}$ must vanish for any piecewise constant virtual temperature field.

The closed range property of $\nabla_{\text{CONF}} \in BL(\text{CONF}; \mathcal{L}^2(\mathbf{\Omega}; V))$ leads to the following existence result of the cold flow vector field $\mathbf{q} \in \mathcal{L}^2(\mathbf{\Omega}; V)$. Although its opposite $-\mathbf{q} \in \mathcal{L}^2(\mathbf{\Omega}; V)$, the heat flow vector field, is classically considered in Continuum Thermodynamics, considering the cold flow vector field as the *alter ego* of the stress tensor field in Continuum Mechanics, avoids an unpleasant minus sign in the constitutive equation for thermal conduction.

Theorem 1 (Virtual thermal work) *For any fixed linear subspace of conforming temperature fields* CONF $\subset$ TEMP*, the axiom of thermal equilibrium implies that:*

$$\langle \mathcal{F}_{\mathcal{G}}, \delta\theta \rangle = 0, \quad \forall \delta\theta \in \ker \nabla_{\mathrm{CONF}},$$

and this is equivalent to state the existence of a (not necessarily unique) square integrable vector field $\mathbf{q} \in \mathcal{L}^2(\boldsymbol{\Omega}; V)$*, the cold flow vector field, which performs, for the regular part of the distributional gradient of a conforming virtual temperature field, a virtual thermal work equal to the one that the thermal force performs for the conforming virtual temperature field:*

$$\langle \mathcal{F}_{\mathcal{G}}, \delta\theta \rangle = \int_{\mathrm{PAT}(\boldsymbol{\Omega})} \mathbf{g}(\mathbf{q}, \nabla\delta\theta)\boldsymbol{\mu}, \quad \forall \delta\theta \in \mathrm{CONF}.$$

Cold flow vector fields fulfilling the condition above are said to be in thermal equilibrium with the given $\mathcal{F}_{\mathcal{G}} \in (\ker \nabla)^{\circ}$*. The affine manifold of these fields is denoted by* EQUIL*.*

Proof The property $\mathcal{F}_{\mathcal{G}} \in (\ker \nabla)^{\circ} \subset (\ker \nabla_{\mathrm{CONF}})^{\circ} = (\ker \nabla \cap \mathrm{CONF})^{\circ} = \nabla^{*}_{\mathrm{CONF}}(\mathcal{L}^2(\boldsymbol{\Omega}; V))$ means that there exists a vector field $\mathbf{q} \in \mathcal{L}^2(\boldsymbol{\Omega}; V)$, the cold flow vector field, such that $\mathcal{F}_{\mathcal{G}} = \nabla^{*}_{\mathrm{CONF}}\mathbf{q}$, i.e.

$$\langle \mathcal{F}_{\mathcal{G}}, \delta\theta \rangle = \langle \nabla^{*}\mathbf{q}, \delta\theta \rangle = \int_{\mathrm{PAT}(\boldsymbol{\Omega})} \mathbf{g}(\mathbf{q}, \nabla\delta\theta)\boldsymbol{\mu}, \quad \forall \delta\theta \in \mathrm{CONF},$$

in variational terms. The converse implication is trivial. □

Let us now observe that the virtual thermal work

$$\int_{\mathrm{PAT}_{\delta\theta}(\boldsymbol{\Omega})} \mathbf{g}(\mathbf{q}, \nabla\delta\theta)\boldsymbol{\mu}, \quad \delta\theta \in \mathrm{TEMP},$$

is well defined for any (even non-conforming) temperature field $\delta\theta \in$ TEMP. Each cold flow vector field $\mathbf{q} \in$ EQUIL induces then a reactive thermal force $\mathcal{R}(\mathcal{F}_{\mathcal{G}}, \mathbf{q}) \in \mathrm{TEMP}^{*}$ given by:

$$\langle \mathcal{R}, \delta\theta \rangle := \int_{\mathrm{PAT}_{\delta\theta}(\boldsymbol{\Omega})} \mathbf{g}(\mathbf{q}, \nabla\delta\theta)\boldsymbol{\mu} - \langle \mathcal{F}_{\mathcal{G}}, \delta\theta \rangle, \quad \forall \delta\theta \in \mathrm{TEMP},$$

with the characteristic property that the virtual thermal work, performed for any conforming virtual temperature field, vanishes:

$$\langle \mathcal{R}, \delta\theta \rangle = 0, \quad \forall \delta\theta \in \mathrm{CONF} \iff \mathcal{R} \in (\mathrm{CONF})^{\circ}.$$

The statement dual to Theorem 1 provides the compatibility condition to be imposed on a square integrable vector field of *thermal gradients* $\boldsymbol{\theta} \in \mathcal{L}^2(\boldsymbol{\Omega}; V)$, in analogy to the kinematic compatibility condition for tensor fields of linearized strains in Continuum Mechanics. The question to be answered is the following: Given a vector field $\boldsymbol{\theta} \in \mathcal{L}^2(\boldsymbol{\Omega}; V)$ of thermal gradients, does it exist an admissible temperature field $\theta \in \mathrm{ADM} = \bar{\theta} + \mathrm{CONF}$ such that $\boldsymbol{\theta} = \nabla\theta$? Thermal gradients fulfilling this property are said to be *thermally compatible*. The property can be equivalently expressed by requiring the existence of a $\bar{\theta} \in$ TEMP such that $\boldsymbol{\theta} - \nabla\bar{\theta} \in \nabla(\mathrm{CONF})$. This issue, which seems not to have been dealt with before in Continuum Thermodynamics literature, where only compatible thermal gradients are considered, is a by-product of the newly proposed variational approach to the First Principle and is at the basis of complementary formulations and related computational methods [27]. Thermal compatibility, according to the general formulation above, can only be treated in variational terms, due to the fact that differential conditions of integrability cannot take conformity to linear boundary constraints into account.

Theorem 2 (Thermal compatibility) *The requirement that a square integrable field of thermal gradients $\boldsymbol{\theta} \in \mathcal{L}^2(\boldsymbol{\Omega}; V)$ be thermally compatible is equivalent to the variational condition*

$$\int_{\boldsymbol{\Omega}} \mathbf{g}(\delta\mathbf{q}, \boldsymbol{\theta})\boldsymbol{\mu} = \int_{\boldsymbol{\Omega}} \mathbf{g}(\delta\mathbf{q}, \nabla\bar{\theta})\boldsymbol{\mu}, \quad \forall\delta\mathbf{q} \in Ker\nabla^*_{\mathrm{CONF}},$$

where $Ker\nabla^*_{\mathrm{CONF}} := \{\delta\mathbf{q} \in \mathcal{L}^2(\boldsymbol{\Omega}; V) : \int_{\mathrm{PAT}(\boldsymbol{\Omega})} \mathbf{g}(\delta\mathbf{q}, \nabla\delta\theta)\boldsymbol{\mu} = 0, \quad \forall\delta\theta \in \mathrm{CONF}\}$ *is the subspace of thermally selfequilibrated cold flow fields, parallel to the affine manifold* EQUIL *of thermally equilibrated cold flow fields.*

Proof The closedness of the linear subspace $\nabla(\mathrm{CONF}) \subset \mathcal{L}^2(\boldsymbol{\Omega}; V)$ is equivalent to the orthogonality property $\nabla(\mathrm{CONF}) = (\mathrm{Ker}\nabla^*_{\mathrm{CONF}})^\circ$. Then the compatibility condition writes $\boldsymbol{\theta} - \nabla\bar{\theta} \in (\mathrm{Ker}\nabla^*_{\mathrm{CONF}})^\circ$, whose variational expression is the condition in the statement. The converse implication is trivial. □

3 Boundary-value problems

The basic tool in boundary-value problems (BVPs) governed by a linear partial differential operator DIFF of order n, is Green's formula of integration by parts, which formally may be written as:

$$\int_{\mathrm{PAT}(\boldsymbol{\Omega})} (\bullet, \mathrm{DIFF}\circ)\boldsymbol{\mu} = \int_{\mathrm{PAT}(\boldsymbol{\Omega})} (\mathrm{ADJDIFF}\bullet, \circ)\boldsymbol{\mu} + \oint_{\partial\mathrm{PAT}(\boldsymbol{\Omega})} (\mathrm{FLUX}\bullet, \mathrm{VAL}\circ)\partial\boldsymbol{\mu},$$

where $\mathrm{PAT}(\boldsymbol{\Omega})$ is a fixed patchwork, $\partial\mathrm{PAT}(\boldsymbol{\Omega})$ is its boundary, $\partial\boldsymbol{\mu}$ is the volume $(n-1)$-form induced on the surfaces $\partial\mathrm{PAT}(\boldsymbol{\Omega})$ and all the integrals are assumed to take a finite value. The differential operator ADJDIFF of order n is the *formal adjoint* of DIFF. The boundary integral acts on the duality pairing between the two fields FLUX • and VAL∘ with the differential operators FLUX and VAL being n-tuples of normal derivatives of order from 0 to $n-1$ in inverse sequence, to that the duality pairing is the sum of n terms, whose kth term is the pairing of normal derivatives of two fields of order k and $n-1-k$.

BVPs are characterized by the property that the closed linear subspace CONF of conforming test fields includes the whole linear subspace $\ker(\mathrm{VAL})$ of test fields in TEMP with vanishing boundary values on $\partial\mathrm{PAT}(\boldsymbol{\Omega})$, i.e. by the property that $\ker(\mathrm{VAL}) \subseteq \mathrm{CONF}$. Let us assume that the time rate of change of the internal energy $\dot{\mathcal{E}}(\boldsymbol{\Omega})$ be expressed in terms of a bulk density $\dot{\varepsilon} \in \mathcal{L}^2(\boldsymbol{\Omega}; \mathcal{R})$:

$$\dot{\mathcal{E}}(\boldsymbol{\Omega}) = \langle \mathcal{F}_{\dot{\mathcal{E}}}, 1_{\boldsymbol{\Omega}} \rangle := \int_{\boldsymbol{\Omega}} \rho\dot{\varepsilon}\boldsymbol{\mu},$$

where $\rho \in \mathcal{L}^2(\boldsymbol{\Omega}; \mathcal{R})$ is the mass density and the heat power $\mathcal{Q}(\boldsymbol{\Omega})$ supplied to the body is expressed in terms of a bulk density $q \in \mathcal{L}^2(\boldsymbol{\Omega}; \mathcal{R})$ and of a superficial density $\partial q \in \mathcal{L}^2(\partial\mathrm{PAT}(\boldsymbol{\Omega}); \mathcal{R})$:

$$\mathcal{Q}(\boldsymbol{\Omega}) = \langle \mathcal{F}_{\mathcal{Q}}, 1_{\boldsymbol{\Omega}} \rangle := \int_{\boldsymbol{\Omega}} \rho q\boldsymbol{\mu} + \oint_{\partial\mathrm{PAT}(\boldsymbol{\Omega})} \partial q\,\partial\boldsymbol{\mu}.$$

The mechanical power is expressed, in terms of the stress tensor field $\mathbf{T} \in \mathcal{L}^2(\boldsymbol{\Omega}; L(V; V))$ and of the Euler operator evaluated on the velocity field $\mathbf{v} \in \mathrm{SOB}^1_{\mathbf{v}}$ of the body, by the formula:

$$\mathcal{M}(\boldsymbol{\Omega}) = \langle \mathcal{F}_{\mathcal{M}}, 1_{\boldsymbol{\Omega}} \rangle := \int_{\boldsymbol{\Omega}} (\mathbf{T}, \mathrm{sym}\nabla\mathbf{v})_{\mathbf{g}}\boldsymbol{\mu},$$

where $\text{SOB}^1_{\mathbf{v}}$ is the product of the Sobolev spaces $H^1(\mathcal{P}; V)$ with $\mathcal{P} \in \text{PAT}_{\mathbf{v}}(\boldsymbol{\Omega})$ and $(\mathbf{T}, \text{sym}\nabla\mathbf{v})_{\mathbf{g}}$ is the inner product between tensors induced by the metric. The bounded linear functionals $\mathcal{F}_{\dot{\mathcal{E}}}$, $\mathcal{F}_{\mathcal{M}}$ and $\mathcal{F}_{\mathcal{Q}}$ may then be univocally extended to the whole space TEMP by setting:

$$\langle \mathcal{F}_{\dot{\mathcal{E}}}, \delta\theta \rangle := \int_{\boldsymbol{\Omega}} \rho\dot{\varepsilon}\delta\theta\boldsymbol{\mu},$$

$$\langle \mathcal{F}_{\mathcal{M}}, \delta\theta \rangle := \int_{\boldsymbol{\Omega}} (\mathbf{T}, \text{sym}\nabla\mathbf{v})_{\mathbf{g}}\delta\theta\boldsymbol{\mu},$$

$$\langle \mathcal{F}_{\mathcal{Q}}, \delta\theta \rangle := \int_{\boldsymbol{\Omega}} \rho q\delta\theta\boldsymbol{\mu} + \oint_{\partial\text{PAT}_\theta(\boldsymbol{\Omega})} \partial q \text{VAL}(\delta\theta)\partial\boldsymbol{\mu}$$

for any $\theta \in \text{TEMP}$. Defining the bulk energy-rate gap field as

$$p := (\mathbf{T}, \text{sym}\nabla\mathbf{v})_{\mathbf{g}} + \rho q - \rho\dot{\varepsilon},$$

the thermal force $\mathcal{F}_{\mathcal{G}} \in \text{TEMP}^*$ is given by:

$$\langle \mathcal{F}_{\mathcal{G}}, \delta\theta \rangle = \int_{\boldsymbol{\Omega}} p\delta\theta\boldsymbol{\mu} + \oint_{\partial\text{PAT}_{\delta\theta}(\boldsymbol{\Omega})} \partial q \text{VAL}(\delta\theta)\partial\boldsymbol{\mu}, \quad \forall\delta\theta \in \text{TEMP}.$$

Due to the basic property $\ker(\text{VAL}) \subseteq \text{CONF}$ of BVPs, the variational condition stated in the virtual thermal work theorem can be localized to yield differential and jump conditions. Although the procedure is standard, we report hereafter the statement and the proof of the basic results for the sake of completeness. Moreover a detailed presentation of these results at this level of generality is not easily found in the literature. Let us denote by COLD the linear subspace of Green-regular cold flow vector fields $\mathbf{q} \in \mathcal{L}^2(\boldsymbol{\Omega}; V)$, characterized by the property that their distributional divergence is piecewise square integrable $\text{DIV}\mathbf{q} \in \mathcal{L}^2(\text{PAT}_{\mathbf{q}}(\boldsymbol{\Omega}); \mathcal{R})$. Then all the terms in the relevant Green's formula are well defined:

$$\int_{\text{PAT}_{\theta\mathbf{q}}(\boldsymbol{\Omega})} \mathbf{g}(\mathbf{q}, \nabla\theta)\boldsymbol{\mu} = \int_{\text{PAT}_{\theta\mathbf{q}}(\boldsymbol{\Omega})} (-\text{DIV}\mathbf{q})\theta\boldsymbol{\mu} + \oint_{\partial\text{PAT}_{\theta\mathbf{q}}(\boldsymbol{\Omega})} \mathbf{g}(\mathbf{q}, \mathbf{n})\text{VAL}(\theta)\partial\boldsymbol{\mu}, \quad \begin{cases} \forall\, \theta \in \text{TEMP}, \\ \forall\, \mathbf{q} \in \text{COLD}, \end{cases}$$

where $\text{PAT}_{\theta\mathbf{q}}(\boldsymbol{\Omega}) = \text{PAT}_\theta(\boldsymbol{\Omega}) \wedge \text{PAT}_{\mathbf{q}}(\boldsymbol{\Omega})$ and FLUX $\mathbf{q} = \mathbf{g}(\mathbf{q}, \mathbf{n})$, with $\mathbf{n}$ outward unit normal to the boundary $\partial\text{PAT}_{\theta\mathbf{q}}(\boldsymbol{\Omega})$ and $\text{VAL}(\theta)$ boundary value of the field $\theta \in \text{TEMP}$ on $\partial\text{PAT}_{\theta\mathbf{q}}(\boldsymbol{\Omega})$.

This formula may be also written in terms of jumps at the interfaces of a regularity patchwork. Indeed a boundary $\partial\text{PAT}(\boldsymbol{\Omega})$ may be considered as the union of the boundary of $\boldsymbol{\Omega}$ and of the pairs of positive and negative faces of each interface between elements of $\text{PAT}(\boldsymbol{\Omega})$, i.e.: $\partial\text{PAT}(\boldsymbol{\Omega}) = \partial\boldsymbol{\Omega} + \text{SING}(\text{PAT})$. Then, setting $\mathbf{n} = \mathbf{n}^+$, outward normal to the $+$ face, and defining the jump:

$$[[\mathbf{g}(\mathbf{q}, \mathbf{n})]] := \mathbf{g}(\mathbf{q}^+, \mathbf{n}^+) + \mathbf{g}(\mathbf{q}^-, \mathbf{n}^-) = \mathbf{g}(\mathbf{q}^+, \mathbf{n}^+) - \mathbf{g}(\mathbf{q}^-, \mathbf{n}^+),$$

across the interfaces, with the boundary $\partial\boldsymbol{\Omega}$ as a $+$ face, Green's formula may be written as:

$$\int_{\text{PAT}_{\theta\mathbf{q}}(\boldsymbol{\Omega})} \mathbf{g}(\mathbf{q}, \nabla\theta)\boldsymbol{\mu} = \int_{\text{PAT}_{\theta\mathbf{q}}(\boldsymbol{\Omega})} (-\text{DIV}\mathbf{q})\theta\boldsymbol{\mu} + \oint_{\partial\boldsymbol{\Omega}} \mathbf{g}(\mathbf{q}, \mathbf{n})\text{VAL}(\theta)\partial\boldsymbol{\mu}$$
$$+ \int_{\text{SING}(\text{PAT}_{\theta\mathbf{q}}(\boldsymbol{\Omega}))} [[\mathbf{g}(\mathbf{q}, \mathbf{n})]]\text{VAL}(\theta)\partial\boldsymbol{\mu}, \quad \begin{cases} \forall\, \theta \in \text{TEMP}, \\ \forall\, \mathbf{q} \in \text{COLD}. \end{cases}$$

Then we have the following result.

Theorem 3 (Localization) *In a boundary value problem of heat conduction, a cold flow vector field* $\mathbf{q} \in \mathrm{EQUIL}$*, i.e. fulfilling the identity*

$$\int_{\mathrm{PAT}(\mathbf{\Omega})} \mathbf{g}(\mathbf{q}, \nabla\delta\theta)\boldsymbol{\mu} = \int_{\mathbf{\Omega}} p\delta\theta\boldsymbol{\mu} + \oint_{\partial\mathrm{PAT}(\mathbf{\Omega})} \partial q \mathrm{VAL}(\delta\theta)\partial\boldsymbol{\mu}, \quad \forall\delta\theta \in \mathrm{CONF},$$

has a distributional divergence $\mathrm{DIV}\mathbf{q}$ *whose restriction to each element* $\mathcal{P} \in \mathrm{PAT}(\mathbf{\Omega})$ *of the patchwork is* $\mathbf{g}$*-square integrable with* $-\mathrm{DIV}\,\mathbf{q} = p$ *in* $\mathrm{PAT}(\mathbf{\Omega})$ *and the jump* $[[\mathbf{g}(\mathbf{q}, \mathbf{n})]]$ *of the flux across the boundary of the domain* $\mathbf{\Omega}$ *and across the interfaces of the patchwork* $\mathrm{PAT}(\mathbf{\Omega})$ *fulfills the conditions:*

$$\begin{aligned} &\mathbf{g}(\mathbf{q}, \mathbf{n}) \quad \in \partial q + \mathrm{CONF}^{\circ}, \quad \text{on} \quad \partial\mathbf{\Omega}, \\ &[[\mathbf{g}(\mathbf{q}, \mathbf{n})]] \in \partial q^{+} + \partial q^{-} + \mathrm{CONF}^{\circ}, \quad \text{on} \quad \mathrm{SING}(\mathrm{PAT}(\mathbf{\Omega})), \end{aligned}$$

where the fields ∂q *of superficial cold supply are taken to be zero outside their domain of definition.*

Proof The statement of the virtual thermal work theorem may be written as:

$$\int_{\mathrm{PAT}(\mathbf{\Omega})} \mathbf{g}(\mathbf{q}, \nabla\delta\theta)\boldsymbol{\mu} = \int_{\mathbf{\Omega}} p\delta\theta\boldsymbol{\mu} + \oint_{\partial\mathrm{PAT}(\mathbf{\Omega})} \partial q \mathrm{VAL}(\delta\theta)\partial\boldsymbol{\mu}, \quad \forall\delta\theta \in \mathrm{CONF}.$$

In BVPs, the linear space $\mathrm{C}_0^{\infty}(\mathrm{PAT}(\mathbf{\Omega}))$ of infinitely differentiable scalar fields with compact support in each element of $\mathrm{PAT}(\mathbf{\Omega})$ is included in CONF, so that

$$\int_{\mathrm{PAT}(\mathbf{\Omega})} \mathbf{g}(\mathbf{q}, \nabla\delta\theta)\boldsymbol{\mu} = \int_{\mathbf{\Omega}} p\delta\theta\boldsymbol{\mu}, \quad \forall\delta\theta \in \mathrm{C}_0^{\infty}(\mathrm{PAT}(\mathbf{\Omega})),$$

which means that $-\mathrm{DIV}\mathbf{q} = p \in \mathcal{L}^2(\mathrm{PAT}(\mathbf{\Omega}); \mathcal{R})$ in the sense of distributions. Hence $\mathbf{q} \in \mathrm{COLD}$. Green's formula then holds and gives

$$\oint_{\partial\mathrm{PAT}(\mathbf{\Omega})} (\mathbf{g}(\mathbf{q}, \mathbf{n}) - \partial q)\mathrm{VAL}(\delta\theta)\partial\boldsymbol{\mu} = 0, \quad \begin{cases} \forall\, \delta\theta \in \mathrm{CONF}, \\ \forall\, \mathbf{q} \in \mathrm{COLD}, \end{cases}$$

and the result follows. □

The reactive thermal force $\mathcal{R}(\partial q, p, \mathbf{q}) \in \mathrm{TEMP}^*$, associated with a vector field $\mathbf{q} \in \mathrm{EQUIL}$, in thermal equilibrium with a bulk energy-rate gap p, and a superficial heat supply ∂q, is given by:

$$\begin{aligned} \langle \mathcal{R}, \delta\theta \rangle &:= \int_{\mathrm{PAT}_{\delta\theta}(\mathbf{\Omega})} \mathbf{g}(\mathbf{q}, \nabla\delta\theta)\boldsymbol{\mu} - \int_{\mathrm{PAT}_{\delta\theta}(\mathbf{\Omega})} p\delta\theta\boldsymbol{\mu} - \oint_{\partial\mathrm{PAT}_{\delta\theta}(\mathbf{\Omega})} \partial q \mathrm{VAL}(\delta\theta)\partial\boldsymbol{\mu} \\ &= \int_{\mathrm{PAT}_{\delta\theta}(\mathbf{\Omega})} -(\mathrm{DIV}\mathbf{q} + p)\,\delta\theta\boldsymbol{\mu} + \oint_{\partial\mathrm{PAT}_{\delta\theta}(\mathbf{\Omega})} (\mathbf{g}(\mathbf{q}, \mathbf{n}) - \partial q)\mathrm{VAL}(\delta\theta)\partial\boldsymbol{\mu} \\ &= \oint_{\partial\mathrm{PAT}_{\delta\theta}(\mathbf{\Omega})} (\mathbf{g}(\mathbf{q}, \mathbf{n}) - \partial q)\mathrm{VAL}(\delta\theta)\partial\boldsymbol{\mu}, \quad \forall\delta\theta \in \mathrm{TEMP}. \end{aligned}$$

Defining the reactive superficial heat supply as $\partial r(\mathbf{q}, \partial q) := \mathbf{g}(\mathbf{q}, \mathbf{n}) - \partial q$, Theorem 1 ensures that

$$\oint_{\partial\mathrm{PAT}(\mathbf{\Omega})} \partial r(\mathbf{q}, \partial q)\mathrm{VAL}(\delta\theta)\partial\boldsymbol{\mu} = 0, \quad \forall\delta\theta \in \mathrm{CONF}.$$

Hence, in particular, $\partial r(\mathbf{q}, \partial q) = 0$ on any piece of boundary where virtual temperatures are not prescribed. The bulk equation $\mathrm{DIV}\,\mathbf{q} = -p$ is known in literature as the reduced equation of conservation of the energy. The boundary equation $\mathbf{g}(\mathbf{q}, \mathbf{n}) = \partial q$, in absence of boundary constraints on the temperature fields, is known as the heat flow principle of FOURIER-STOKES.

4 Variational formulations of heat conduction BVPs

The variational conditions of thermal equilibrium and compatibility, stated in Theorems 1 and 2, lead to the following primary and complementary formulations of BVPs of heat conduction. Let us assume a generalized form of FOURIER's law [28] of *heat conduction* which is pointwise expressed, in terms of a convex potential $\boldsymbol{\phi}: V \to \mathcal{R}$, by the variational inequality $\mathbf{g}(\mathbf{q}_{\mathbf{x}}, \delta\boldsymbol{\theta}_{\mathbf{x}}) \leq \mathbf{g}(d^+\boldsymbol{\phi}(\boldsymbol{\theta}_{\mathbf{x}}), \delta\boldsymbol{\theta}_{\mathbf{x}})$ for all $\delta\boldsymbol{\theta}_{\mathbf{x}} \in V$, where d^+ is the unilateral derivative [29]. The validity of this law a.e. in $\boldsymbol{\Omega}$ is equivalent [30] to the global variational inequality

$$\langle \mathbf{q}, \delta\boldsymbol{\theta} \rangle \leq \langle d^+\boldsymbol{\Phi}(\boldsymbol{\theta}), \delta\boldsymbol{\theta} \rangle, \quad \forall \delta\boldsymbol{\theta} \in \mathcal{L}^2(\boldsymbol{\Omega}; V),$$

involving the fields $\mathbf{q} \in \mathcal{L}^2(\boldsymbol{\Omega}; V)$ and $\boldsymbol{\theta} \in \mathcal{L}^2(\boldsymbol{\Omega}; V)$ with the global convex potential given by

$$\boldsymbol{\Phi}(\boldsymbol{\theta}) := \int_{\boldsymbol{\Omega}} \boldsymbol{\phi}(\boldsymbol{\theta})\boldsymbol{\mu}.$$

The primary variational formulation of BVPs of heat conduction is obtained by inserting FOURIER's law in the virtual thermal work of Theorem 1, to get the variational inequality

$$\langle d^+\boldsymbol{\Phi}(\nabla\theta), \nabla\delta\theta \rangle \geq \int_{\boldsymbol{\Omega}} p\delta\theta\boldsymbol{\mu} + \oint_{\partial \mathrm{PAT}(\boldsymbol{\Omega})} \partial q \mathrm{VAL}(\delta\theta)\partial\boldsymbol{\mu}, \quad \forall \delta\theta \in \mathrm{CONF},$$

in which the basic unknown is the admissible temperature field $\theta \in \mathrm{ADM}$. This is equivalent to the minimum principle for the functional

$$\int_{\boldsymbol{\Omega}} \boldsymbol{\phi}(\nabla\theta)\boldsymbol{\mu} - \int_{\boldsymbol{\Omega}} p\theta\boldsymbol{\mu} - \oint_{\partial \mathrm{PAT}(\boldsymbol{\Omega})} \partial q \mathrm{VAL}(\theta)\partial\boldsymbol{\mu}, \quad \theta \in \mathrm{CONF}.$$

The conjugate global convex potential is given by

$$\boldsymbol{\Psi}(\mathbf{q}) := \int_{\boldsymbol{\Omega}} \boldsymbol{\psi}(\mathbf{q})\boldsymbol{\mu},$$

with $\boldsymbol{\psi}: V \to \mathcal{R}$ and $\boldsymbol{\Psi}: \mathcal{L}^2(\boldsymbol{\Omega}; V) \to \mathcal{R}$ conjugate to $\boldsymbol{\phi}: V \to \mathcal{R}$ and $\boldsymbol{\Phi}: \mathcal{L}^2(\boldsymbol{\Omega}; V) \to \mathcal{R}$, according to the Fenchel–Legendre transform [14]. Substituting the converse of the global heat conduction law

$$\langle d^+\boldsymbol{\Psi}(\mathbf{q}), \delta\mathbf{q} \rangle \geq \langle \boldsymbol{\theta}, \delta\mathbf{q} \rangle, \quad \forall \delta\mathbf{q} \in \mathcal{L}^2(\boldsymbol{\Omega}; V),$$

in the thermal compatibility condition of Theorem 2, we get the complementary variational formulation

$$\langle d^+\boldsymbol{\Psi}(\mathbf{q}), \delta\mathbf{q} \rangle \geq \oint_{\partial \mathrm{PAT}(\boldsymbol{\Omega})} \mathbf{g}(\delta\mathbf{q}, \mathbf{n})\mathrm{VAL}\bar{\theta}\partial\boldsymbol{\mu}, \quad \forall \delta\mathbf{q} \in \mathrm{Ker}\nabla^*_{\mathrm{CONF}},$$

in which the basic unknown is the cold flow vector field $\mathbf{q} \in \mathrm{EQUIL}$. This equivalent to the minimum principle for the functional

$$\int_{\boldsymbol{\Omega}} \boldsymbol{\psi}(\mathbf{q})\boldsymbol{\mu} - \int_{\partial \mathrm{PAT}(\boldsymbol{\Omega})} \mathbf{g}(\mathbf{q}, \mathbf{n})\mathrm{VAL}\bar{\theta}\partial\boldsymbol{\mu}, \qquad \mathbf{q} \in \mathrm{EQUIL}.$$

Computational issues may lead to prefer a mixed formulation in which the temperature scalar field $\theta \in \mathrm{ADM}$ and the cold flow vector field $\mathbf{q} \in \mathcal{L}^2(\boldsymbol{\Omega}; V)$ are assumed as basic unknowns. Accordingly, the boundary value problem of heat conduction is formulated as a mixed variational inequality

$$\begin{cases} \int_{\boldsymbol{\Omega}} \mathbf{g}(\mathbf{q}, \nabla\delta\theta)\boldsymbol{\mu} = \int_{\boldsymbol{\Omega}} p\delta\theta\boldsymbol{\mu} + \oint_{\partial \mathrm{PAT}(\boldsymbol{\Omega})} \langle \partial q, \mathrm{VAL}\delta\theta \rangle \partial\boldsymbol{\mu}, \quad \forall \delta\theta \in \mathrm{CONF}, \\ \int_{\boldsymbol{\Omega}} \mathbf{g}(d^+\boldsymbol{\psi}(\mathbf{q}), \delta\mathbf{q})\boldsymbol{\mu} \geq \int_{\boldsymbol{\Omega}} \mathbf{g}(\nabla\theta, \delta\mathbf{q}), \boldsymbol{\mu}, \qquad \forall \delta\mathbf{q} \in \mathcal{L}^2(\boldsymbol{\Omega}; V), \end{cases}$$

equivalent to a saddle point principle for the functional

$$F(\mathbf{q},\theta) := -\boldsymbol{\Psi}(\mathbf{q}) + \int_{\boldsymbol{\Omega}} \mathbf{g}(\mathbf{q},\nabla\theta)\boldsymbol{\mu} - \int_{\boldsymbol{\Omega}} p\theta\boldsymbol{\mu} - \oint_{\partial \mathrm{PAT}(\boldsymbol{\Omega})} \partial q \mathrm{VAL}(\theta)\partial\boldsymbol{\mu} \quad \begin{cases}\theta \in \mathrm{CONF},\\ \mathbf{q} \in \mathcal{L}^2(\boldsymbol{\Omega}; V).\end{cases}$$

Classical formulations of heat conduction, with the relevant potentials differentiable, or even quadratic, are recovered by considering the usual bilateral derivative and changing the inequalities to equalities.

5 Conclusions

The First Principle of Thermodynamics has been formulated, by a straight but tricky reasoning, as a variational condition in which the test fields are piecewise constant virtual temperature fields. Based on the theorem of Lagrange multipliers, the virtual thermal work theorem provides the existence of a heat flow vector field in the body. In classical treatments (e.g. [18–20,31] the existence of a heat flow is instead assumed as a separate axiom of Continuum Thermodynamics. The primary and complementary variational formulations of the first principle have been shown to lead in a direct way to governing principles of heat conduction and to the related computational methods. The treatment performed in this article may be similarly applied to any balance law in Continuum Physics. For instance, the principle of mass conservation leads to a variational formulation in which Lagrange multipliers are vector fields describing the mass flow through a control volume [32].

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