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Author for correspondence:
Paolo Maria Mariano
e-mail: paolomaria.mariano@unifi.it

Influence of material microstructures on heat transfer: universal effects

Daniele La Pegna[1] and Paolo Maria Mariano[2]

[1]Scuola Normale Superiore, Piazza dei Cavalieri 7, I-56126 Pisa, Italy
[2]DICEA, Università di Firenze, via Santa Marta 3, I-50139 Firenze, Italy

PMM, 0000-0002-3841-8408

We develop a nonlinear framework in which finite-speed heat propagation emerges naturally from microstructural effects, even without invoking ad hoc modifications of Fourier's law. A structural invariance requirement of the Clausius–Duhem inequality under general diffeomorphism-based observer changes is adopted to derive thermodynamically consistent evolution equations that incorporate manifold-valued phase fields to represent internal microstructure. Internal constraints between temperature and microstructural variables give rise to non-linear hyperbolic structures, reflecting wave-like thermal dynamics. We discuss the theoretical foundations of this viewpoint not considering strain and propose appropriate simulations to corroborate the theoretical findings. The key point of our work is that, within the framework we establish, the derived microstructural effects on heat transfer are universal in the sense that they do not depend on specific microstructural shapes.

1. Introduction

Fourier's law links the heat flux $\mathfrak{q}$ and the temperature gradient through a factor k, the conductivity, here assumed to be scalar and constant, that is, $\mathfrak{q} = -k\nabla\theta$, where θ is the absolute temperature. With this law and in the absence of sources, the balance of energy reduces to the classical parabolic equation $c_v\dot{\theta} = k\Delta\theta$, where c_v is the specific heat at constant volume.

Although widely used in technology, the scheme foresees heat propagation at infinite speed, which contradicts the everyday experience of heating bodies.

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Indeed, in a one-dimensional ambient, with $\hat{k} = k/c_v$ and under conditions $\theta(x,0) = 0$, for $x \neq 0$ and $\theta(0,0) = 1$, a fundamental solution of the above heat equation is $\theta(x,t) = (4\pi\hat{k}t)^{-1/2} \exp(-x^2/(4\hat{k}t))$, so that for $|x|$ as large as we wish and for any $t > 0$, we have $\theta(x,t) > 0$. Hence, the equation predicts that heat propagates from $x = 0$ to any $x \neq 0$ in an arbitrarily small interval of time; thus, at infinite speed.

The history of attempts aimed at overcoming such a physical inconsistency is not trivially branched. Different but not necessarily mutually excluding viewpoints have been proposed. They are based on at least one of the following claims:

(i) Intended as a constitutive equation, Fourier's law is insufficient. The description of non-equilibrium states requires to be refined.
(ii) The relation between heat flux and temperature is, instead, a balance law, not a constitutive structure, and should be derived as such.
(iii) The physical evidence that temperature variations propagate at finite speed depends on the presence of temperature-dependent microstructures in real bodies.

The present work focuses on the third claim.

To account for "independent" microstructural events on a low spatial scale, say λ, that influence global behaviour, a natural way is to introduce appropriate descriptors ν of the microstructural morphology (*phase fields*), which depend on space and time. They are considered observable. The relevant bulk and contact actions are defined by the power they perform in a time rate of ν. These interactions satisfy balance equations that can be postulated in the local form [1] or weak form [2], or *derived* from invariance requirements [3–7]. The microstructural actions enter the balance of energy. Their presence determines finite speed heat propagation when the phase field is subject to appropriate internal constraints. Those of interest for this aspect are of twofold nature: (i) ν is a differentiable function of the heat flux or a perturbation of it with respect to the Fourier law; (ii) ν is a differentiable function of θ. In the former case, the balance of microstructural interactions can be reduced, as proven in [8,9] (see also [10]), to the Guyer-Krumhansl equation, originally derived from the Boltzmann equation [11,12]. In the latter case, from the balance of energy, we may derive further different specific models of hyperbolic (that is, finite speed) heat propagation [13]. Considering temperature-dependent phase fields is appropriate, e.g. for ceramics based on strontium titanate, the class $Ba_{1-x}Sr_xTiO_3$. They experience temperature-induced polarization even in the absence of strain [14]. Also, heating-induced polarization occurs in quartz, lead titanate ($PbTiO_3$), barium titanate ($BaTiO_3$), lead zirconate titanate and other materials (pertinent data are in [15]). This effect is what we commonly call *pyroelectricity*: (meta)equilibrium of polar crystals in a relaxed state is altered by thermal atomic fluctuations with the consequent appearance of electrical polarization—-bound charges on the crystal surface [16, ch. 4]. In addition, symmetry addresses polarization [17]. In all these cases, ν represents the polarization vector and the internal constraint $\nu = \gamma(\theta)$ applies, with γ a differentiable vector-valued map.

Temperature-dependent polarization also occurs in the chiral smectic phases C* and H* of liquid crystals. For them, in addition to the polarization vector field, other phase fields must be added to describe the layered arrangement of stick molecules tilted with respect to the normal layer (smectic C* phase; data are in [18]) or arrangements in which the average molecular direction follows a short-pitch helix (smectic H* phase) [19].

Besides these special prominent cases, the effect we discuss here is universal in the sense that it is independent of the specific description of the microstructure. Thus, our analyses do not exploit specific datasets; they have only conceptual character.

In particular, in §2 we provide an account of other conceptual views on the propagation of heat at finite speed, with the aim of placing our work in a perspective that allows appropriate comparisons. Then, in §3 we discuss again the theoretical foundations of our proposal in a way different from a previous analysis presented in [13]. Indeed, in [13], the balance of microstructural

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interactions is derived from an invariance requirement for the external power of actions under SO(3)-based changes of observers. That approach does not cover the case in which the phase field is scalar. Instead, the view adopted here also covers the scalar case. It is based on a requirement of structure-invariance for the second law, a viewpoint introduced in [7] with anticipation in [20]. The main focus of this paper is, indeed, a refinement of the general proposal in [13]. Linear and nonlinear *special* offspring of this are analysed in §4 and 5. We provide for them relevant numerical simulations. Section 6 collects concluding remarks.

2. Notation and a few preliminary notions

As for the notation used, we shall adopt an interposed dot to indicate duality pairing; when we refer to orthonormal frames of reference, as we do in the numerical analyses below, the interposed dot can be identified with the scalar product. A superposed dot will indicate the time derivative. Always concerning notations, in what follows, we first develop the analysis in a generic frame of reference; then, we restrict the treatment to an orthonormal frame of reference. In the former case, the operator D will indicate a derivative with respect to the space variable; it will coincide with the gradient ∇ in an orthonormal frame of reference, while generically D and ∇ are distinguished by the connection.

Specifically, consider a scalar product $\langle \cdot, \cdot \rangle$ in $\mathbb{R}^3$ and a basis $\{\mathbf{e}_i\}$, with associated metric $\boldsymbol{g}$ whose components are $g_{ij} = \langle \mathbf{e}_i, \mathbf{e}_j \rangle$. Let also $\{\mathbf{e}^j\}$ be the dual basis of $\{\mathbf{e}_i\}$ defined—in terms of the duality pairing—by $\mathbf{e}^i \cdot \mathbf{e}_j = \delta^i_j$, where δ^i_j is the Kronecker symbol; $i, j = 1, 2, 3$. With $x \longmapsto \mathsf{v} := \tilde{\mathsf{v}}(x) \in \mathbb{R}^3$ a differentiable vector function, for all frames of reference we have $D\mathsf{v} = \frac{\partial \mathsf{v}^i}{\partial x^j} \mathbf{e}_i \otimes \mathbf{e}^j$ while, at least for a specific choice of $\{\mathbf{e}_i\}$, we have $\nabla \mathsf{v} = (\partial \mathsf{v}^i / \partial x)^j \mathbf{e}_i \otimes \mathbf{e}_j$, where the convection summation over repeated indices is adopted here and in the rest of this paper. In other words, $D\mathsf{v}$ is always a 1-covariant, 1-contravariant linear operator, while there exists at least one frame of reference in which $\nabla \mathsf{v}$ is a 2-contravariant operator associated with $D\mathsf{v}$ by the inverse metric $\boldsymbol{g}^{-1}$, with components g^{ij}, that is, $(D\mathsf{v})\boldsymbol{g}^{-1} = \nabla \mathsf{v}$. The product $\boldsymbol{g} D\mathsf{v} \cdot \nabla \mathsf{v}$ is naturally defined: the result is the value taken over $\nabla \mathsf{v}$, an element of a linear space, by an element of the relevant dual space, that is, $D\mathsf{v}$; so, the interposed dot means, indeed, $\boldsymbol{g} D\mathsf{v}(\nabla \mathsf{v})$. When we consider a specific scalar product, $\langle \nabla \mathsf{v}, \nabla \mathsf{v} \rangle = g_{jk} (\nabla \mathsf{v})^{ki} g_{ki} (\nabla \mathsf{v})^{ij} = g_{jk} (D\mathsf{v})^k_i (\nabla \mathsf{v})^{ij}$. For general frames of reference, we have, instead, $(\nabla \mathsf{v})^{ij} = (D\mathsf{v})^i_k g^{kj} + \Gamma^i_{kh} \mathsf{v}^h g^{kj}$, where Γ indicates the connection. When $\boldsymbol{g}$ depends smoothly on x, the Levi-Civita connection associated with it is given by $\Gamma^i_{kh} = \frac{1}{2} g^{ij} (D_\alpha g_{kj} + D_h g_{kj} - D_j g_{kh})$. Here, we consider ∇ as $D^\sharp = D\boldsymbol{g}^{-1}$, that is, we avoid referring to covariant derivatives ∇ and consider ∇ as the vector operator associated with the derivative D (with covector component) in at least one frame of reference.

Finally, $|\cdot|$ will be used to indicate the absolute value of scalars, the modulus of vectors, the Frobenius norm of second or higher order tensors.

3. A short account of other attempts to overcome Fourier's paradox

(a) Looking at Fourier's law in terms of constitutive structures

Commenting on the description of heat transfer, in 1872 Maxwell wrote as follows [21, p. 240]. "[. . .] in calculating the temperature of the point P, we must take into account the temperature of every other point Q, however distant and how short the time may be during which the propagation of heat has been going on. Hence, in a strict sense, the influence of a heated part of the body extends to the most distant parts of the body in an incalculably short time, so that it is impossible to assign to the propagation of heat a definite velocity." Then, he concluded that "the sensible propagation of heat, so far from being instantaneous, is an excessively slow process, and that the time required to produce a similar change of temperature in two similar 'systems of different dimensions is proportional to the square of the linear dimensions."

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In 1948 [22], Cattaneo analysed the problem starting from Boltzmann's analysis of the transport in a gas of a generic quantity with an average value (say) G [23, p. 69]. When we identify G with θ, the path indicated by Boltzmann leads to Fourier's law. We have no evidence that Cattaneo had read Maxwell's 1872 remarks; in any case he considered for G a finite delay. Thus, Cattaneo obtained an evolution equation for the heat flux that reads as

$$\hat{\tau}\dot{\mathfrak{q}} + \mathfrak{q} = -k\nabla\theta. \tag{3.1}$$

Maxwell had already obtained a similar expression [24, eqn. 143], but then he cast out $\dot{\mathfrak{q}}$, considering it to be negligible. Equation (3.1) is a first-order approximation of $\mathfrak{q}(x, t-\hat{\tau}) = -k\nabla\theta(x,t)$, under the assumption that $\mathfrak{q}$ is differentiable. A natural extension foresees the introduction of two delays, namely $\hat{\tau}_q$ and $\hat{\tau}_T$ such that $\mathfrak{q}(x, t-\hat{\tau}_q) = -k\nabla\theta(x, t-\hat{\tau}_T)$, as in [25,26]. However, accepting this dual phase lag view, the first and second order expansion of $\mathfrak{q}(x, t-\hat{\tau}_q) = -k\nabla\theta(x, t-\hat{\tau}_T)$ could admit solutions that foresee negative values for θ, as shown in [27,28].

Apart from these last aspects, the Maxwell-Cattaneo scheme, namely the combination of equation (3.1) with the energy balance, has so far stimulated a large body of work (see the critical review in [29–31]). It requires knowledge of both $\theta(x,0)$ and $\dot{\theta}(x,0)$, two data points that are difficult to realize in pairs as arbitrary entities in experiments.

In 1968, Gurtin and Pipkin proposed to consider a distributed time delay [32]; they presumed that, for a rigid conductor, free energy, entropy, and heat flux have to be considered as functionals depending on temperature, its history, and the history of its gradient. For the heat flux they thus suggested the integral form

$$\mathfrak{q}(x,t) = -\int_{-\infty}^{t} \mathcal{K}(t-t')\nabla\theta(x,t')\,\mathrm{d}t', \tag{3.2}$$

with a bounded kernel $\mathcal{K}(0)$. By refining the approach in 1989, Joseph and Preziosi considered Jeffery's-type kernels made by the sum of a bounded operator and a Dirac delta [29]. Cattaneo's equation [22] emerges as a special case of the integral approach. However, a question is as follows: How can we concretely know the memory of a natural material, or one newly manufactured?

(b) Further descriptions of non-equilibrium states

The condition $\mathfrak{q} \neq 0$ is pertinent to non-equilibrium states. In discussing Brillouin's theory of specific and latent heats, Truesdell and Toupin considered the introduction of non-equilibrium fluxes in the list of state variables [33, §250]. In 1967, Müller [34] adopted the idea for the description of heat transfer and suggested including fluxes as $\mathfrak{q}$ itself and the dissipative stress component (viscous-type) in the list of state variables. There was a subsequent need to introduce a non-equilibrium entropy with an associated notion of temperature. The connection between equilibrium and nonequilibrium temperatures was then a pertinent question [35, p. 171] (see also [36]).

In 1972, Müller proved [37] that the constitutive structures he proposed for the heat conduction in fluids fail to be objective in the sense that a spin term emerges when we consider isometric changes of observers. Thus, Müller concluded rejecting the universal validity of the objectivity principle for constitutive equations (indeed, the heat flux fails to be objective, as we can show by deriving it from the Boltzmann equation, but the question raised in Müller's work was much more general). We could formally change the notion of objectivity by admitting the occurrence of these spin-type terms, but a consequent question would be to find an unquestionable reason for such a change. Also, in the previous scheme, the resulting equations are not always genuinely hyperbolic [34], so they do not necessarily cover the whole scenario of shocks and second sound; regularity of initial data does not necessarily imply analogous regularity of the solutions.

Further non-observable variables (so-called *internal*) can be considered as peculiar descriptors of non-equilibrium states [38]; they are assumed to satisfy phenomenological evolution laws, which can be selected so as to determine hyperbolicity, with the consequent finite-speed heat propagation [39]. Defined to be non-observable, internal variables are insensitive to observer

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changes; so, as such, they do not contribute to loss of objectivity. A question is whether their evolution laws can be derived from first principles (and what kind of principles), or they are postulated only on the basis of phenomenological suggestions or mere matter of convenience.

(c) Evolution laws for the heat flux as balance equations

At the beginning of the 1980s, Bressan [40] and Ruggeri [35,41] independently proposed to consider the evolution laws for the heat flux and the dissipative component of the stress as true field equations. In this way, these laws would not necessarily be subject to the objectivity principle. If we accept the view, the physical origin of such a character should be clarified.

A shortcut answer could be that one accepts from the outset a system of balance equations with hyperbolic character. So did Liu and Müller in 1983, looking at "a phenomenological theory of dilute gases" [42, p. 287]. Taking moments of the distribution function of placement and velocities, which is the unknown variable in the Boltzmann equation, they obtained a hierarchy of hyperbolic field equations overcoming Grad's 13 moments procedure. The treatises [43,44] provide a critical account of the relevant literature.

When some suitable relaxation time goes close to zero and can be neglected, the moment expansion of the velocity distribution provides Fourier's, Fick's, and Darcy's laws, the stress dissipative component linear dependence on the velocity gradient in the presence of viscous effects, and a diffusion equation for multi-temperature mixtures, all in a hierarchy of balance equations. The procedure "preserves the entropy principle at least for processes not far from equilibrium" [45, p. 609]. However, it does not include cases in which the stress has an energetic-type component, such as in the presence of (say) elastic molecular bonds. In addition, Boillat and Ruggeri crucially showed in 1997 [46] that in a classical space-time the hierarchy of balance laws emerging by the expansion in terms of moments of the velocity distribution tends to recover the parabolic character of the classical heat transfer description, as the number of moments increases.

(d) Other offspring from the Boltzmann equation and the effects of random walks

A different view on the Boltzmann equation can be adopted when we consider that in the isotropic dispersionless case temperature deviation and heat flux are related to the zero-eigenvalue eigenfunctions of the normal-process collision operator. So, solving the linearized Boltzmann equation for the pure phonon field in terms of eigenvectors of the collision operator, Guyer and Krumhansl obtained in 1966 [11,12] an evolution equation for the heat flux that explicitly incorporates the phonon mean free path into the governing equations and provides a link between kinetic and continuum models on the basis of well-defined physical parameters. This equation has been extensively analysed and falls within the scheme that we discuss here when the phase field is linked to the heat flux by an internal constraint [8].

Diffusion can also be related to a random walk. The probabilities of reaching a place for the m and $m+1$ steps are related by a recursion formula. For sufficiently large steps, the probability itself can be replaced by a continuous function whose expansion (at least in a one-dimensional ambient) leads to a Fokker-Planck equation augmented by the second time derivative of the unknown probability. When the random scattering is isotropic, such an equation reduces to the classical heat equation varied by a second time derivative. Thus, as shown by Weymann, it provides the random basis of a hyperbolic variant of the heat equation postulated by Morse & Feshbach [47]. A connection among Cattaneo's scheme, Guyer and Krumhansl's approach, and the viewpoint we adopt here can be established, as in [8,9,48]. The main idea is that a refined description of the matter evidences interactions at different scales; they give the necessary contribution to overcome Fourier's paradox. This refinement is obtained by introducing observable fields in the way that we explain below.

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4. Foundations of the description of microstructural effects on heat propagation

Let $\mathcal{B} \subset \mathbb{R}^3$ be an open connected bounded set with non-zero volume and a surface-like boundary $\partial\mathcal{B}$, oriented by the outward unit normal n everywhere but a finite number of corners and edges. We call a *part* of $\mathcal{B}$ any connected subset $\mathfrak{b}$ of $\mathcal{B}$ with non-vanishing volume and surface-like boundary $\partial\mathfrak{b}$ oriented as $\partial\mathcal{B}$.

(a) Observable fields

We do not consider here macroscopic deformations. The body that occupies $\mathcal{B}$ has a microstructure endowed with its own internal degrees of freedom at a microscopic scale λ, whose definition depends on specific cases. In every place x and time $t \in [t_0, t_1]$ these degrees of freedom are relative to the material element that occupies x. They are represented by a differentiable phase field

$$\tilde{\nu} : \mathcal{B} \times [t_0, t_1] \longmapsto \mathcal{M}, \tag{4.1}$$

where $\mathcal{M}$ is a finite-dimensional Riemannian manifold, generically not embedded in any linear space. We write ν for the value $\tilde{\nu}(x, t)$. This view is sufficiently general to allow the description of wide classes of material structures—indeed, the variable ν can be a scalar, a vector, a tensor, or any other geometrical object belonging to a finite-dimensional Riemannian manifold. The specification of the nature of ν depends on specific physical circumstances (in the case of pyroelectric materials, ν is the polarization vector). Due to the variety of possible cases and with the intention of providing a view as comprehensive as possible, we do not specify the nature of ν, leaving it generic. The type of analysis that we develop allows this approach.

(b) Observers

As already declared, we consider $\nu = \tilde{\nu}(x, t)$ as *observable*. In the present scheme, an observer is the choice of reference frames over $\mathbb{R}^3$, the manifold $\mathcal{M}$ and a time scale. We consider changes of observers in the physical space described by generic diffeomorphisms of $\mathbb{R}^3$ onto itself, whose set is indicated by $\mathrm{Diff}(\mathbb{R}^3, \mathbb{R}^3)$. Precisely, we take a map $[0, +\infty) \ni s \mapsto \mathrm{f}_s \in \mathrm{Diff}(\mathbb{R}^3, \mathbb{R}^3)$, which we assume to be smooth and such that $\mathrm{f}_0 = id$, where id is the identity in $\mathrm{Diff}(\mathbb{R}^3, \mathbb{R}^3)$. We define the flux $\mathrm{f}_{t,s} := \mathrm{f}_t \circ \mathrm{f}_s^{-1}$ and indicate by $\bar{\mathrm{v}}$ the derivative

$$\bar{\mathrm{v}} := \left.\frac{\mathrm{d}\mathrm{f}_{t,s}}{\mathrm{d}s}\right|_{t=s}.$$

Since ν represents on $\mathcal{M}$ observable degrees of freedom that are in the physical space, we need to represent over $\mathcal{M}$ how different observers record ν. To this end, following [5,7], we refer to a class of differentiable homomorphisms $\tilde{\mathcal{F}} := \{\phi : \mathrm{Diff}(\mathbb{R}^3, \mathbb{R}^3) \longrightarrow \mathrm{Diff}(\mathcal{M}, \mathcal{M})\}$ such that $\phi(id) = \mathrm{id}$, where id is the identity in $\mathrm{Diff}(\mathcal{M}, \mathcal{M})$, the Lie group of diffeomorphisms of $\mathcal{M}$ onto itself. Every $\phi \in \tilde{\mathcal{F}}$ characterizes a class of changes of observers. Through the elements of $\tilde{\mathcal{F}}$, at every t the flux $\mathrm{f}_{t,s}$ induces a smooth curve over $\mathrm{Diff}(\mathcal{M}, \mathcal{M})$, that is, $[0, +\infty) \ni s \mapsto \phi_{\mathrm{f}_{t,s}} \in \mathrm{Diff}(\mathcal{M}, \mathcal{M})$; thus, at every t, a smooth curve $s \mapsto \nu_{t,s} := \phi_{\mathrm{f}_{t,s}}(\nu) \in \mathcal{M}$. By construction, $\nu_{t,s}$ is differentiable with respect to s and we write υ for the derivative defined by

$$\upsilon := \left.\frac{\mathrm{d}\nu_{t,s}}{\mathrm{d}s}\right|_{t=s}. \tag{4.2}$$

Thus, for the time rate of the microstructure, we consider the transformation rule

$$\dot{\nu} \longmapsto \dot{\nu}^{\circ} := \dot{\nu} + \upsilon \tag{4.3}$$

under a change of observer, as described above. We strictly assume that $|\upsilon|$ is *bounded* at all t and is differentiable with respect to x.

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When $\mathsf{f}_{t,s}$ is an element of $SO(3) \subset \mathrm{Diff}(\mathbb{R}^3, \mathbb{R}^3)$, we have the following:

$$\bar{\mathrm{v}} = \left.\frac{\mathrm{d}Q_s}{\mathrm{d}s}\right|_{s=0} = \left.\frac{\mathrm{d}\exp(s\mathbf{e}q)}{\mathrm{d}s}\right|_{s=0} = \mathbf{e}q,$$

where $\mathbf{e}$ is Ricci's symbol and $q \in \mathbb{R}^3$ is the axial vector of the skew-symmetric tensor $q\times = \mathbf{e}q$. Thus, we obtain

$$v = \mathcal{A}(\nu)q, \quad \text{with} \quad \mathcal{A}(\nu) := \left.\frac{\mathrm{d}\phi_{Q_s}(\nu)}{\mathrm{d}Q_s}\right|_{s=0} \mathbf{e}.$$

$\mathcal{A}(\nu)$ is a linear operator from $\mathbb{R}^3$ to $T_\nu\mathcal{M}$, that is, in short, $\mathcal{A}(\nu) \in \mathrm{Hom}(\mathbb{R}^3, \mathcal{T}_\nu\mathcal{M})$. The transformation rule (4.3) thus reads

$$\dot{\nu} \longmapsto \dot{\nu}^\diamond = \dot{\nu} + \mathcal{A}(\nu)q. \tag{4.4}$$

For example, when ν is a three-dimensional vector, as when it represents the polarization in pyroelectric materials, then $\phi \equiv \mathsf{id}$ and we have

$$\mathcal{A}(\nu) = \left.\frac{\mathrm{d}(Q_s\nu)}{\mathrm{d}Q_s}\right|_{s=0} \mathbf{e} = -\nu \times .$$

We can obtain the same result in another way. With ν still a three-dimensional vector, let $\nu' = Q(t)\nu$ be the value recorded by the observer $\mathcal{O}'$ that rotates with respect to $\mathcal{O}$ whose measure of the time rate is $\dot{\nu}$. Consider the map $t \longmapsto Q(t)$ to be smooth. Thus, we compute $\dot{\nu}' = \dot{\nu} + \dot{Q}\nu$. By pulling $\dot{\nu}'$ into $\mathcal{O}$, we obtain a new vector $\dot{\nu}^\diamond := Q^\mathsf{T}\dot{\nu}'$ given by $\dot{\nu}^\diamond = \dot{\nu} + q \times \nu$, which is (4.4).

(c) Actions

Actions on a generic body part $\mathfrak{b}$ have bulk and contact nature. They are defined by the external power $\mathcal{P}^{\mathrm{ext}}_{\mathfrak{b}}$ that they perform in the time rate $\dot{\nu}$, a power given by

$$\mathcal{P}^{\mathrm{ext}}_{\mathfrak{b}}(\dot{\nu}) := \int_{\mathfrak{b}} \boldsymbol{\beta}^\ddagger \cdot \dot{\nu}\, \mathrm{d}x + \int_{\partial\mathfrak{b}} \boldsymbol{\tau}_\partial \cdot \dot{\nu}\, \mathrm{d}\mathcal{H}^2(x), \tag{4.5}$$

where $\mathrm{d}\mathcal{H}^2$ is the two-dimensional Hausdorff measure (area), $\boldsymbol{\beta}^\ddagger$ represents bulk actions and is generically assumed to be the sum of inertial and noninertial components, say $\boldsymbol{\beta}^\ddagger = \beta + \beta^{in}$, where the superscript *in* means inertial, while $\boldsymbol{\tau}_\partial$ represents contact microstructural actions that depend on x, t and the boundary $\partial\mathfrak{b}$, a circumstance indicated by the subscript ∂.

(d) The first law of thermodynamics

The power $\mathcal{P}^{ext}_{\mathfrak{b}}$ enters the first law of thermodynamics. We indicate by e the internal energy density per unit volume and write the first law of thermodynamics as

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathfrak{b}} e\, \mathrm{d}x - \mathcal{P}^{\mathrm{ext}}_{\mathfrak{b}}(\dot{\nu}) - \int_{\mathfrak{b}} \tilde{r}\, \mathrm{d}x + \int_{\partial\mathfrak{b}} \mathfrak{q} \cdot n\, \mathrm{d}\mathcal{H}^2(x) = 0, \tag{4.6}$$

where $\tilde{r}$ is the heat source, and $\mathfrak{q} = \tilde{\mathfrak{q}}(x,t)$ once again is the *heat flux* through the boundary $\partial\mathfrak{b}$.

We assume $\tilde{\mathfrak{q}} \in C^1(\mathcal{B}, \mathbb{R}^3) \cup C(\bar{\mathcal{B}}, \mathbb{R}^3)$ so that the balance (4.6) becomes

$$\int_{\mathfrak{b}} \dot{e}\, \mathrm{d}x - \mathcal{P}^{ext}_{\mathfrak{b}}(\dot{\nu}) - \int_{\mathfrak{b}} (\tilde{r} - \mathrm{div}\mathfrak{q})\, \mathrm{d}x = 0. \tag{4.7}$$

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(e) The second law of thermodynamics

We indicate by $\eta = \tilde{\eta}(x,t)$ the entropy density per unit volume and assume that $\tilde{\eta}$ is continuous and continuously differentiable in time, while the derivatives of $\tilde{\eta}$ are bounded over $\mathcal{B}$ at every t. The entropy inequality reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathfrak{b}} \eta \,\mathrm{d}x + \int_{\partial\mathfrak{b}} \ell_\partial \,\mathrm{d}\mathcal{H}^2(x) - \int_{\mathfrak{b}} \mathfrak{s}\,\mathrm{d}x \geq 0 \tag{4.8}$$

that we presume to hold for any choice of $\mathfrak{b}$. The boundary term ℓ_∂ is a *scalar entropy flux*, while $\mathfrak{s}$ is an *entropy source*. In more detail, ℓ_∂ depends on x, t, and the boundary $\partial\mathfrak{b}$.

If also $\mathfrak{s}$ is bounded over $\mathcal{B}(t)$ at every t as $\dot{\eta}$ is by assumption, we get

$$\left|\int_{\partial\mathfrak{b}} \ell_\partial \,\mathrm{d}\mathcal{H}^2(x)\right| \leq C\mathrm{vol}(\mathfrak{b}),$$

where C is a constant and $\mathrm{vol}(\mathfrak{b})$ is the volume of $\mathfrak{b}$. Thus, by the Cauchy theorem we find that ℓ_∂ depends on $\partial\mathfrak{b}$ only through n at all places in which n is well-defined, namely there exists a function $\tilde{\ell}$ such that $\ell_\partial(x,t) = \tilde{\ell}(x,t,n) = -\tilde{\ell}(x,t,-n)$. Moreover, there exists a *vector entropy flux* $\tilde{\mathfrak{h}}$ with values $\mathfrak{h} = \tilde{\mathfrak{h}}(x,t)$ such that

$$\ell_\partial(x,t) = \tilde{\ell}(x,t,n) = \tilde{\mathfrak{h}}(x,t)\cdot n = \mathfrak{h}\cdot n.$$

Consequently, we write the entropy inequality as

$$\int_{\mathfrak{b}} \dot{\eta}\,\mathrm{d}x + \int_{\partial\mathfrak{b}} \mathfrak{h}\cdot n \,\mathrm{d}\mathcal{H}^2(x) - \int_{\mathfrak{b}} \mathfrak{s}\,\mathrm{d}x \geq 0. \tag{4.9}$$

We take $\tilde{\mathfrak{h}}(\cdot,t) \in C^1(\mathcal{B},\mathbb{R}^3)\cup C(\bar{\mathcal{B}},\mathbb{R}^3)$ and assume that both $\dot{\eta}$ and s are continuous; therefore, due to the arbitrariness of $\mathfrak{b}$, we get the *local entropy inequality*

$$\dot{\eta} \geq \mathfrak{s} - \mathrm{div}\mathfrak{h} \tag{4.10}$$

in $\mathcal{B}$. Thus, we assume that

$$\mathfrak{s} = \frac{\tilde{r}}{\theta} \quad \text{and} \quad \mathfrak{h} = \frac{\mathfrak{q}}{\theta} + \bar{\boldsymbol{\omega}},$$

where $\bar{\boldsymbol{\omega}}$ is an additional flux of entropy. The presence of $\bar{\boldsymbol{\omega}}$ has been first postulated for generic bodies in [37]. Here, we adopt that proposal by explicitly attributing its presence to loss of information induced by microstructural changes.

By inserting these relations into the local entropy inequality (4.10), we get

$$\theta\dot{\eta} + \theta\mathrm{div}\bar{\boldsymbol{\omega}} - \frac{1}{\theta}\mathfrak{q}\cdot D\theta \geq \tilde{r} - \mathrm{div}\mathfrak{q}.$$

Thus, once we introduce Helmoltz's *free energy density* $\psi := e - \theta\eta$, we find a version of the Clausius-Duhem inequality that is appropriate for what we are discussing here:

$$\int_{\mathfrak{b}} (\dot{\psi} + \eta\dot{\theta})\,\mathrm{d}x - \mathcal{P}^{\mathrm{ext}}_{\mathfrak{b}}(\dot{v}) + \int_{\mathfrak{b}} (\theta^{-1}\mathfrak{q}\cdot D\theta - \theta\mathrm{div}\bar{\boldsymbol{\omega}})\,\mathrm{d}x \leq 0. \tag{4.11}$$

The presence of $\bar{\boldsymbol{\omega}}$ is justified by generality. As clearly emerges from the following analyses, the microstructural effects imply heat transfer with finite speed even when $\bar{\boldsymbol{\omega}} = 0$ and the heat flux is expressed only by the Fourier law.

(f) The energy content under generic observer changes

When $\mathfrak{f}_s$ is an isometry, the free energy density is required to be invariant, that is, objective. However, when $\mathfrak{f}_s$ is a generic diffeomorphism of the physical space $\mathbb{R}^3$ on itself, the two observers it links may record a different time rate of the energy per unit volume changed by $\mathfrak{f}_s$. By indicating

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with ς a list of state variables left unspecified for the moment, we thus accept, according to [7], a transformation rule given by

$$(\dot{\psi} + \eta\dot{\theta}) \longmapsto (\dot{\psi} + \eta\dot{\theta}) + \varphi(\varsigma; D\bar{\mathrm{v}}, \upsilon, D\upsilon, \dots), \tag{4.12}$$

where the dots indicate possible dependence on higher derivatives of v and υ. By assumption, the function φ is bounded and vanishes when $\bar{\mathrm{v}} = q\times$ and $\upsilon = \mathcal{A}(\nu)q$, with q the rotation vector. These assumptions grant that the energy is objective. (Equation (4.12) corrects a failure in the symbology adopted in [7], which, however, does not affect the result in that reference.) Also, since we have assumed $\mathrm{f}_0 = id$, for $\mathfrak{q}_{\mathrm{f}_{t,s}}$ the value of the heat flux after an observer change, we have $\mathfrak{q}_{\mathrm{f}_{t,s}}|_{t=s} = \mathfrak{q}$ and $\bar{\boldsymbol{\omega}}_{\mathrm{f}_{t,s}}|_{t=s} = \bar{\boldsymbol{\omega}}$.

(g) Covariance axiom

Assume that the change of observer $\mathcal{O} \longrightarrow \mathcal{O}'$ is induced by $\mathrm{f}_s \in \mathrm{Diff}(\mathbb{R}^3, \mathbb{R}^3)$, with the consequences on $\mathcal{M}$ described above. Let $\mathfrak{A} \le 0$ be a short form of the inequality (4.11) referred to $\mathcal{O}$. For $\mathcal{O}'$ we have (formally) $\mathfrak{A}' \le 0$. The pull-back induced by f_s^{-1} of $\mathfrak{A}'$ into $\mathcal{O}$ gives $\mathfrak{A}^\circ \le 0$, with $\mathfrak{A}^\circ = \mathfrak{A} + \mathfrak{A}^\dagger$, where $\mathfrak{A}^\dagger$ involves υ in (4.3). If we reverse the process and consider the change $\mathcal{O}' \longrightarrow \mathcal{O}$ as induced by f_s^{-1}, the pull-back of $\mathfrak{A} \le 0$ into the frame defining $\mathcal{O}'$ reads $\mathfrak{A}' + \mathfrak{A}^\ddagger \le 0$, where $\mathfrak{A}^\ddagger$ *is in principle different from* $\mathfrak{A}^\dagger$. Thus, we accept the following axiom.

Axiom 4.1 (*Covariance principle* [7,20]). In any diffeomorphism-based observer change, the additional term arising after pulling back the Clausius-Duhem inequality (4.11) as evaluated by one observer in a frame defining another observer is always nonpositive and vanishes when observer changes are rigid.

Formally, the axiom prescribes $\mathfrak{A}^\dagger \le 0$ and $\mathfrak{A}^\ddagger \le 0$. Thus, if an observer $\mathcal{O}$ records that a given process does not produce energy, any other observer $\mathcal{O}'$, which deforms smoothly with respect to $\mathcal{O}$, records that the same process does not produce energy.

(h) Consequences: the local balance of microstructural actions

With the rules (4.12) and (4.3), the covariance axiom implies

$$\int_{\mathfrak{b}} \varphi \, \mathrm{d}x - \int_{\mathfrak{b}} \boldsymbol{\beta}^\ddagger \cdot \upsilon \, \mathrm{d}x - \int_{\partial\mathfrak{b}} \boldsymbol{\tau}_\partial \cdot \upsilon \, \mathrm{d}\mathcal{H}^2(x) \le 0. \tag{4.13}$$

Assume that $|\boldsymbol{\beta}^\ddagger|$ is bounded at every t over $\mathcal{B}$. There exists a constant $\bar{c} > 0$ such that

$$\left| \int_{\partial\mathfrak{b}} \boldsymbol{\tau}_\partial \cdot \upsilon \, \mathrm{d}\mathcal{H}^2(x) \right| \le \bar{c}\,\mathrm{vol}(\mathfrak{b}). \tag{4.14}$$

For simplicity, assume that $\boldsymbol{\tau}_\partial(\cdot, t)$ is continuous for every t. Cauchy's theorem applies. Thus, since υ does not depend on $\partial\mathfrak{b}$, there is a map $\tilde{\boldsymbol{\tau}}$ such that $\boldsymbol{\tau}_\partial(x,t) = \tilde{\boldsymbol{\tau}}(x,t,n)$ and $\upsilon \cdot (\tilde{\boldsymbol{\tau}}(x,t,n) + \tilde{\boldsymbol{\tau}}(x,t,-n))$ for every υ, which implies $\tilde{\boldsymbol{\tau}}(x,t,n) = -\tilde{\boldsymbol{\tau}}(x,t,-n)$, the difference living in the cotangent space to $\mathcal{M}$ at $\nu = \tilde{\nu}(x,t)$, indicated by $T^*_{\tilde{\nu}(x,t)}\mathcal{M}$. It is the space of linear forms over the tangent space $T_{\tilde{\nu}(x,t)}\mathcal{M}$ and is linear, so the sum $\tilde{\boldsymbol{\tau}}(x,t,n) + \tilde{\boldsymbol{\tau}}(x,t,-n)$ is well defined and belongs to the same space. We also find that $\upsilon \cdot \tilde{\boldsymbol{\tau}}(x,t,n)$ is linear with respect to n. So, there is a linear map $\tilde{\mathcal{S}}$ from $\mathbb{R}^3$ onto $T^*_{\tilde{\nu}(x,t)}\mathcal{M}$, with values $\mathcal{S} := \tilde{\mathcal{S}}(x,t)$, such that

$$\boldsymbol{\tau} := \tilde{\boldsymbol{\tau}}(x,t,n) = \tilde{\mathcal{S}}(x,t)n = \mathcal{S}n. \tag{4.15}$$

$\mathcal{S}$ is called a *microstress*. It is related to the scale λ, to which ν refers. Specifically, indicating by lower case Greek indices the coordinates referred to charts over $\mathcal{M}$, we have $\mathcal{S} = \mathcal{S}^A_\alpha \hat{\mathbf{e}}^\alpha \otimes \mathbf{e}_A$, with $\hat{\mathbf{e}}^\alpha$ an element of the dual basis on a chart referred to a neighborhood of $\tilde{\nu}(x,t)$, and $\mathbf{e}_A$ the *Ath* element of a vector basis in $\mathbb{R}^3$, so that $\boldsymbol{\tau}_\alpha = \mathcal{S}^A_\alpha n_A$. (The theorem can be re-obtained by weakening

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the requirement of continuity for $\boldsymbol{\tau}(\cdot,t)$.) When $\mathcal{S}(\cdot,t)$ is C^1 over $\mathcal{B}$ and continuous over $\partial\mathcal{B}$, the inequality (4.13) becomes

$$\int_{\mathfrak{b}} \varphi \,\mathrm{d}x - \int_{\mathfrak{b}} (\upsilon \cdot (\boldsymbol{\beta}^{\ddagger} + \mathrm{Div}\mathcal{S}) + \mathcal{S} \cdot D\upsilon)\,\mathrm{d}x \leq 0 \tag{4.16}$$

and must be satisfied for any choice of υ; also, $D\upsilon$ is the spatial derivative of υ. Since φ depends on υ, we can only say that in the bulk there is $z := \tilde{z}(x,t) \in T^*_{\tilde{\nu}(x,t)}\mathcal{M}$ such that

$$\boldsymbol{\beta}^{\ddagger} + \mathrm{div}\mathcal{S} = z \tag{4.17}$$

and

$$\int_{\mathfrak{b}} \varphi \,\mathrm{d}x - \int_{\mathfrak{b}} (z \cdot \upsilon + \mathcal{S} \cdot D\upsilon)\,\mathrm{d}x \leq 0. \tag{4.18}$$

Equation (4.17) is what we call *local balance of microstructural actions*. All its addenda belong at x and t to the cotangent space $T^*_{\tilde{\nu}(x,t)}\mathcal{M}$ of $\mathcal{M}$ at $\nu := \tilde{\nu}(x,t)$.

According to (4.4), assume now that $\upsilon = \mathcal{A}q$; for a while we exclude the possibility that ν is scalar. In this case, since φ vanishes under rigid observer changes and the equality sign holds by definition, the covariance axiom implies from (4.18)

$$\int_{\mathfrak{b}} (\mathcal{A}^* z + (D\mathcal{A}^*)^t \mathcal{S})\,\mathrm{d}x = 0,$$

where the asterisk and t in superscript position indicate, respectively, the formal adjoint of $\mathcal{A}$ and the minor right transposition (the one of last two components) of a third-rank tensor. The arbitrariness of $\mathfrak{b}$ implies

$$\mathcal{A}^* z + (D\mathcal{A}^*)^t \mathcal{S} = 0.$$

This last equation plays the role of local balance of microstructural couples; when ν is a scalar, we have $\mathcal{A} = 0$. The local balance of microstructural actions (4.17) also implies

$$\int_{\mathfrak{b}} \boldsymbol{\beta}^{\ddagger} \cdot \dot{\nu}\,\mathrm{d}x + \int_{\partial\mathfrak{b}} \boldsymbol{\tau} \cdot \dot{\nu}\,\mathrm{d}\mathcal{H}^2(x) = \int_{\mathfrak{b}} (z \cdot \dot{\nu} + \mathcal{S} \cdot D\dot{\nu})\,\mathrm{d}x, \tag{4.19}$$

a relation assumed to hold for any choice of the time rates involved. We indicate the right-hand term by $\mathcal{P}^{int}_{\mathfrak{b}}(\dot{\nu})$ and call it the *internal power*, so that equation (4.19) is a weak form of the balance equations. Then, from (4.7), the arbitrariness of $\mathfrak{b}$ and an assumption of continuity for the integrand imply the local energy balance

$$\dot{e} - z \cdot \dot{\nu} - \mathcal{S} \cdot D\dot{\nu} + \mathrm{div}\mathfrak{q} - r = 0. \tag{4.20}$$

We could get these results by imposing objectivity (that is, invariance with respect to the transformation $\dot{\nu} \longmapsto \dot{\nu}^{\diamond}$) on the external power alone, as done in [13]. However, such a choice would not include the case in which ν is a scalar because for it $\mathcal{A}(\nu) = 0$. The path followed here includes the scalar case and maintains distinguished balance equations from the specification of constitutive structures.

(i) Further consequences

Since the integral densities have been assumed to be continuous, due to the arbitrariness of $\mathfrak{b}$ and the identity (4.19), from the inequality (4.11) we obtain the local dissipation inequality

$$\dot{\psi} + \eta\dot{\theta} - z \cdot \dot{\nu} - \mathcal{S} \cdot D\dot{\nu} + \theta^{-1}\mathfrak{q} \cdot D\theta - \theta\mathrm{div}\bar{\boldsymbol{\omega}} \leq 0. \tag{4.21}$$

Set $\varsigma = (\nu, N, \theta)$, where $N := D\nu$ is the spatial derivative of $\tilde{\nu}(x,t)$. We assume that ψ, η, z, $\mathcal{S}$ are values of differentiable maps that depend on ς. Then, from (4.21), the arbitrariness of the time

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rates involved implies, in the standard way,

$$\eta = -\frac{\partial \psi}{\partial \theta}, \quad z = \frac{\partial \psi}{\partial \nu}, \quad \mathcal{S} = \frac{\partial \psi}{\partial N}, \quad \theta^{-1}\mathfrak{q} \cdot D\theta - \theta \mathrm{div}\bar{\boldsymbol{\omega}} \leq 0.$$

The last inequality is compatible with

$$\mathfrak{q} = -\kappa \nabla\theta + \bar{\mathfrak{q}} \tag{4.22}$$

with $\bar{\mathfrak{q}}$ a vector that satisfies the identity

$$\bar{\mathfrak{q}} \cdot D\theta = \theta^2 \mathrm{div}\bar{\boldsymbol{\omega}}, \tag{4.23}$$

where $\bar{\boldsymbol{\omega}}$ is assigned constitutively, so that

$$\bar{\mathfrak{q}} = \frac{\theta^2 \mathrm{div}\bar{\boldsymbol{\omega}}}{|\nabla\theta|^2}\nabla\theta + \check{\mathfrak{q}}, \tag{4.24}$$

with $\check{\mathfrak{q}}$ a vector depending on $D\theta$ such that $\check{\mathfrak{q}} \cdot D\theta = 0$. We assume $\check{\mathfrak{q}} = 0$.

5. Emergence of finite speed heat propagation in linearized structures

(a) Derivation

For the sake of simplicity, from now on we will refer to orthonormal frames of reference. We identify contravariant and covariant components, that is, we do not distinguish between covectors and vectors. Thus, we substitute the derivative D with the gradient ∇ in those specific frames. In this context, the formal adjoint, indicated above by an asterisk, coincides with the transpose, denoted by a superscript $\top$. We assume the following:

(H1) there is a differentiable internal constraint of type $\nu = \gamma(\theta)$, where γ is a differentiable map that takes values in $\mathcal{M}$;
(H2) direct bulk actions on the microstructure are absent, namely $\boldsymbol{\beta}^{\ddagger} = 0$.

From equation (4.17), the assumption H2 implies

$$z \cdot \dot{\nu} + \mathcal{S} \cdot \nabla\dot{\nu} = \mathrm{div}(\mathcal{S}^{\top}\dot{\nu})$$

and we set $\mathfrak{p} := \mathcal{S}^{\top}\dot{\nu} - \bar{\mathfrak{q}}$, so that, under the above conditions, the local form of the energy balance (4.20) reads

$$\dot{e} + \mathrm{div}(\mathfrak{q} - \mathfrak{p}) - \tilde{r} = 0. \tag{5.1}$$

The assumption H1 implies $e = \tilde{e}(\nu, N, \theta) = \hat{e}(\theta, \nabla\theta)$ and $\mathfrak{p} = \tilde{\mathfrak{p}}(\nu, N, \theta, \dot{\nu}) = \hat{\mathfrak{p}}(\theta, \nabla\theta, \dot{\theta})$. Thus, the equation (5.1) becomes

$$\boldsymbol{\zeta} \cdot \nabla\dot{\theta} - k\Delta\theta + \bar{c}_v\dot{\theta} + \boldsymbol{\xi} \cdot \nabla\theta - \frac{\partial \mathfrak{p}}{\partial \nabla\theta} \cdot \nabla\nabla\theta - \tilde{r} = 0, \tag{5.2}$$

where

$$\bar{c}_v := \frac{\partial e}{\partial \theta}, \quad \boldsymbol{\xi} := -\frac{\partial \mathfrak{p}}{\partial \theta}, \quad \boldsymbol{\zeta} := \frac{\partial e}{\partial \nabla\theta} - \frac{\partial \mathfrak{p}}{\partial \dot{\theta}}.$$

If we neglect the term that involves $\nabla\nabla\theta$, set $\tilde{r} = 0$ and assume to evaluate in a specific state the functions that multiply the derivatives of θ, we get a linear equation with constant coefficients:

$$\boldsymbol{\zeta} \cdot \nabla\dot{\theta} - k\Delta\theta + \bar{c}_v\dot{\theta} + \boldsymbol{\xi} \cdot \nabla\theta = \tilde{r}. \tag{5.3}$$

The characteristic matrix of (5.3) is

$$C = \begin{pmatrix} 0 & \zeta^1 & \zeta^2 & \zeta^3 \\ \zeta^1 & -k & 0 & 0 \\ \zeta^2 & 0 & -k & 0 \\ \zeta^3 & 0 & 0 & -k \end{pmatrix},$$

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where ζ^i are the components of $\boldsymbol{\zeta}$. The eigenvalues are

$$\lambda_{1,2} := \frac{1}{2}\left(-k \pm \sqrt{|\boldsymbol{\zeta}|^2 + k^2}\right), \quad \lambda_3 := -k.$$

λ_1, λ_2, λ_3 are distinct and nonzero because $k < \sqrt{|\boldsymbol{\zeta}|^2 + k^2}$, whenever $|\boldsymbol{\zeta}| \neq 0$. λ_1 and λ_2 are simple roots of the characteristic polynomial $\det(C - \lambda I)$. Thus, they have algebraic and geometric multiplicity 1. The eigenvalue λ_3 has algebraic multiplicity 2. The linearly independent eigenvectors of C

$$w_1 = \begin{cases} (0, 0, \zeta^3, -\zeta^2)^T & \text{if } \zeta^3 \neq 0 \\ (0, \zeta^2, -\zeta^1, 0)^T & \text{otherwise,} \end{cases} \qquad w_2 = \begin{cases} (0, \zeta^3, 0 - \zeta^1)^T & \text{if } \zeta^3 \neq 0 \\ (0, 0, 0, 1)^T & \text{otherwise,} \end{cases}$$

span the eigenspace of λ_3 whenever $|\boldsymbol{\zeta}| \neq 0$. The signature of C is $(+, -, -, -)$. Therefore, since C is nonsingular and indefinite, (5.3) is hyperbolic when $|\boldsymbol{\zeta}| \neq 0$ and $k \neq 0$. Despite the presence of mixed derivatives, two bounded characteristic velocities are associated with it.

The equation (5.3) has already been derived in [13], and further discussed in [48]. Here, we analyze it numerically, visualizing the way heat propagates, according to it, and further comment on its nature after undimensionalizing it.

(b) Dimensionless structure

Let $\mathbf{x}^*$, θ^*, $\tilde{r}^*$ and t^* be dimensionless variables defined by

$$\mathbf{x}^* = \frac{1}{L}\mathbf{x}, \quad \theta^* = \frac{\theta}{\theta_0}, \quad \tilde{r}^* = \frac{\tilde{r}}{\tilde{r}_0}, \quad t^* = \frac{\bar{c}_v \theta_0}{\tilde{r}_0}$$

where L is a characteristic length, θ_0 is a reference temperature, $\tilde{r}_0$ a scalar with the dimension of heat source, and t^* represents the time it takes for a body exposed to the heat source $\tilde{r}_0$ to increase its temperature by $\delta\theta = \theta_0$. Thus, the dimensionless form of (5.3) is

$$\boldsymbol{\zeta}^* \cdot \nabla^*\left(\frac{\mathrm{d}\theta^*}{\mathrm{d}t^*}\right) - k^* \Delta^* \theta^* + \frac{\mathrm{d}\theta^*}{\mathrm{d}t^*} + \boldsymbol{\xi}^* \cdot \nabla^* \theta^* + \tilde{r}^* = 0, \tag{5.4}$$

where $\nabla^*(\cdot) = L\nabla(\cdot)$, $\Delta^*(\cdot) = L^2\Delta(\cdot)$ and

$$\boldsymbol{\zeta}^* := \frac{1}{\bar{c}_v L}\boldsymbol{\zeta}, \quad k^* := \frac{k\tau}{\bar{c}_v L^2}, \quad \boldsymbol{\xi}^* := \frac{\tau}{\bar{c}_v L}\boldsymbol{\xi}.$$

k^* represents the ratio between heat transmitted by conduction and heat absorbed by the body. With a little abuse of notation, in what follows we will avoid repeating the superscript * , although we will refer to dimensionless quantities.

(c) A benchmark solution and related stability

Consider the homogeneous version of (5.3) in dimensionless form:

$$\boldsymbol{\zeta} \cdot \nabla\dot{\theta} - k\Delta\theta + \dot{\theta} + \boldsymbol{\xi} \cdot \nabla\theta = 0. \tag{5.5}$$

Assume

$$\theta(x, t) = \mathrm{Re}\{a\, \mathrm{e}^{\mathrm{i}(\boldsymbol{\kappa} \cdot \mathbf{x} - \omega t)}\}, \tag{5.6}$$

where i is the imaginary unit, $\boldsymbol{\kappa} \in \mathbb{R}^3$ the wave vector, $\omega \in \mathbb{C}$ the frequency, and $a \in \mathbb{R}$ a constant. From equation (5.5) we get

$$(\omega\boldsymbol{\zeta} \cdot \boldsymbol{\kappa} + k|\boldsymbol{\kappa}|^2 - i\omega + i\boldsymbol{\xi} \cdot \boldsymbol{\kappa}) a\, e^{i(\boldsymbol{\kappa} \cdot \mathbf{x} - \omega t)} = 0.$$

For a non-trivial solution we must have

$$\omega = \frac{\boldsymbol{\xi} - (k|\boldsymbol{\kappa}|^2)\boldsymbol{\zeta}}{(\boldsymbol{\zeta} \cdot \boldsymbol{\kappa})^2 + 1} \cdot \boldsymbol{\kappa} - i\frac{k|\boldsymbol{\kappa}|^2 + \boldsymbol{\xi} \cdot (\boldsymbol{\kappa} \otimes \boldsymbol{\kappa})\boldsymbol{\zeta}}{(\boldsymbol{\zeta} \cdot \boldsymbol{\kappa})^2 + 1}.$$

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Consequently, we obtain $\theta(\mathbf{x},t)=a\,\cos(\boldsymbol{\kappa}\cdot(\mathbf{x}-\mathbf{v}t))e^{\hat{\beta}t}$, with

$$\mathbf{v}:=\frac{\boldsymbol{\xi}-(k|\boldsymbol{\kappa}|^2)\boldsymbol{\zeta}}{(\boldsymbol{\zeta}\cdot\boldsymbol{\kappa})^2+1}\quad\text{and}\quad\hat{\beta}=-\frac{k|\boldsymbol{\kappa}|^2+\boldsymbol{\xi}\cdot(\boldsymbol{\kappa}\otimes\boldsymbol{\kappa})\boldsymbol{\zeta}}{(\boldsymbol{\zeta}\cdot\boldsymbol{\kappa})^2+1}. \tag{5.7}$$

$\mathbf{v}$ is the velocity of propagation of the temperature wave while $\hat{\beta}\in\mathbb{R}$ is the decaying time constant. The solution is stable if $\hat{\beta}\le 0$, otherwise an arbitrarily small perturbation is amplified to infinity. The factors $\boldsymbol{\xi}$ and $\boldsymbol{\zeta}$ must satisfy the inequality

$$(\boldsymbol{\xi}\otimes\boldsymbol{\zeta})\cdot(\boldsymbol{\kappa}\otimes\boldsymbol{\kappa})\ge -k|\boldsymbol{\kappa}|^2, \tag{5.8}$$

for all wave vectors $\boldsymbol{\kappa}\in\mathbb{R}^3$. In the one-dimensional space, $\zeta,\ \xi,\ \kappa\in\mathbb{R}$ and we have $\theta(x,t)=a\,\cos(\kappa(x-vt))e^{\hat{\beta}t}$, where

$$v:=\frac{\mathrm{Re}\{\omega\}}{\kappa}=\frac{\xi-k\zeta\kappa^2}{(\zeta\kappa)^2+1}\quad\text{and}\quad\hat{\beta}:=\mathrm{Im}\{\omega\}=-\kappa^2\frac{k+\zeta\xi}{(\zeta\kappa)^2+1}, \tag{5.9}$$

so that (5.8) reduces to $\xi\zeta\ge -k$. The function $\theta(x,t)=a\,\cos(\kappa(x-vt))e^{\hat{\beta}t}$ solves the following one-dimensional differential problem with periodic boundary conditions

$$\begin{cases}\zeta\theta_{,xt}-k\theta_{,xx}+\theta_{,t}+\xi\theta_{,x}=0, & x\in[0,1),\quad t\in(0,T_f],\\ \theta(0,t)=\theta(1,t), & t>0,\\ \theta_{,x}(0,t)=\theta_{,x}(1,t), & t>0,\\ \theta(x,0)=\cos(\kappa x), & x\in[0,1),\end{cases} \tag{5.10}$$

where the comma as a subscript means partial derivative with respect to the variable following it.

Remark 5.1. If $\zeta\xi=-k$, the equation (5.10) reduces to

$$\frac{\partial}{\partial t}\left(\zeta\frac{\partial\theta}{\partial x}+\theta\right)+\xi\frac{\partial}{\partial x}\left(\zeta\frac{\partial\theta}{\partial x}+\theta\right)=0, \tag{5.11}$$

which is the one-dimensional advection equation

$$\frac{\partial w}{\partial t}+\xi\frac{\partial w}{\partial x}=0,\quad\text{for}\quad w(x,t):=\zeta\frac{\partial\theta}{\partial x}(x,t)+\theta(x,t).$$

A general solution is $w(x,t)=f(x-\xi t)$. Thus, in this case, the temperature $\theta(x,t)$ satisfies

$$\zeta\frac{\partial\theta}{\partial x}(x,t)+\theta(x,t)=f(x-\xi t).$$

We can obtain a particular solution to (5.11) by substituting $k=-\xi\zeta$ into (5.9), so that

$$v=\frac{\xi+\xi(\zeta\kappa)^2}{(\zeta\kappa)^2+1}=\xi\quad\text{and}\quad\hat{\beta}=-\kappa^2\frac{-\zeta\xi+\zeta\xi}{(\zeta\kappa)^2+1}=0;$$

hence, $\theta(x,t)=a\,\cos(\kappa(x-\xi t))$.

(d) Comparison with the standard heat equation

The differential operator involved in equation (5.10) is

$$\mathfrak{L}_h:=\frac{\partial}{\partial t}-k\frac{\partial^2}{\partial x^2}+\zeta\frac{\partial^2}{\partial t\partial x}+\xi\frac{\partial}{\partial x},$$

while the one pertaining to the standard heat equation is

$$\mathfrak{L}_p:=\frac{\partial}{\partial t}-k\frac{\partial^2}{\partial x^2}.$$

The eigenvalues of these two operators—say, λ_h and λ_f—are given by

$$\mathfrak{L}_h\theta=\lambda_h\theta\quad\text{and}\quad\mathfrak{L}_p\theta=\lambda_p\theta.$$

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where $\theta(x,t)$ must satisfy some given boundary conditions. Take $\theta(x,t)=\exp(\kappa x-\omega t)$. We have

$$\lambda_h=-\omega-k\kappa^2-\zeta\kappa\omega+\xi\kappa \quad \text{and} \quad \lambda_p=-\omega-k\kappa^2.$$

When $\xi\neq\zeta\omega$, $\lambda_h\longrightarrow\lambda_p$, as $\xi,\zeta\longrightarrow 0$, and so behave the eigenfunctions. Consider the differential problems

$$\mathfrak{L}_p\theta=0 \quad \text{and} \quad \mathfrak{L}_h\theta=0, \tag{5.12}$$

with periodic boundary and initial conditions given by

$$\theta(0,t)=\theta\left(\frac{2\pi}{\kappa},t\right), \quad \theta_{,x}(0,t)=\theta_{,x}\left(\frac{2\pi}{\kappa},t\right), \quad \theta(x,0)=\exp(i\kappa x).$$

They admit as solutions $\theta(x,t)=\exp(i(\kappa x-\omega t))$. Then, from $(5.12)_1$, we get

$$\omega=-ik\kappa^2=:\omega_p$$

while from $(5.12)_2$ we obtain

$$\omega=\frac{\xi\kappa+k\zeta\kappa^2}{1+(\zeta\kappa)^2}-i\frac{(k-\xi\zeta)\kappa^2}{1+(\zeta\kappa)^2}:=\omega_h.$$

As $\xi,\zeta\longrightarrow 0$, $\omega_h\longrightarrow\omega_p$. Therefore, as $\xi,\zeta\longrightarrow 0$ the solution of $(5.12)_2$ converges to that of $(5.12)_1$.

(e) Computational analysis in two-dimensional ambient setting

(i) Spatial discretization

Write $\mathbf{x}:=(x,y)$ for a generic point of the unit square Ω.[1] Consider

$$\begin{cases}\boldsymbol{\zeta}\cdot\nabla\dot{\theta}-k\Delta\theta+\dot{\theta}+\boldsymbol{\xi}\cdot\nabla\theta=0, & \mathbf{x}\in\Omega, \quad t\in(0,T_f],\\ \theta(0,y,t)=\theta(1,y,t), & \nabla\theta(0,y,t)=\nabla\theta(1,y,t), \quad y\in(0,1), \quad t>0,\\ \theta(x,0,t)=\theta(x,1,t), & \nabla\theta(x,0,t)=\nabla\theta(x,1,t), \quad x\in(0,1), \quad t>0,\\ \theta(0,0,t)=\theta(0,1,t)=\theta(1,0,t)=\theta(1,1,t), & t>0,\\ \theta(x,y,0)=\cos(\boldsymbol{\kappa}\cdot\mathbf{x}), & \mathbf{x}\in\Omega,\end{cases} \tag{5.13}$$

with $\boldsymbol{\kappa}\in\mathbb{R}^2$ a given wave vector. The boundary conditions are periodic in the x and y directions. This is tantamount to solving the evolution equation on a torus. The function $\theta(x,y,t)=\cos(\boldsymbol{\kappa}\cdot(\mathbf{x}-\mathbf{v}t))e^{\hat{\beta}t}$, with $\mathbf{v}$ and $\hat{\beta}$ as in (5.7), is a solution.

We define a uniform mesh on Ω with constant size $\boldsymbol{\delta}x=\boldsymbol{\delta}y=h=1/\mathtt{N}+1$. The mesh nodes are given by

$$x_i=ih, \quad i=0:\mathtt{N}+1, \quad y_j=jh, \quad j=0:\mathtt{N}+1.$$

The periodicity of the boundary conditions implies that we can identify all the nodes with coordinates (x_0,y_j) $j=0:\mathtt{N}+1$ with the nodes $(x_{\mathtt{N}+1},y_j)$ $j=0:\mathtt{N}+1$, and the nodes (x_i,y_0) $i=0:\mathtt{N}+1$ with the nodes $(x_i,y_{\mathtt{N}+1})$ $i=0:\mathtt{N}+1$. Moreover, the four vertices of the unit square correspond to

[1]In the previous sections, x indicated a generic point in $\mathcal{B}$, which can be chosen in spaces of various dimensions (typically 1, 2, 3). Here, with abuse of notation, we indicate by x only one coordinate in the plane.

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the same node (x_0, y_0). By writing $\theta_{ij}(t)$ for the approximate temperature at $\mathbf{x} = [x_i, y_j]^\top$ and time t, namely $\theta_{ij}(t) \simeq \theta(x_i, y_j, t)$, the vector of unknowns is thus

$$\mathbf{u}(t) = \begin{bmatrix} \mathbf{u}_0(t) \\ \mathbf{u}_1(t) \\ \vdots \\ \mathbf{u}_N \end{bmatrix}, \quad \text{where } \mathbf{u}_j = \begin{bmatrix} \theta_{0j}(t) \\ \theta_{1j}(t) \\ \vdots \\ \theta_{\mathtt{N}j}(t) \end{bmatrix}. \tag{5.14}$$

By adopting a standard centred scheme for the spatial derivatives, with h the mesh size, from equation (5.13), we obtain a system of $(\mathtt{N}+1)^2$ ordinary differential equations:

$$\mathbf{M}\dot{\mathbf{u}}(t) + \mathbf{K}\mathbf{u}(t) = 0, \tag{5.15}$$

where $\mathbf{M} \in \mathbb{R}^{(\mathtt{N}+1)^2 \times (\mathtt{N}+1)^2}$ and $\mathbf{K} \in \mathbb{R}^{(\mathtt{N}+1)^2 \times (\mathtt{N}+1)^2}$.

(ii) Time integration and convergence analysis

We adopt the Crank-Nicolson (CN) scheme, which is implicit and of second order. The time interval is subdivided into $\mathtt{N}_\ell$ steps with $\delta t = T_f/\mathtt{N}_\ell$. Referring to system (5.15), indicating by $\mathbf{u}^n \simeq \mathbf{u}(t^n)$ the solution at $t^n = n\delta t$, we update it by

$$\left(\mathbf{M} + \frac{\delta t}{2}\mathbf{K}\right)\mathbf{u}^{n+1} = \left(\mathbf{M} - \frac{\delta t}{2}\mathbf{K}\right)\mathbf{u}^n.$$

Since the iteration matrix $\mathbf{M} + \frac{\delta t}{2}\mathbf{K}$ is constant, we can factorize it only once.

To evaluate the error, we refer to the one-dimensional ambient and compare the numerical results with the benchmark solution in §5c. Also, we refer to a second-order upwind scheme (II-UP) in which, if the gradient coefficient is positive, the spatial derivative is approximated by a finite backward difference, while, if it is negative, we use a finite forward difference. To obtain a numerical scheme with truncation error of order $O(h^2)$ for $\zeta \frac{\partial^2\theta}{\partial t \partial x}$, we proceed as follows:

— if $\zeta > 0$, $\frac{\partial \dot{\theta}}{\partial x}(x_i, t) \simeq \frac{3\dot{\theta}_i(t) - 4\dot{\theta}_{i-1}(t) + \dot{\theta}_{i-2}(t)}{2h}$;
— if $\zeta < 0$, $\frac{\partial \dot{\theta}}{\partial x}(x_i, t) \simeq \frac{-3\dot{\theta}_i(t) + 4\dot{\theta}_{i+1}(t) - \dot{\theta}_{i+2}(t)}{2h}$.

We make an analogous choice for the term $\xi \frac{\partial \theta}{\partial x}$. Thus, if $\zeta < 0$, $\mathbf{M} = \mathbf{I} + \zeta\mathbf{G}_+$ while if $\zeta > 0$, $\mathbf{M} = \mathbf{I} + \zeta\mathbf{G}_-$ and the same for the stiffness matrix: $\mathbf{K} = k\mathbf{L} + \xi\mathbf{G}_+$ or $\mathbf{K} = k\mathbf{L} + \xi\mathbf{G}_-$ whether $\xi < 0$ or $\xi > 0$, respectively. Here, $\mathbf{I}$ is the identity matrix, $\mathbf{L}$ the discrete Laplacian while the subscripts "+" and "−" indicate the discrete gradient $\mathbf{G}$ obtained by forward or backward finite differences, respectively.

Consider the two following discrete L^p norms ($p = 2, \infty$) for $\mathbf{v} \in \mathbb{R}^n$:

$$||\mathbf{v}||_{\Delta,2} = \left(h \sum_{j=1:n} |v_j|^2\right)^{1/2} \quad \text{and} \quad ||\mathbf{v}||_{\Delta,\infty} = \max_{j=1:n} |v_j|. \tag{5.16}$$

At (x_j, t^n), the error $\hat{e}_i^n$ is the difference between computed and exact solutions θ^*:

$$\hat{e}_i^n = |\theta_i^n - \theta^*(x_j, t^n)|.$$

Figure 1 shows the discrete L^2 norm of the error, evaluated at $t = T_f$, as the spacing $h \to 0$. Both the considered numerical schemes are second-order accurate in space, that is,

$$||\hat{e}(x, T_f)||_{\Delta,2} = O(h^2).$$

We obtain the same behaviour for the discrete L^∞ norm. Both schemes are also second-order accurate in time (see figure 1), so

$$||\hat{e}(x, T_f)||_{\Delta,2} = O(h^2 + \delta t^2).$$

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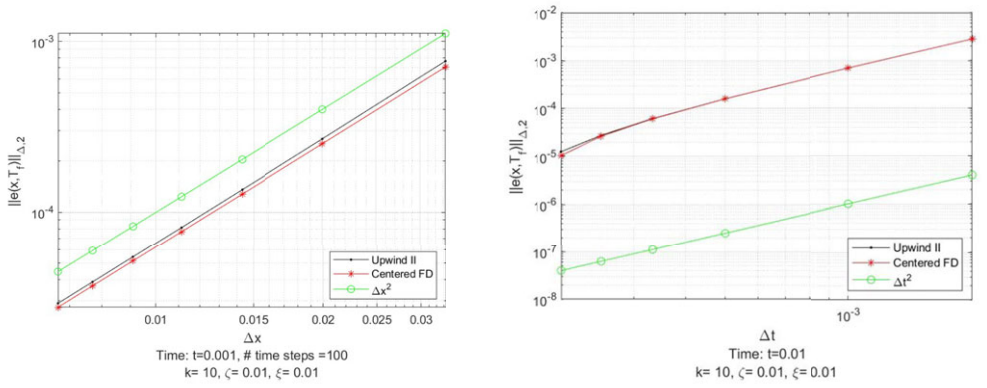

Figure 1. Discrete L^2 norm of the error as (a) $h \longrightarrow 0$ and (b) $\delta t \longrightarrow 0$.

Since the centred finite difference scheme is more accurate than the II-UP procedure, we adopt it.

(iii) Simulation: two-dimensional setting with periodic boundary conditions

We first refer to system (5.13) and choose the initial condition as a Gaussian distribution given by

$$\theta(x,y,0) = \frac{0.8}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-0.5)^2+(y-0.5)^2}{2\sigma^2}},$$

where $\sigma^2 = 0.003$. Figure 2 shows simulations for the following choice of the non-dimensional parameters:

$$k = 1, \quad \boldsymbol{\zeta} = 0.1\left[\cos\left(\frac{7}{4}\pi\right), \sin\left(\frac{7}{4}\pi\right)\right]^\top, \quad \boldsymbol{\xi} = \mathbf{0}. \tag{5.17}$$

They evidence that the temperature travels in the direction of $\boldsymbol{\zeta}$, but in the opposite way. An approximation of the velocity at which the peak is traveling is calculated by dividing the distance traveled by the maximum value of the temperature distribution in a certain number n of time steps by the elapsed time $n\boldsymbol{\delta}t$. Increasing the number of nodes, the computed velocity oscillates about a mean value. For the values in (5.17), we obtain $\langle v \rangle \simeq 3.6$. Figure 3 shows the phase portrait for nodes $(0,0)$ and $(0.5,0.5)$ (temperature $\theta(t^n)$ and temperature time rate $\dot{\theta}(t^n)$ at each time t^n have been rescaled).

The temperature evolution over Ω becomes similar to the one predicted by the standard Fourier heat equation as $|\boldsymbol{\zeta}|$ decreases (see figure 4).

(iv) Prescribing fluxes at the boundary

Heat fluxes can be readily prescribed on the boundary of a specimen in laboratory settings. The circumstance renders the analysis of Neumann-type boundary conditions of practical relevance. To show how we can implement the relevant numerical analysis, we consider a one-dimensional ambient and the following system:

$$\begin{cases} \zeta \dfrac{\partial^2\theta}{\partial t \partial x} - k\dfrac{\partial^2\theta}{\partial x^2} + \dfrac{\partial\theta}{\partial t} + \xi\dfrac{\partial\theta}{\partial x} = 0, \quad x \in (0,1), \quad t \in (0, T_f], \\ \theta(x,0) = 1, \quad x \in (0,1), \\ \dfrac{\partial\theta}{\partial x}(0,t) = 0, \dfrac{\partial\theta}{\partial x}(1,t) = -\dfrac{1}{k}\mathfrak{q}(t), \quad t \in (0, T_f], \end{cases} \tag{5.18}$$

where $\mathfrak{q}(t)$ is a prescribed function of time. Space and time are discretized by a uniform mesh $x_i = ih$, $i = 0 : \mathtt{N}+1$, and $t^n = n\delta t$, $n = 1 : \mathtt{N}_p$ where $h = 1/(\mathtt{N}+1)$ and $\delta t = T_f/\mathtt{N}_p$, with $\mathtt{N}_p$ the number

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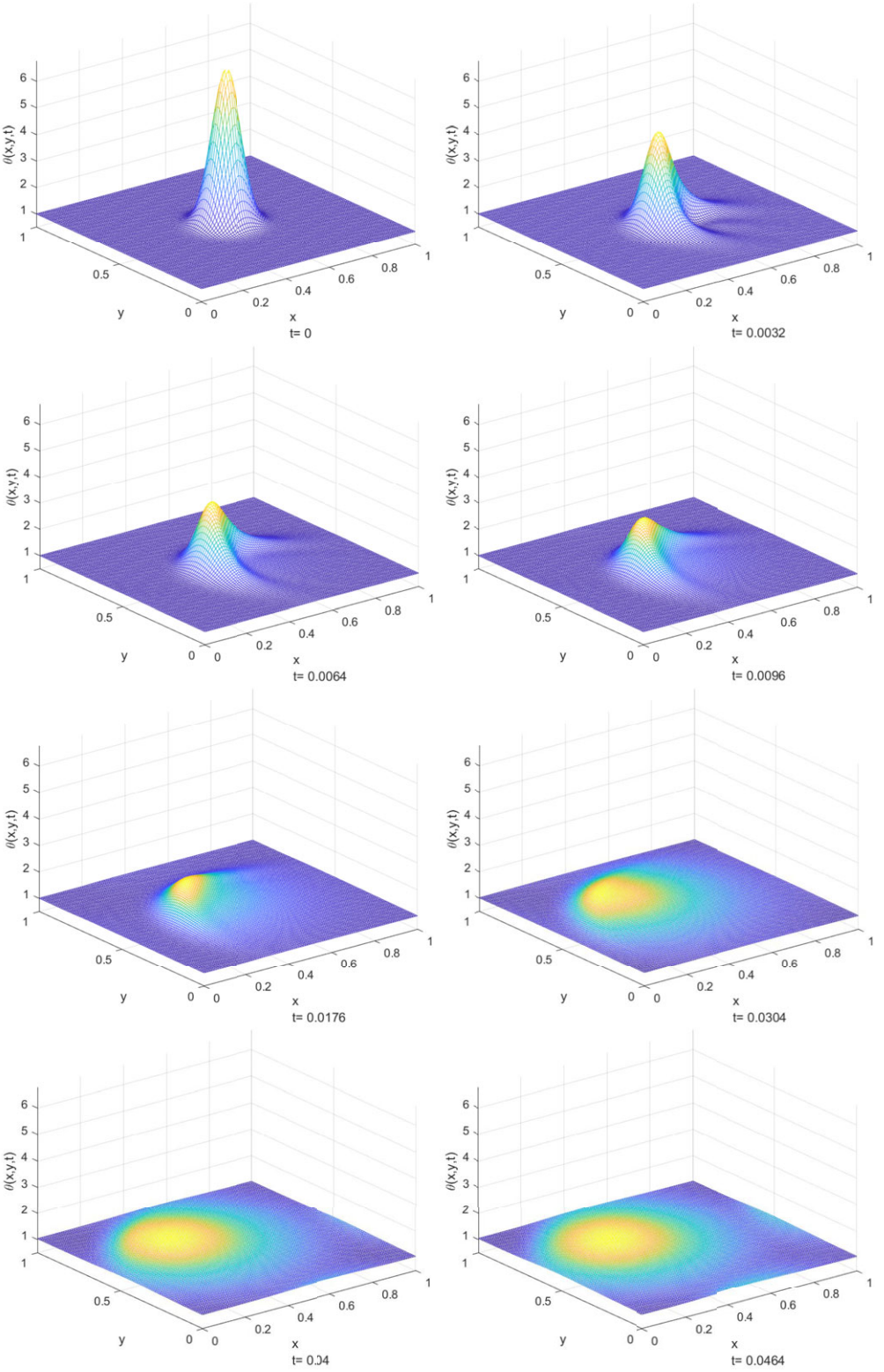

Figure 2. Two-dimensional problem with periodicity boundary conditions. $||\zeta||_2 = 0.1k$.

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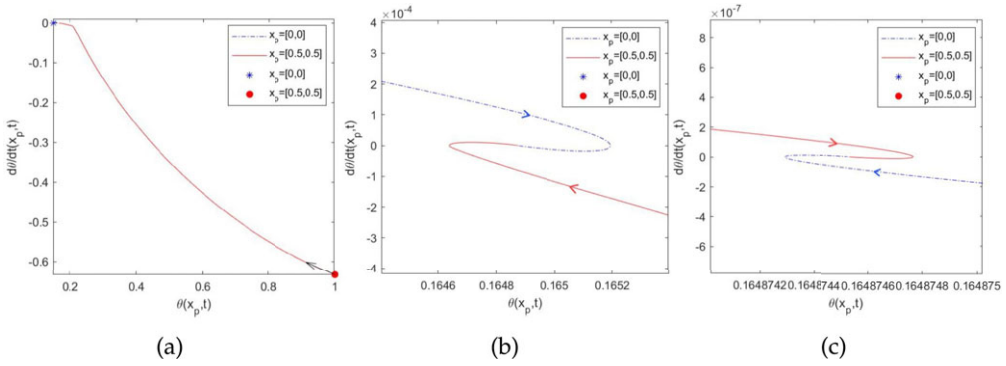

Figure 3. Phase space of the periodic problem with $k = 1, ||\boldsymbol{\zeta}|| = 0.1, \xi = 0$. (b) and (c) shows a zoom close to the stationary condition reached for long times.

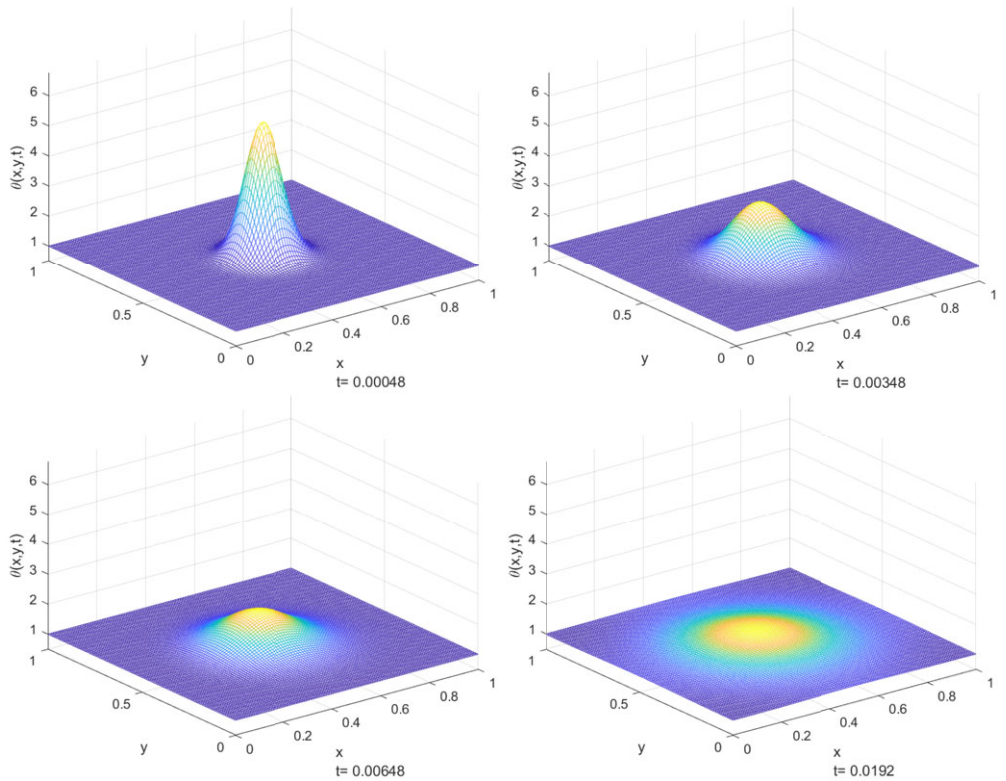

Figure 4. Two-dimensional problem with periodicity boundary conditions. $||\boldsymbol{\zeta}||_2 = 0.01k$.

of time steps. Once again, we adopt a centred scheme for the derivatives. The Neumann boundary conditions imply

$$\theta_0(t) = \theta_1(t) \quad \text{and} \quad \theta_{N+1}(t) = \theta_N(t) - \frac{h}{k}q(t). \tag{5.19}$$

Thus, we end up with the following system:

$$\mathbf{M}\dot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{f}, \tag{5.20}$$

where $\mathbf{u} = [\theta_1(t), \ldots, \theta_N(t)]^\top \in \mathbb{R}^N$, $\mathbf{f}(t) = [0, \ldots, 0, (\frac{\zeta}{2\kappa}\dot{q}(t) + (\frac{\xi}{\kappa} - \frac{1}{h})q(t))]^\top$ and $\mathbf{M}, \mathbf{K} \in \mathbb{R}^{N\times N}$.

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6. Explicit analysis of the reactive actions

(a) Reactive microstructural actions

Above, we have not explicitly expressed the reactive components of the actions (microstress and self-action), associated with the presence of the internal constraint γ. In order to render these components explicit, we refer to the general theory of internal constraints in continua as proposed in [49,50]. So, we accept the pertinent principle of determinism. It states that (1) every functional depending on state, say $\mathcal{F}$ (free energy, entropy, stress, etc.), admits additive decomposition into active $\overset{a}{\mathcal{F}}$ and reactive $\overset{r}{\mathcal{F}}$ components; (2) only the active components are connected by suitable constitutive rules to the independent thermokinetic variables; (3) the reactive terms depend on the specific processes under analysis; they are fields in the orthogonal complement of the respective active functionals, orthogonality defined in some suitable way.

In the present setting, an internal constraint is said to be *perfect* when, in the absence of a discontinuity surface, the pertinent reactive entities identically satisfy the identity

$$\dot{\overset{r}{\psi}} + \overset{r}{\eta}\,\dot{\theta} - \overset{r}{z}\cdot\dot{\nu} - \overset{r}{\mathcal{S}}\cdot\nabla\dot{\nu} - \frac{1}{\theta}\,\overset{r}{\mathfrak{q}}\cdot\nabla\theta - \theta\,\mathrm{div}\,\overset{r}{\bar{\boldsymbol{\omega}}} = 0. \tag{6.1}$$

Accepting the constraint $\nu = \gamma(\theta)$, and excluding for a while the assumption H2 for the sake of generality, we define

$$\gamma' := \frac{\mathrm{d}\gamma(\theta)}{\mathrm{d}\theta}, \tag{6.2}$$

so that $\dot{\nu} = \gamma'\dot{\theta}$, and consider $|\gamma'| \neq 0$. Thus, equation (6.1) becomes

$$\dot{\overset{r}{\psi}} + \overset{r}{\eta}\,\dot{\theta} - \overset{r}{z}\cdot\gamma'\dot{\theta} - (\overset{r}{S}{}^{\top}\gamma')\cdot\nabla\dot{\theta} - (\overset{r}{\mathcal{S}}\cdot\nabla\gamma')\dot{\theta} - \frac{1}{\theta}\,\overset{r}{\mathfrak{q}}\cdot\nabla\theta - \theta\,\mathrm{div}\,\overset{r}{\bar{\boldsymbol{\omega}}} = 0. \tag{6.3}$$

The arbitrariness of the fields involved implies the following:

$$-\overset{r}{\eta} + \overset{r}{z}\cdot\gamma' + \overset{r}{\mathcal{S}}\cdot\nabla\gamma' = 0, \quad \overset{r}{S}{}^{\top}\gamma' = 0, \quad \dot{\overset{r}{\psi}} = 0, \quad \overset{r}{\mathfrak{q}} = 0, \quad \mathrm{div}\,\overset{r}{\bar{\boldsymbol{\omega}}} = 0. \tag{6.4}$$

We assume that $\overset{a}{\psi}$, $\overset{a}{\eta}$, $\overset{a}{P}$, $\overset{a}{z}$, and $\overset{a}{\mathcal{S}}$, all depend on (θ, ν, N, θ). So, due to the internal constraint, the list of state variables reduces to $(\theta, \nabla\theta)$. The Clausius-Duhem inequality thus reads as follows:

$$\frac{\partial\overset{a}{\psi}}{\partial\theta}\,\dot{\theta} + \frac{\partial\overset{a}{\psi}}{\partial\nabla\theta}\cdot\nabla\dot{\theta} + \overset{a}{\eta}\,\dot{\theta} - \overset{a}{z}\cdot\gamma'\dot{\theta} - (\overset{a}{S}{}^{\top}\gamma')\cdot\nabla\dot{\theta} - (\overset{a}{\mathcal{S}}\cdot\nabla\gamma')\dot{\theta} + \frac{1}{\theta}\,\overset{a}{\mathfrak{q}}\cdot\nabla\theta - \theta\,\mathrm{div}\,\overset{a}{\bar{\boldsymbol{\omega}}} \leq 0. \tag{6.5}$$

Once again, arbitrariness of the rate fields involved implies

$$-\frac{\partial\overset{a}{\psi}}{\partial\theta} - \overset{a}{\eta} + \overset{a}{z}\cdot\gamma' + \overset{a}{\mathcal{S}}\cdot\nabla\gamma' = 0, \tag{6.6}$$

$$-\frac{\partial\overset{a}{\psi}}{\partial\nabla\theta} + \overset{a}{S}{}^{\top}\gamma' = 0 \tag{6.7}$$

and

$$\frac{1}{\theta}\,\overset{a}{\mathfrak{q}}\cdot\nabla\theta - \theta\,\mathrm{div}\,\overset{a}{\bar{\boldsymbol{\omega}}} \leq 0. \tag{6.8}$$

The last inequality is compatible with $\mathfrak{q} = -k\nabla\theta + \bar{\mathfrak{q}}$, with $\bar{\mathfrak{q}}$ which satisfies (4.23). By summing up active and reactive components and neglecting for a while assumption H2, we get

$$S^{\top}\gamma' = \frac{\partial\overset{a}{\psi}}{\partial\nabla\theta} \quad \text{and} \quad \eta = -\frac{\partial\overset{a}{\psi}}{\partial\theta} + \mathrm{div}\left(\frac{\partial\overset{a}{\psi}}{\partial\nabla\theta}\right) + \gamma'\cdot\beta^{\ddagger}. \tag{6.9}$$

Also, if we set $\overset{r}{\psi} = 0$, which is compatible with $(6.4)_3$, the first identity (6.9) implies

$$S = \frac{\gamma'}{|\gamma'|^2} \otimes \frac{\partial\psi}{\partial\nabla\theta}. \tag{6.10}$$

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Thus, with the use of (6.9) and (6.10), from the local balance (4.17) we obtain

$$z = \left(\operatorname{div}\left(\frac{\partial\psi}{\partial\nabla\theta}\right) + \gamma'\cdot\beta^{\ddagger} - \left(\frac{\gamma'}{|\gamma'|^2}\otimes\frac{\partial\psi}{\partial\nabla\theta}\right)\cdot\nabla\gamma'\right)\frac{\gamma'}{|\gamma'|^2}.$$

When we consider H2, the previous expression obviously reduces to

$$z = \left(\operatorname{div}\left(\frac{\partial\psi}{\partial\nabla\theta}\right) - \left(\frac{\gamma'}{|\gamma'|^2}\otimes\frac{\partial\psi}{\partial\nabla\theta}\right)\cdot\nabla\gamma'\right)\frac{\gamma'}{|\gamma'|^2}.$$

From identity (6.10), and taking into account the internal constraint, we obtain

$$\mathcal{S}^{\top}\dot{\gamma} = \left(\frac{\partial\psi}{\partial\nabla\theta}\otimes\frac{\gamma'}{|\gamma'|^2}\right)\gamma'\dot{\theta} = \frac{\partial\psi}{\partial\nabla\theta}\dot{\theta}. \tag{6.11}$$

Thus, we explicitly rewrite the local energy balance as

$$\dot{e} - k\Delta\theta - \operatorname{div}\left(\frac{\partial\psi}{\partial\nabla\theta}\dot{\theta} - \bar{\mathfrak{q}}\right) - \tilde{r} = 0. \tag{6.12}$$

The derivation of interaction reactive components has also been done in [51], a paper dedicated to the analysis of thermoelastic acceleration waves in constrained general complex media.

(b) Some prominent nonlinear cases

(i) Isotropic behaviour in the absence of heat sources and perturbation of the Fourier law

Under the assumed internal constraint, we have $\psi = \tilde{\psi}(\theta, \nu, \nabla\nu) = \mathfrak{f}(\theta, \nabla\theta)$. As a special choice, we set ψ to be

$$\psi = \frac{1}{2}\mathfrak{a}|\nabla\theta|^2 + u(\theta), \tag{6.13}$$

where $\mathfrak{a}$ is a positive constant and u is differentiable function; ψ refers to a homogeneous and isotropic body. Since the internal energy density e is given by $e = \psi + \theta\eta$, from (6.9) and (6.13) we obtain the following expression:

$$e = \frac{1}{2}\mathfrak{a}|\nabla\theta|^2 + u(\theta) - \theta u'(\theta) + \mathfrak{a}\theta\Delta\theta. \tag{6.14}$$

Also, consider $\tilde{r} = 0$ and $\bar{\mathfrak{q}} = 0$. Under these assumptions, the energy balance (6.12) reduces to

$$\bar{c}_v\dot{\theta} - k\Delta\theta + \mathfrak{a}\theta\Delta\dot{\theta} = 0, \tag{6.15}$$

where $\bar{c}_v := -\theta u''(\theta)$. Notice that the microstructural effect is naturally nonlinear.

(ii) Role of the heat perturbation flux only

Consider the case in which, possibly after a transient process, the microstructure evolution is as uniform (ordered) as to render negligible the contribution of $\nabla\nu$ to the energy. It means that the energetic component of the microstress is vanishingly small with respect to the microstructural self-action z. In fact, the microstress describes first-neighbour interactions at the spatial scale of microstructure. In this approximation, we have

$$\psi = u(\theta),$$

with u a differentiable function. So, when $\boldsymbol{\beta}^{\ddagger} = 0$, as we assume here, the entropy (6.9) reduces to $\eta = -u'$, and the internal energy density $e = \psi + \theta\eta$ is

$$e = u(\theta) - \theta u'(\theta).$$

We assume

$$\tilde{r} = 0 \quad \text{and} \quad \breve{\mathfrak{q}} = 0$$

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and $\bar{\boldsymbol{\omega}}$ such that

$$\mathrm{div}\bar{\boldsymbol{\omega}} = \mathfrak{a}\dot{\theta}\frac{|\nabla\theta|^2}{\theta^2}.$$

Consequently, from (4.23), we have

$$\bar{\mathfrak{q}} = \mathfrak{a}\dot{\theta}\nabla\theta$$

and the energy balance (6.12) reduces to the following nonlinear equation:

$$\mathfrak{a}\nabla\theta\cdot\nabla\dot{\theta} - k\Delta\theta + \mathfrak{a}\dot{\theta}\Delta\theta + \bar{c}_v\dot{\theta} = 0, \tag{6.16}$$

which can be rewritten as

$$\bar{c}_v\dot{\theta} = \mathrm{div}(k\nabla\theta - \mathfrak{a}\dot{\theta}\nabla\theta).$$

Remark 6.1. If we still consider (6.13) and take $\bar{\mathfrak{q}} = \mathfrak{a}\dot{\theta}\nabla\theta$, the equation (6.16) can be formally obtained in two cases: (i) when we consider $\tilde{r}$ as a live load given by $\tilde{r} = \mathfrak{a}\theta\Delta\dot{\theta}$, or (ii) when, still taking $\tilde{r} = 0$, the vector field $\nabla\dot{\theta}$ is divergence free. In the case (i), $\tilde{r}$ plays the role of a compensating source that is necessary to recompose the "uniformity" of the microstructural behaviour, as intended above.

(iii) Influence of a possible dissipative microstress component

Above, the active component of microstress $\mathcal{S}$ has been considered energy-dependent. Assume that a viscous stress component $\mathcal{S}^v$ can be attributed to $\overset{a}{\mathcal{S}}$, so that $\mathcal{S} = \mathcal{S}^e + \mathcal{S}^v + \overset{r}{\mathcal{S}}$. The stress component $\mathcal{S}^v$ is intrinsically dissipative. It means that

$$\mathcal{S}^v\cdot\nabla\dot{\nu} \geq 0$$

for any choice of $\nabla\dot{\nu}$, with a condition that the equality sign holds only when $\nabla\dot{\nu} = 0$. The inequality is compatible with a structure given by $\mathcal{S}^v = \varpi\nabla\dot{\nu}$, where $\varpi > 0$ is a constant. In the presence of the internal constraint $\nu = \gamma(\theta)$, we have

$$\mathcal{S}^{v\top}\dot{\nu} = \varrho(\theta)\dot{\theta}^2\nabla\theta + \bar{\varrho}(\theta)\dot{\theta}\nabla\dot{\theta}, \tag{6.17}$$

where $\varrho(\theta) := \varpi\gamma''\gamma'$ and $\bar{\varrho}(\theta) := \varpi\gamma'^2$. The local energy balance (6.12) becomes

$$\dot{e} - k\Delta\theta - \mathrm{div}\left(\frac{\partial\psi}{\partial\nabla\theta}\dot{\theta} + \mathcal{S}^{v\top}\dot{\nu} - \bar{\mathfrak{q}}\right) - \tilde{r} = 0. \tag{6.18}$$

Assume

$$\bar{\mathfrak{q}} = 0 \quad \text{and} \quad \tilde{r} = 0.$$

Taking into account (6.14) and (6.17), the local energy balance (6.18) becomes

$$\bar{c}_v\dot{\theta} - k\Delta\theta + \mathfrak{a}\theta\Delta\dot{\theta} - \varrho\dot{\theta}^2\Delta\theta - (2\varrho + \bar{\varrho}')\dot{\theta}\nabla\theta\cdot\nabla\dot{\theta} - \varrho'\dot{\theta}^2|\nabla\theta|^2 - \bar{\varrho}\dot{\theta}\Delta\dot{\theta} - \bar{\varrho}|\nabla\dot{\theta}|^2 = 0. \tag{6.19}$$

When there is uniform heating speed so that $|\nabla\dot{\theta}|$ is so small that can be considered negligible, (6.19) may be simplified as follows:

$$\bar{c}_v\dot{\theta} - k\Delta\theta + \mathfrak{a}\theta\Delta\dot{\theta} - \varrho\dot{\theta}^2\Delta\theta - \varrho'\dot{\theta}^2|\nabla\theta|^2 = 0. \tag{6.20}$$

We do not further analyze this special case.

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(c) Computational analysis of a nonlinear hyperbolic heat propagation

(i) Boundary value problem

In the one-dimensional setting, (6.16) reads

$$\bar{c}_v\theta_t - k\theta_{xx} + \mathtt{a}(\theta_t\theta_x)_x = 0. \tag{6.21}$$

We seek possible solutions of the form $\theta(x,t) = f(x) + g(t)$, where f and g are differentiable. Indicating by a prime the spatial derivative, from equation (6.21) we get

$$\bar{c}_v\dot{g} - kf'' + \mathtt{a}\dot{g}f'' = 0,$$

which gives

$$\dot{g} = \frac{kf''}{\bar{c}_v + \mathtt{a}f''} = \alpha \in \mathbb{R},$$

provided that

$$\bar{c}_v + \mathtt{a}f'' \neq 0, \tag{6.22}$$

as we assume here. Obviously, α must be constant because g depends only on time, while the fraction on the right-hand side is a function of the space variable only. Thus, we have

$$g(t) = \alpha t + \bar{c} \quad \text{and} \quad f'' = \frac{\alpha\bar{c}_v}{k - \mathtt{a}\alpha}, \tag{6.23}$$

so that

$$\theta(x,t) = \alpha t + \frac{\alpha\bar{c}_v}{2(k-\mathtt{a}\alpha)}x^2 + c_1x + c_0, \tag{6.24}$$

where c_1 and c_0 are arbitrary constants that include $\bar{c}$ and $\alpha \in \mathbb{R}$ must be such that $k - \mathtt{a}\alpha \neq 0$. The condition (6.22) thus reduces to $k \neq 0$.

For the boundary value problem

$$\begin{cases} \bar{c}_v\theta_t - k\theta_{xx} + \mathtt{a}(\theta_t\theta_x)_x = 0, & x \in (0,1), \quad t \in \mathbb{R}^+, \\ \theta(x,0) = \dfrac{\mathtt{q}}{2}x^2, & x \in (0,1), \\ \partial_x\theta(0,t) = 0, & \\ \partial_x\theta(1,t) = \mathtt{q}, & \mathtt{q} \in \mathbb{R}, \end{cases} \tag{6.25}$$

we have an analytical solution:

$$\theta(x,t) = \frac{k\mathtt{q}}{\bar{c}_v + \mathtt{a}\mathtt{q}}t + \frac{\mathtt{q}}{2}x^2, \tag{6.26}$$

where $\mathtt{q}$ is a constant heat flux at the boundary. For a time interval $(0,T]$, we consider $\theta(x,t) \in \mathtt{H}^1((0,1)\times(0,T])$, select test functions $\varphi \in \mathcal{C}^\infty(\Omega)$ and integrate over $\Omega = (0,1)$. The boundary conditions imply

$$\int_0^1 \bar{c}_v\theta_t\varphi\,\mathrm{d}x + \int_0^1 k\theta_x\varphi'\,\mathrm{d}x - k\mathtt{q}\varphi(1) + \mathtt{a}\mathtt{q}\theta_t(1)\varphi(1) - \int_0^1 \mathtt{a}\theta_x\theta_t\varphi'\,\mathrm{d}x = 0.$$

For every t, we need $\Omega \ni x \mapsto \theta(x,t) \in \mathtt{H}^1(0,1)$ e $\Omega \ni x \mapsto \theta_t(x,t) \in \mathtt{H}^1(0,1)$. Set $\mathcal{V} := \mathtt{H}^1(\Omega)$. We have the following problem: *For every $t \in (0,T]$ find $\theta(t) \in \mathcal{V}$ such that $\forall\varphi \in \mathcal{V}$*

$$\int_0^1 \bar{c}_v\theta_t\varphi\,\mathrm{d}x + \int_0^1 k\theta_x\varphi'\,\mathrm{d}x - \int_0^1 \mathtt{a}\theta_x\theta_t\varphi'\,\mathrm{d}x - k\mathtt{q}\varphi(1) + \mathtt{a}\mathtt{q}\theta_t(1)\varphi(1) = 0.$$

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(ii) Semi-discretization with the Faedo-Galerkin method

Let $\mathcal{V}_h \subset \mathrm{H}^1(0,1)$ be a subspace of finite dimension and $\{\varphi_i\}_{i=1}^{\mathtt{N}}$ a pertinent basis. For every $t \in (0,T]$, we look for $\theta_h(\cdot,t) \in \mathcal{V}_h$ such that, for every φ_i, $i = 1:\mathtt{N}$,

$$\theta_h(x,t) = \sum_{j=1}^{\mathtt{N}} v_j(t)\varphi_j(x).$$

After the discretization associated with the choice of $\theta_h(x,t)$, the considered differential problem reduces to a system of ordinary differential equations given by

$$M\dot{\mathbf{v}} + K\mathbf{v} - (\mathbb{A}\mathbf{v})\dot{\mathbf{v}} = \mathbf{f}, \tag{6.27}$$

where

$$\tilde{M}_{ij} = \int_0^1 \bar{c}_v \varphi_i \varphi_j \,\mathrm{d}x + \mathtt{q}\,\mathtt{a}\,\varphi_i(1)\varphi_j(1), \quad K_{ij} = \int_0^1 k\varphi_i'\varphi_j' \,\mathrm{d}x, \quad i,j = 1:\mathtt{N},$$

and

$$\mathbb{A}_{ijk} = \int_0^1 \mathtt{a}\varphi_i'\varphi_j\varphi_k' \,\mathrm{d}x, \quad i,j,k = 1:\mathtt{N},$$

while the entries of $\mathbf{v}(t) \in \mathbb{R}^{\mathtt{N}}$ are the coefficients of $\theta_h(x,t)$ in the basis $\{\varphi_i\}_{i=1}^{\mathtt{N}}$, that is, $v_i(t)$, $i = 1:\mathtt{N}$ and those of $\mathbf{f} \in \mathbb{R}^{\mathtt{N}}$ are given by $\mathtt{f}_i = kq\varphi_i(1), \quad i = 1:\mathtt{N}$.

(iii) Finite elements

We choose $\mathtt{N}$ nodes $x_i = ih$, $i = 1:\mathtt{N}$ with $h = 1/(\mathtt{N}-1)$ being the constant length of the elements $\mathcal{I}_i := (x_i, x_{i+1})$, $i = 1:N-1$. For the basis of $\mathcal{V}_h$ we choose standard piece-wise linear functions with compact support. The load vector is $\mathbf{f} = k\mathtt{q}\,\mathbf{e}_{\mathtt{N}}$, where $\mathbf{e}_{\mathtt{N}}$ is the $\mathtt{N}^{th}$ vector of canonical basis. The nonlinear term in the equation (6.27) can be written as $A\dot{\mathbf{v}}$, where A is a matrix $\mathtt{N} \times \mathtt{N}$, whose ij-th element is defined by $A_{ij} = \sum_{k=1}^{\mathtt{N}} \mathbb{A}_{ijk} v_k$. In other words, A is the matrix given by the linear combination of the slices of $\mathbb{A}_{ij\hat{k}}$ for $\hat{k} = 1,\ldots,\mathtt{N}$ with coefficients equal to the components of vector $\mathbf{v}$.

(iv) Time integration with implicit Euler

We employ the backward Euler method. We fix a constant time step $\boldsymbol{\delta}t$ and denote by $\mathbf{v}^n \approx \mathbf{v}(t^n)$ the solution at time $t^n = n\boldsymbol{\delta}t$. Approximating the time derivative in (6.27) with a backward difference, we get a nonlinear system for $\mathbf{v}^{n+1}$ given by

$$(M + \boldsymbol{\delta}t\,K - \mathbb{A}\mathbf{v}^{n+1})\mathbf{v}^{n+1} = \boldsymbol{\delta}t\,\mathbf{f} + (M - \mathbb{A}\mathbf{v}^{n+1})\mathbf{v}^n. \tag{6.28}$$

For it we adopt a fixed point alghorithm:

1. Set $\mathbf{w}^{(0)} = \mathbf{v}^n$; % Initial guess: solution at previous time.
2. For $k = 0, 1, \ldots$ until convergence
3. $A^{(k)} = \mathbb{A}\mathbf{w}^{(k)}$;
4. $T^{(k)} = M + \boldsymbol{\delta}tK - A^{(k)}$;
5. $\mathbf{b}^{(k)} = \boldsymbol{\delta}t\mathbf{f} + (M - A^{(k)})\mathbf{v}^n$;
6. Solve $T^{(k)}\mathbf{w}^{(k+1)} = \mathbf{b}^{(k)}$;
7. Check for convergence $||T^{(k+1)}\mathbf{w}^{(k+1)} - \mathbf{b}^{(k+1)}||_2 < \tau$;
8. end For.

Convergence is achieved when the norm of the residual is smaller than a fixed tolerance $\tau > 0$, that is, when

$$||(M + \boldsymbol{\delta}tK - A^{(k)})\mathbf{w}^{(k)} - (M - A^{(k)})\mathbf{v}^n - \boldsymbol{\delta}t\mathbf{f}||_2 \le \tau,$$

where $||\cdot||_2$ is the Euclidean norm of vectors.

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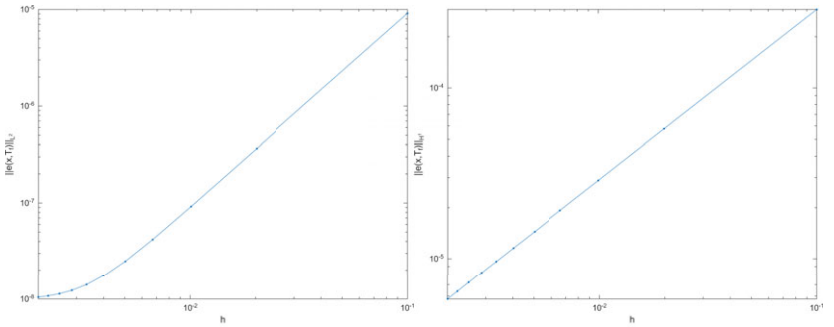

(a) L^2-norm (b) H^1-norm

Figure 5. L^2-norm and H^1-norm of the error function after 100 time steps as the mesh size h goes to zero.

Notice that, in the one-dimensional space, we do not need to save $\mathbb{A}$ because we can easily construct the three diagonals $A = \mathbb{A}\mathbf{w}$ for every vector $\mathbf{w}$.

In principle, problem (6.28) can be solved with other numerical methods for nonlinear systems of equations, for example, the Newton method. However, in the numerical experiment conducted, the approach adopted converged in fewer than 4 iterations at every time step.

(v) Convergence analysis

A convergence analysis of the finite element method described above was carried out on problem (6.25), whose analytical solution is given by equation (6.26). Take

$$k = 0.9, \quad \mathfrak{a} = 0.001, \quad \mathfrak{q} = 0.5.$$

The final time is fixed at $T = 0.1$ while the time step is $\delta t = 10^{-5}$. A convergence analysis, based on the discrete L^2 and H^1 norms of

$$e^n(x) = \theta(x, t^n) - \sum_{i=1}^{N} v_i(t^n)\varphi_i(x),$$

reveals that the error exhibits quadratic convergence in h with respect to the norm L^2, and linear convergence with respect to the norm H^1 (see figure 5). At each fixed-point iteration we have to solve a linear system, and the condition number of the matrix of the system grows as $\mathcal{O}(\frac{1}{h})$.

(vi) Heat flux at the boundary: an example

In the linearized equation (5.3), the mixed term $\boldsymbol{\zeta} \cdot \nabla\dot{\theta}$ introduces an anisotropy. In contrast, in the scheme leading to equation (6.16), the temperature gradient alone drives the heat transfer. Consider the *heat flux experiment*, which is a boundary value problem with nonhomogeneous time-varying Neumann boundary conditions. In one-dimensional space, the differential problem reads

$$\begin{cases} \bar{c}_v \dfrac{\partial\theta}{\partial t} - k\dfrac{\partial^2\theta}{\partial x^2} + \mathfrak{a}\dfrac{\partial}{\partial x}\left(\dfrac{\partial\theta}{\partial t}\dfrac{\partial\theta}{\partial x}\right) = 0, & x \in (0,1), \quad t \in \mathbb{R}^+, \\ \theta(x,0) = 1, & x \in (0,1) \quad \text{(homogeneous initial condition)} \\ \dfrac{\partial\theta}{\partial x}(0,t) = 0, & t \in (0,T_f] \quad \text{(adiabatic wall)} \\ \dfrac{\partial\theta}{\partial x}(1,t) = -\dfrac{1}{k}\mathfrak{q}(t) & \text{(prescribed heat flux)} \end{cases}.$$

Here, $\mathfrak{q} : \mathbb{R} \to \mathbb{R}$ is a heat flux that varies in time applied to the boundary $x = 1$, while we assume that at $x = 0$ the behaviour is adiabatic. The values of non-dimensional material parameters are

$$k = 1, \quad \bar{c}_v = 1, \quad \mathfrak{a} = 0.005, \quad \zeta = 0.01,$$

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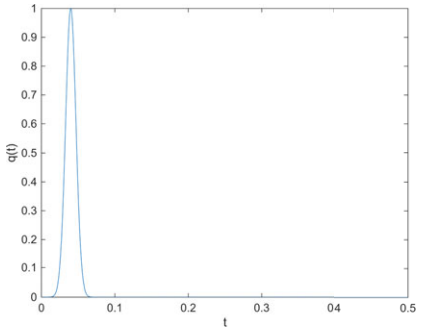

Figure 6. Heat flux boundary condition for $\tau = 10^4, \phi = 0.04$.

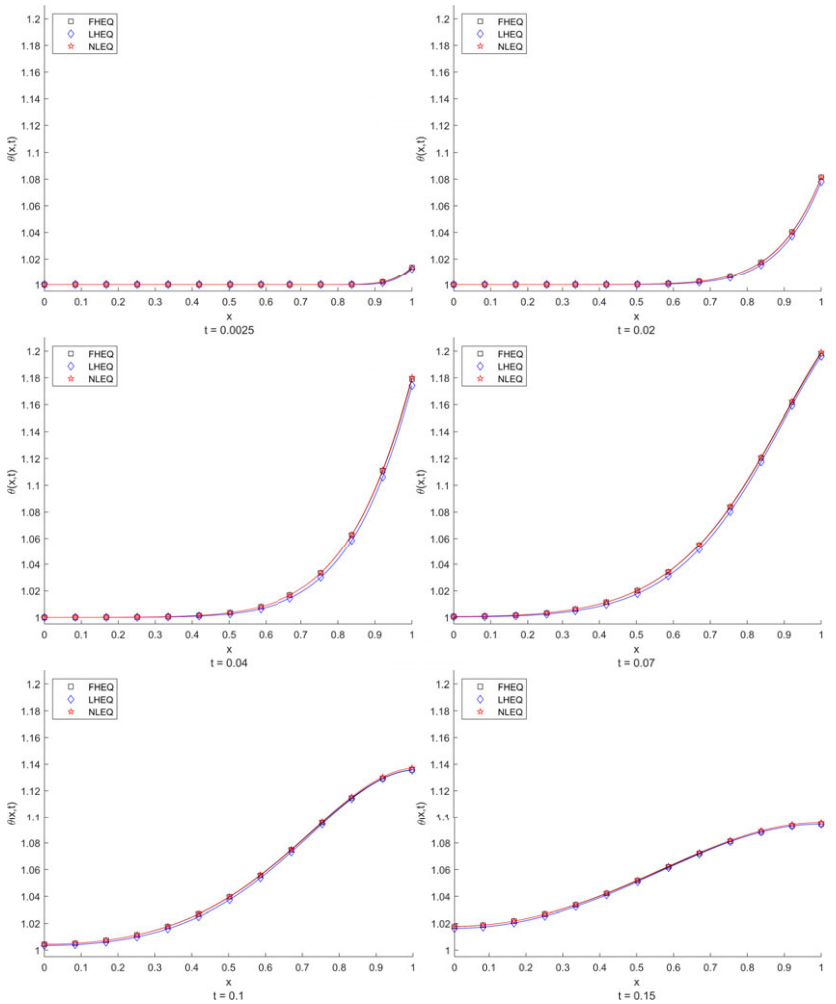

Figure 7. Numerical solution of the Neumann boundary value problem: comparison at different instants of the Fourier (parabolic) heat equation (FHEQ), the hyperbolic heat equation (5.3) (LHEQ), and the nonlinear heat equation (6.16) (NLEQ).

and the following heat flux is applied (see figure 6):

$$\mathrm{q}(t) = e^{-\tau(t-\phi)^2}, \quad \tau = 10^4, \quad \phi = 0.04. \tag{6.29}$$

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The integration domain is the interval $[0, 0.5]$. The time step is $\delta t = 10^{-4}$. The mesh size is $h = 5 \cdot 10^{-3}$. The results are in figure 7. From a qualitative viewpoint, when the material parameters related to the material microstructure are small with respect to the (nondimensional) thermal conductivity, the temperature profiles dictated by both the considered hyperbolic nonlinear and linear descriptions agree with the standard parabolic one; however, although the microstructural effects are small in these simulations, they determine a propagation of heat with finite speed.

7. Conclusion

The analyses developed so far apply directly to pyroelectric materials when the strain is negligible. They can be naturally extended to account for small and large strains. However, the view goes beyond the pyroelectric case. In fact, the above analyses do not depend on a particular microstructure. Every time a phase field is involved in the description of a body and the underlying physics allows us to admit an internal constraint that expresses the phase field as a function of temperature (with the possible addition of its derivatives), a structure as the one described in this paper may occur; it describes the experimentally recorded finite-speed heat propagation, although we accept the Fourier law.

Data accessibility. This article has no additional data.

Declaration of AI use. We have not used AI-assisted technologies in creating this article.

Authors' contributions. D.L.P.: formal analysis, investigation, methodology, software, validation, visualization, writing—original draft, writing—review and editing; P.M.M.: conceptualization, formal analysis, investigation, methodology, supervision, validation, writing—original draft, writing—review and editing.

Both authors gave final approval for publication and agreed to be held accountable for the work performed therein.

Conflict of interest declaration. We declare we have no competing interests.

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