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# Boundary Conditions for Diffusive-Hyperbolic Systems in Non-Equilibrium Thermodynamics [1]

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Dedicated to Professor Wolfgang Muschik on the occasion of his 65-th birthday.

*A model of a heat conductor with an internal variable, describing thermodiffusion as well as thermal wave propagation is developed. Boundary conditions for the obtained diffusive-hyperbolic system are derived from the second law of thermodynamics. Propagation of weak and strong discontinuities for the hyperbolic sub-system is analyzed.*

## 1 Introduction

The Causality Principle states that two events which are causally correlated cannot happen at the same time but the cause must precede the effect. From the mathematical point of view this implies that the differential equations of nature should exclude instantaneous propagation, i. e. these should be cast in the hyperbolic form. Yet, some equations of classical continuum mechanics and thermodynamics - those of Navier-Stokes and Fourier - are parabolic. Despite their apparent contrast with the Causality Principle these equations play a central role in thermodynamics. In fact:
- Fourier's and Navier-Stokes' theories are able to describe heat conduction and shear stress propagation in a wide range of pressure and temperature;
- in a fully Newtonian framework there is no limit for the admissible speeds of propagation of disturbances;
- in the linear case the thermomechanical signals result from the superposition of different contributions, propagating with finite and infinite speed, respectively. However, the second ones are strongly damped and become neglegible after a short interval of time (Fichera, 1992).

On the other hand in some cases, such as second sound propagation at low temperature, the parabolic theories are not in agreement with the experimental evidence (Narayanamurti and Dynes, 1972). In these phenomena the hyperbolic regime is present only in the vicinity of some critical values of the physical fields while outside that short interval the diffusive situation is restored. For instance, in dielectric crystals heat waves appear only at a given critical temperature (3.8 K for bismuth) while outside a short interval around the critical point the classical thermodiffusion takes place (Narayanamurti and Dynes, 1972). The latter example suggests that in non-equilibrium thermodynamics it would be desirable to construct models which are controlled by systems of equations containing some free parameters whose value determines the nature (parabolic or hyperbolic) of the system itself.

In the present paper we develop a nonlocal diffusive-hyperbolic model of a rigid heat conductor by applying a gradient theory of internal variable. To accomplish that task we need a reformulation of the causality requirement for the constitutive equations which is compatible with both hyperbolic and parabolic models. Furthermore, gradient theories of internal variable, when applied to bounded domains, require suitable boundary conditions. Such conditions, in turn, are difficult to assign since the internal variables are not controllable, i.e. their value on the boundary cannot be adjusted through a direct action of surface or body forces (Maugin and Muschik, 1994).

In what follows we provide a weak formulation of the Causality Constitutive Principle postulated in modern non-equilibrium thermodynamics (Muschik et al., 2001). Then we apply the aforesaid point of view in the derivation of a diffusive-hyperbolic model of heat conductor. We also prove that, in such a case, the boundary conditions follow from the set of the thermodynamic restrictions. In other words, the value of the internal variable on the boundary is controlled by the second law of thermodynamics. Further, we provide an example of a diffusive-hyperbolic system of equations by considering a one-dimensional heat conductor. We analyze the properties of the hyperbolic sub-system and calculate the speeds of propagation of weak and strong discontinuities. The selection rules for physical shocks are derived as well.

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## 2 Basic Laws and Constitutive Principles

Let $B$ denote a rigid body which occupies a compact and simply connected fixed region $C$ of an Euclidean point space $E^3$. A vector $\mathbf{x}$ of the associated vector space $\mathbf{E}^3$ denotes the position of the points of $C$. A thermodynamical process involving $B$ is represented by a curve, regular almost everywhere, in the thermodynamic state space $\Sigma$ spanned by the absolute temperature $\theta$, a scalar internal variable $\alpha$ together with their gradients $\mathbf{g} = grad\theta$ and $\mathbf{a} = grad\alpha$. Along with Muschik et al. (2001), we call $\theta$ and $\alpha$ the *wanted fields* while $\theta$, $\alpha$, $\mathbf{g}$, and $\mathbf{a}$ constitute the *basic fields.* The local balance of energy for a rigid heat conductor reads

$$\rho\dot{\epsilon} = -div\mathbf{q} + \rho r, \tag{2.1}$$

where $\rho$ is the mass density, $\epsilon$ the specific internal energy, $r$ the heat supply per unit of mass and $\mathbf{q}$ the heat flux vector (Coleman and Owen, 1974).
Moreover, the Clausius-Duhem inequality takes the form

$$-\rho\dot{\Psi} - \rho S\dot{\theta} - \frac{1}{\theta}\mathbf{q}\cdot\mathbf{g} \geq 0, \tag{2.2}$$

where $S$ means the specific entropy and $\Psi = \epsilon - \theta S$ defines the Helmholtz free energy, (Coleman and Owen, 1974). Finally, we postulate the following nonlocal evolution equation for $\alpha$

$$\dot{\alpha} = f(\theta, \dot{\theta}, \alpha, \mathbf{a}). \tag{2.3}$$

Because of the presence of $\mathbf{a}$ as an argument of $f$, (2.3) is a partial differential equation, requiring thus suitable boundary conditions. Additional memory effects are due to $\dot{\theta}$ appearing among the arguments of $f$. Equations (2.1) and (2.3) allow, in principle, the determination of the wanted fields $\theta$ and $\alpha$, i.e. the evolution of the system in $\Sigma$, once a suitable set of constitutive equations for the functions $(r, \epsilon, \Psi, \mathbf{q})$ and a suitable set of initial and boundary conditions for $\theta$ and $\alpha$ are assigned. Let us postulate the following constitutive equations:

$$\Phi = \Phi^*(\theta, \alpha, \mathbf{g}, \mathbf{a}). \tag{2.4}$$

Beside the material symmetry and suitable transformation properties by changing the observer (Muschik et al., 2001) the equations above must satisfy the following constitutive principles:

**Dissipation Principle** (Coleman and Owen, 1974)
*The constitutive equations (2.4) must be assigned in a form such that the local entropy inequality (2.2) is satisfied in any thermodynamic process.*

**Weak Causality Constitutive Principle** (Cimmelli, 2001)
*The constitutive equations (2.4) cannot enlarge the set of the admissible speeds following from the symmetry group of space-time transformations.*

Let us append some short comments to the requirements above. The first one follows from the second law of thermodynamics and it is used in the literature for a very long time (Coleman and Mizel, 1964; Coleman and Owen, 1974). However, only recently it received a rigorous theoretical justification by Muschik and Ehrentraut (1996), as a consequence of the *no-reversible direction axiom.* The second principle reformulates in a weak sense the strong causality requirement of extended non-equilibrium thermodynamics, (Müller and Ruggeri, 1998; Jou et al., 1996), proposed in the literature as a general material axiom of continuum thermodynamics (Muschik et al., 2001). The present formulation forces the constitutive equations to conserve the upper limit for the admissible speeds, if any. For instance, in relativistic continuum thermodynamics the symmetry group is that of the Minkowski space-time transformations and the hyperbolic property holds true inside the light cones. Such a property must be conserved by the constitutive equations for the energy-momentum tensor $T^{\alpha\beta}$ which is a material dependent property (Israel, 1976). In other cases the constitutive equations may restrict the set of the admissible speeds, such as in the extended theories (Müller and Ruggeri, 1998; Jou et al., 1996), or may not, such as in the classical theory of gravitation, which is elliptic, or in Fourier's and Navier-Stokes' theories, which are parabolic.

## 3 Boundary Conditions as Thermodynamic Restrictions

Exploitation of (2.2), in order to restric the constitutive equations, may be performed by several procedures (Muschik et al., 2001). Here we apply a slight modification of the Coleman-Gurtin technique (Coleman and Gurtin, 1967), which works in the presence of internal variables. To this end let us take the gradient of (2.3) which yields

$$\dot{\mathbf{a}} = \frac{1}{\tau}\mathbf{g} - \frac{1}{\mu}\dot{\mathbf{g}} + \frac{1}{\nu}\mathbf{a} + \frac{\partial f}{\partial \mathbf{a}}\nabla\mathbf{a}, \tag{3.1}$$

where

$$\frac{1}{\tau} =: \frac{\partial f}{\partial \theta},\ \frac{1}{\mu} =: -\frac{\partial f}{\partial \dot{\theta}},\ \frac{1}{\nu} =: -\frac{\partial f}{\partial \alpha}. \tag{3.2}$$

Once (3.1) is introduced into (2.2) and the time derivative of $\Psi$ is calculated, one obtains

$$\mathbf{B}\cdot\mathbf{y} + \mathbf{C}\cdot\nabla\mathbf{a} + D \geq 0, \tag{3.3}$$

with

$$\mathbf{y}^T =: \left(\dot{\theta}, \dot{\alpha}, \dot{\mathbf{g}}\right), \tag{3.4}$$

$$\mathbf{B} =: \left[-\rho\left(\frac{\partial \Psi}{\partial \theta} + S\right),\ \frac{\partial \Psi}{\partial \alpha},\ \rho\left(\frac{1}{\mu}\frac{\partial \Psi}{\partial \mathbf{a}} - \frac{\partial \Psi}{\partial \mathbf{g}}\right)\right], \tag{3.5}$$

$$\mathbf{C} =: -\left(\rho\frac{\partial \Psi}{\partial \mathbf{a}} \otimes \frac{\partial f}{\partial \mathbf{a}}\right), \tag{3.6}$$

$$D =: \left[\frac{\rho}{\nu}\frac{\partial \Psi}{\partial \mathbf{a}}\cdot\mathbf{a} - \left(\frac{\rho}{\tau}\frac{\partial \Psi}{\partial \mathbf{a}} + \frac{\mathbf{q}}{\theta}\right)\cdot\mathbf{g}\right]. \tag{3.7}$$

As a result of the the Coleman-Gurtin procedure we may conclude that (3.3) is satisfied in any thermodynamic process if the following restrictions hold true

$$\mathbf{B} = \mathbf{0}, \tag{3.8}$$

$$\mathbf{C} = -\mathbf{C}^T, \tag{3.9}$$

$$D \geq 0. \tag{3.10}$$

In particular, equation (3.9) may be trivially satisfied if either $\frac{\partial f}{\partial \mathbf{a}} = \mathbf{0}$ or $\frac{\partial \Psi}{\partial \mathbf{a}} = \mathbf{0}$. In both cases it is easily seen that the evolution equation (2.3) reduces to an ordinary differential equation and no boundary conditions are needed (Cimmelli, 2001). If instead (3.9) is not trivially satisfied the following orthogonality condition ensues

$$\frac{\partial \Psi}{\partial \mathbf{a}}\cdot\frac{\partial f}{\partial \mathbf{a}} = 0. \tag{3.11}$$

A similar restriction has been obtained by Kosiński and Wojno in dealing with a hyperbolic theory of heat conduction (Kosiński and Wojno, 1995). When evaluated on $\partial C$, equation (3.11) will result in a boundary condition for $\alpha$ and $\mathbf{a}$, whose values on the boundary are in such a way controlled by the second law of thermodynamics. As a worked example let us consider the following scalar functions:

$$f = f_1(\theta) + \frac{1}{2}f_2(\alpha)a^2 + \mathbf{d}(\alpha)\cdot\mathbf{a}, \tag{3.12}$$

$$\Psi = \Psi_1(\theta) + \frac{1}{2}\Psi_2(\theta)a^2 + \mathbf{c}(\theta)\cdot\mathbf{a}. \tag{3.13}$$

In (3.12)-(3.13) $\mathbf{c}$ and $\mathbf{d}$ are given vector fields and, as usual in the internal variable theory, both $f$ and $\Psi$ are splitted into a classical part, depending on the observable quantities only, and an intrinsic one, depending also on the internal fields $\alpha$ and $\mathbf{a}$. Then (3.11) leads to the orthogonality condition

$$\mathbf{d} \cdot \mathbf{c} + \Big(\Psi_2 \mathbf{d} + f_2 \mathbf{c} + \Psi_2 f_2 \mathbf{a}\Big) \cdot \mathbf{a} = 0. \tag{3.14}$$

By evaluating equation (3.14) on $\partial C$ the following boundary conditions may be obtained:
1. Dirichlet's type boundary condition:

$$\Psi_2 = f_2 = 0 \ \ on \ \partial C \ \ \Rightarrow \mathbf{d} \cdot \mathbf{c} = 0 \ \ on \ \partial C. \tag{3.15}$$

Equation (3.15) allow to express the boundary value of $\alpha$ as a given function of the absolute temperature $\theta$. Hence it may be regarded as a Dirichlet's boundary condition.
2. Neumann's type boundary condition:

$$\Big(\mathbf{d} = \mathbf{0}, \ \Psi_2 = 0\Big) \ \ on \ \partial C \ \ \Rightarrow \mathbf{c} \cdot \mathbf{a} = 0 \ \ on \ \partial C. \tag{3.16}$$

Equation above yields the component of the gradient of $\alpha$ along the direction of the vector $\mathbf{c}$. Since such a vector is a controllable quantity its value on the boundary may be conditioned, through the action of external forces, in such a way that $\mathbf{c} = c(\theta)\mathbf{n}$. Then the classical Neumann's boundary condition is recovered.
3. Mixed boundary condition:

$$\Psi_2 = 0 \ \ on \ \partial C \ \ \Rightarrow \mathbf{d} \cdot \mathbf{c} + f_2 \mathbf{c} \cdot \mathbf{a} = 0 \ \ on \ \partial C. \tag{3.17}$$

Finally, let us draw again the attention of the reader to the main difficulty in determining the boundary conditions for internal variables. It consists in the lack of their controllability through the direct action of surface or body forces. Thence we need boundary conditions which are necessarily satisfied by virtue of some general physical laws. According to the present approach the value of the internal variable on the boundary is controlled by the second law of thermodynamics. A similar point of view has been applied by Valanis (1996), Waldman (1967) and Drouot and Maugin (2001).

## 4 Shock Wave Formation in the Hyperbolic Regime

In order to better point out the transition from the parabolic to the hyperbolic regime let us consider a one-dimensional rigid heat conductor and let us postulate the following constitutive equations:

$$\epsilon = \epsilon(\theta), \tag{4.1}$$

$$r = r(\theta, \alpha), \tag{4.2}$$

$$q = -\chi_1 \theta_x - \chi_2 \alpha_x, \tag{4.3}$$

with $F_y =: \frac{\partial F}{\partial y}$ while $\chi_1$ and $\chi_2$ are constant. Finally, let us postulate for $\alpha$ the linear evolution equation:

$$k_1 \theta_t + k_2 \alpha_t - \delta_3 \alpha_x = \tau\theta + \sigma\alpha, \tag{4.4}$$

where, again, the material functions $k_1$, $k_2$, $\tau$, $\sigma$ and $\delta_3$ take constant values. By writing

$$\chi_1 = k_1 + \delta_1, \ \ \chi_2 = k_2 + \delta_2, \tag{4.5}$$

we get

$$\rho c_v \theta_t + q_x = \rho r, \tag{4.6}$$

$$q_t + \tau\theta_x + \sigma\alpha_x = -\delta_1\theta_{xt} - \delta_2\alpha_{xt} - \delta_3\alpha_{xx}, \tag{4.7}$$

$$k_1\theta_t + k_2\alpha_t - \delta_3\alpha_x = \tau\theta + \sigma\alpha, \tag{4.8}$$

where $c_v(\theta) = \frac{\partial\epsilon}{\partial\theta} > 0$ is the specific heat. Due to the presence of the operator of diffusion $\delta(x,t) =: -\delta_1\theta_{xt} - \delta_2\alpha_{xt} - \delta_3\alpha_{xx}$ the system above results to be parabolic. However, as $\delta_1$, $\delta_2$ and $\delta_3$ tend to zero, it yields the hyperbolic sub-system

$$\rho c_v\theta_t + q_x = \rho r, \tag{4.9}$$

$$q_t + \tau\theta_x + \sigma\alpha_x = 0, \tag{4.10}$$

$$k_1\theta_t + k_2\alpha_t = \tau\theta + \sigma\alpha. \tag{4.11}$$

Such a system admits the characteristic speeds $U = 0$ and

$$U(\theta) = \frac{-(\rho c_v(\theta) + k_1)}{2} \pm \frac{\sqrt{(\rho c_v(\theta) + k_1)^2 + 4\rho c_v(\theta)k_1}}{2}, \tag{4.12}$$

which depend only on $\theta$ and take real values if $k_1 > 0$. Because of the nonlinear constitutive equations for $\epsilon$ and $r$ the system above is non-linear, allowing thus shock wave formation after a finite time. Such waves are represented by a plane of equation $\phi(x,t) = 0$, the shock front, across which the fields $(\theta, \alpha, q)$ are discontinuous. Let us denote by $\left(\theta_0, \alpha_0, q_0\right)$ the unperturbed state ahead of the shock and by $\left(\theta_1, \alpha_1, q_1\right)$ the perturbed state behind the shock. The Rankine-Hugoniot compatibility conditions read (Boillat, 1965)

$$-\rho s[\epsilon] + [q] = 0, \tag{4.13}$$

$$-s[q] + [\tau\theta + \sigma\alpha] = 0, \tag{4.14}$$

$$-s[k_1\theta + k_2\alpha] = 0, \tag{4.15}$$

where $s$ means the velocity of the shock and $[F] =: F_1 - F_0$. Let us observe that, although both functions $\theta$ and $\alpha$ are discontinuous across the shock, their linear combination $k_1\theta + k_2\alpha$ is not. Moreover, if one assumes $\epsilon(\theta) = \epsilon_0\theta^4$, which represents the Debye's internal energy of crystals at low temperature (Narayanamurti and Dynes, 1972), then the characteristic and shock velocities read

$$U(\theta) = -2\rho\epsilon_0\theta^3 - \frac{k_1}{2} + \sqrt{4\rho^2\epsilon_0^2\theta^6 + \frac{k_1^2}{4} + 6k_1\rho\epsilon_0\theta^3}, \tag{4.16}$$

$$s(\theta_1) = \pm\sqrt{\frac{\tau k_2 - \sigma k_1}{\rho\epsilon_0 k_2\left(\theta_1^2 + \theta_0^2\right)\left(\theta_1 + \theta_0\right)}}. \tag{4.17}$$

Equation (4.17) proves that, once the unperturbed state is known, $s$ depends only on the temperature behind the shock and vanishes if $\tau k_2 - \sigma k_1 = 0$ (characteristic shock), (Boillat, 1965). The physically meaningful shocks among the solutions which are compatible with (4.13)-(4.15) are selected by the Lax condition (Lax, 1973), traducing the physical requirement of non-decreasing entropy across the shock front. It reads

$$U(\theta_1) > s(\theta_1) > U(\theta_0). \tag{4.18}$$

When applied to the present case, the condition above yields

$$-2\rho\epsilon_0\theta_1^3 - \frac{k_1}{2} + \sqrt{4\rho^2\epsilon_0^2\theta_1^6 + \frac{k_1^2}{4} + 6k_1\rho\epsilon_0\theta_1^3} > \tag{4.19}$$

$$\sqrt{\frac{\tau k_2 - \sigma k_1}{\rho\epsilon_0 k_2\left(\theta_1^2 + \theta_0^2\right)\left(\theta_1 + \theta_0\right)}} >$$

$$-2\rho\epsilon_0\theta_0^3 - \frac{k_1}{2} + \sqrt{4\rho^2\epsilon_0^2\theta_0^6 + \frac{k_1^2}{4} + 6k_1\rho\epsilon_0\theta_0^3}$$

for waves propagating in the positive direction and an analogous inequality for waves propagating in the negative direction.

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