



Anisotropic heterogeneous n -D heat equation with boundary control and observation: I. Modeling as port-Hamiltonian system*

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Abstract The aim of this paper is to recast the heat equation with boundary control and observation in the port-Hamiltonian formalism. The anisotropic and heterogeneous case in an n -D geometrical domain is systematically developed. Three different points of view are presented. The first two are thermodynamically founded, taking either entropy or energy as Hamiltonian functional. With the choice of entropy, the second principle can be recovered. With the choice of energy, following Zhou et al. (2017), extra physical variables are introduced allowing to recover the first principle. The third formulation is classical from a mathematical perspective, although less meaningful physically speaking; however the Hamiltonian proves to be a Lyapunov functional, which is useful for boundary control purposes. Moreover, all these three formulations can be discretized with a structure-preserving scheme, as presented in the companion paper Serhani et al. (2019a).

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1. INTRODUCTION

Port-Hamiltonian systems (pHs) have proved very efficient for the modeling and control of complex multiphysics systems (Maschke and van der Schaft (1992); Duindam et al. (2009)). It allows in particular to tackle the problem of model-based controllers design. The approach relies on a functional, namely the Hamiltonian, which encodes physical information about the system; a geometrical interconnection structure is another key ingredient of the approach. This leads to a useful *power balance*, and in particular to the relevant ways to control and observe the system (w.r.t. this choice of Hamiltonian). Modularity is a salient feature of pHs: interconnecting two of them through their *ports* (boundary input/control and boundary output/observation for instance) leads to a new pHs. A Hamiltonian for the obtained pHs is easily computed from the Hamiltonians of the subsystems. Hence the power balance of complex systems can be obtained from the power balances of the simpler subsystems. Furthermore, the pHs formalism allows to tackle non-linear systems (van der Schaft and Jeltsema (2014)).

It has to be noted that this formalism lies half-way between physics and mathematics. It aims at taking into account the geometrical structure of the system under consideration, together with the physical meaning of the variables or fields used for its description. In particular, it puts apart physical laws (such as conservation law, balance

equation, etc.), parameters (such as diffusivity coefficient, mass density, etc.), and constitutive relations (such as Ohm's law, Fourier's law, etc.).

The terminology *pHs* comes from dynamical systems driven by Hamilton's equation in finite dimension. The energy variables are the generalized momenta and positions, and the flows are their time derivatives. Taking the mechanical energy as Hamiltonian, one can derive the efforts through its gradient and obtain a system of the form (1) below: see e.g. van der Schaft and Jeltsema (2014) for an introduction to this formalism.

In the last two decades, a wide literature has grown around pHs formalism. It has been generalized to infinite-dimensional systems (van der Schaft and Maschke (2002); Duindam et al. (2009); Jacob and Zwart (2012)), to tackle space-time dynamics. Other types of Hamiltonians than the physical energy have been used (see for instance van der Schaft and Maschke (2018)), leading to different kinds of information about the system under study. We can note that the description we use here is not the more general framework of pHs, but it is sufficient for our purpose. A more recent topic is to provide accurate discretization methods (both in time and space) to preserve this powerful formalism. Several strategies have been tested to this aim, as the finite difference method (Kotyczka (2018)), the finite volume method (Kotyczka et al. (2018)) and the finite element method (Cardoso-Ribeiro et al. (2018)) for instance. The latter is both an easy to implement and accurate way to proceed in so far as it can be structure-preserving when making use of the Partitioned Finite Element Method (PFEM), as will be

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proved in the companion paper Serhani et al. (2019a); this method is fully detailed in Cardoso-Ribeiro et al. (2019) for conservative systems, and has recently been extended to dissipative systems in Serhani et al. (2019c).

In this work, we aim to apply the pHs formalism to the heat equation in the anisotropic and heterogeneous case, in an n -D geometrical domain; the choice of three different Hamiltonian functionals leads to three different points of view, which prove complementary. The first two are thermodynamically founded: the entropy and the internal energy, while the third one is less meaningful physically speaking, but enjoys an interesting behavior on a mathematical level. The latter should be rather considered as a candidate Lyapunov functional for boundary control purposes. In the three cases, thermodynamical laws (*i.e.* constitutive relations) are needed to close the system; they strongly rely on the context (we can think for instance of Dulong-Petit, Einstein or Debye models, linking the internal energy to the temperature, and to Fourier's law or Cattaneo's law linking the heat flux to the temperature). In other words, relevant constitutive relations are needed for the physical case under study. However, with the pHs formalism, since constitutive relations are put apart, this need can happily be postponed. As will be seen in Serhani et al. (2019a), an interesting consequence at the numerical level is that the work on the discretization of the physical laws comes first, while the discretization of the constitutive relations comes at the end of the strategy.

Mathematically, the Hamiltonian \mathcal{H} depends on what are called *energy variables*, typically *extensive* variables for the problem under study. Taking the variational derivatives (an analogue of the gradient in finite dimension) of \mathcal{H} with respect to the energy variables gives the *co-energy variables*, typically *intensive* variables. Using physical laws, these variables allow to write a system into the following form (which can be called *boundary pHs*)

$$\vec{\mathbf{f}} = \mathcal{J}\vec{\mathbf{e}}, \quad v_\partial = \mathcal{B}\vec{\mathbf{e}}, \quad y_\partial = \mathcal{C}\vec{\mathbf{e}}, \quad (1)$$

where

- $\vec{\mathbf{f}}$ are the *flows*,
- $\vec{\mathbf{e}}$ are the *efforts*,
- \mathcal{J} is a formally skew-symmetric operator,
- \mathcal{B} is a control operator,
- \mathcal{C} is an observation operator,
- v_∂ is the control (or input, or actuation),
- y_∂ is the observation (or output, or measurement).

All vector fields and related quantities will be denoted in bold with an arrow.

Parameters are contained in the definitions of $\vec{\mathbf{f}}$ and $\vec{\mathbf{e}}$, while \mathcal{J} is a structure operator which can involve spatial derivatives but does not contain any parameter.

Moreover, some extra constitutive relations between $\vec{\mathbf{f}}$ and $\vec{\mathbf{e}}$ are needed to close the system (possibly introducing new physical parameters) in order to be able to solve it.

The operators \mathcal{B} and \mathcal{C} are typically boundary operators, such as boundary trace operators (hence the name boundary pHs and the ∂ index for v_∂ and y_∂). In suitable functional spaces, \mathcal{B} and \mathcal{C} have to satisfy a relation with respect to the operator \mathcal{J} ; roughly speaking this relation corresponds to the default of skew-adjointness. We do not

enter in these mathematical considerations further, since this is not the topic of this paper (see for instance Kurula and Zwart (2015)). Keep in mind that this is closely related to the following Green formula in our case of interest:

$$\int_{\Omega} f \operatorname{div}(\vec{\mathbf{g}}) + \int_{\Omega} \overrightarrow{\operatorname{grad}}(f) \cdot \vec{\mathbf{g}} = \int_{\partial\Omega} f \vec{\mathbf{g}} \cdot \vec{\mathbf{n}},$$

where $\Omega \subset \mathbb{R}^n$ is an open connected set and $\vec{\mathbf{n}}$ its outward unit normal.

The paper is organized as follows. In Section 2, the thermodynamical setting is presented and the useful notations are introduced. Then, the three continuous models, based on physical laws, are rewritten in the pHs formalism. In Section 3, the choice of entropy as Hamiltonian leads to an anti-dissipative closed system, or an accrescent open system. In Section 4, the choice of internal energy as Hamiltonian leads to a conservative closed system, or a lossless open system. In Section 5, the choice of a weighted L^2 functional of the internal energy density leads to a dissipative closed system, or a lossy open system. We conclude in Section 6 with a discussion on the comparison of the three points of view, and propose some interesting perspectives.

2. THERMODYNAMICAL HYPOTHESES AND NOTATIONS

All the thermodynamical material listed in this section can be found in e.g. Bird et al. (2002).

Let $\Omega \subset \mathbb{R}^n$ be a bounded open connected set, $n \geq 1$, with mass density $\rho(\mathbf{x})$, for all $\mathbf{x} \in \Omega$; and $\vec{\mathbf{n}}$ denotes the outward unit normal on the boundary $\partial\Omega$. We suppose that this domain does not change over time, *i.e.* we work at *constant volume*. No chemical reactions are to be found in the domain.

Let us denote

- u the internal energy density,
- $\vec{\mathbf{J}}_Q$ the heat flux,
- T the local temperature,
- $\beta := \frac{1}{T}$ the reciprocal temperature,
- s the entropy density,
- $\vec{\mathbf{J}}_S := \beta \vec{\mathbf{J}}_Q$ the entropy flux,
- $C_V := \left(\frac{du}{dT} \right)_V$ the isochoric heat capacity.

The first law of thermodynamics reads

$$\rho(\mathbf{x}) \partial_t u(t, \mathbf{x}) = -\operatorname{div}(\vec{\mathbf{J}}_Q(t, \mathbf{x})), \quad \forall t \geq 0, \mathbf{x} \in \Omega. \quad (2)$$

Under our hypothesis, Gibbs formula reads $dU = T dS$, *i.e.*

$$\partial_t u(t, \mathbf{x}) = T(t, \mathbf{x}) \partial_t s(t, \mathbf{x}), \quad \forall t \geq 0, \mathbf{x} \in \Omega. \quad (3)$$

Considering u as a function of the entropy s , and using Gibbs formula (3), we get for all $t \geq 0$ and all $\mathbf{x} \in \Omega$

$$\rho(\mathbf{x}) \partial_t s(t, \mathbf{x}) = -\operatorname{div}(\vec{\mathbf{J}}_S(t, \mathbf{x})) + \sigma(t, \mathbf{x}), \quad (4)$$

where $\sigma := \overrightarrow{\operatorname{grad}}(\beta) \cdot \vec{\mathbf{J}}_Q$ is the irreversible entropy production.

In the sequel, we will often take a look at what is obtained when using Fourier's law as constitutive relation:

$$\vec{\mathbf{J}}_Q(t, \mathbf{x}) = -\bar{\lambda}(\mathbf{x}) \cdot \overrightarrow{\mathbf{grad}}(T(t, \mathbf{x})), \quad \forall t \geq 0, \mathbf{x} \in \Omega, \quad (5)$$

where $\bar{\lambda}$ is a tensor representing the thermal conductivity; it is a positive symmetric tensor thanks to Onsager's reciprocal relations. Note that the use of a tensor enables dealing with anisotropic media. Usual (*i.e.* isotropic) Fourier's law can be recovered with $\bar{\lambda} = \lambda_0 \bar{I}$, where \bar{I} is the identity tensor.

With the above material, and in particular assuming (5), the classical PDE for the temperature T can be easily recovered: for all $t \geq 0$ and all $\mathbf{x} \in \Omega$,

$$\rho(\mathbf{x}) C_V(t, \mathbf{x}) \partial_t T(t, \mathbf{x}) = \operatorname{div} (\bar{\lambda}(\mathbf{x}) \cdot \overrightarrow{\mathbf{grad}}(T(t, \mathbf{x}))). \quad (6)$$

This equation will serve later as a reference for the numerical simulations, since it is classical and easy to discretize with the finite element method (at least when C_V is time-invariant, as supposed in the Dulong-Petit model).

3. ENTROPY FORMULATION

Let us see the entropy density s as a function of the internal energy density u , and define the entropy of the system as Hamiltonian functional, *i.e.*

$$S(t) := \int_{\Omega} \rho(\mathbf{x}) s(u(t, \mathbf{x})) \, d\mathbf{x}, \quad (7)$$

for all $t \geq 0$, with u as energy variable. By definition, the co-energy variable is given by the variational derivative of S w.r.t. u in the weighted $L^2_{\rho}(\Omega)$ space (*i.e.* with measure $\rho(\mathbf{x}) \, d\mathbf{x}$, an important point to take in account when making use of Riesz representation theorem); by Gibbs formula (3), we get:

$$\delta_u S = \frac{ds}{du} = \beta.$$

Thus, thanks to (3) and (4), one computes

$$\begin{aligned} d_t S(t) &= \int_{\Omega} \rho(\mathbf{x}) \partial_t u(t, \mathbf{x}) \beta(t, \mathbf{x}) \, d\mathbf{x}, \\ &= \int_{\Omega} \rho(\mathbf{x}) \partial_t s(t, \mathbf{x}) \, d\mathbf{x}, \\ &= - \int_{\Omega} \operatorname{div} (\vec{\mathbf{J}}_S(t, \mathbf{x})) \, d\mathbf{x} + \int_{\Omega} \sigma(t, \mathbf{x}) \, d\mathbf{x}, \\ &= - \int_{\partial\Omega} \vec{\mathbf{J}}_S(t, \gamma) \cdot \vec{\mathbf{n}}(\gamma) \, d\gamma + \int_{\Omega} \sigma(t, \mathbf{x}) \, d\mathbf{x}, \\ &= - \int_{\partial\Omega} \beta(t, \gamma) \vec{\mathbf{J}}_Q(t, \gamma) \cdot \vec{\mathbf{n}}(\gamma) \, d\gamma \\ &\quad + \int_{\Omega} \sigma(t, \mathbf{x}) \, d\mathbf{x}. \end{aligned}$$

The last equality comes from the definition of $\vec{\mathbf{J}}_S$. This relation expresses the power balance associated to the entropy as Hamiltonian. In particular, by the second law of thermodynamics, we can see that $\int_{\Omega} \sigma$ has to be positive. However, this requires a constitutive relation, for instance between $\overrightarrow{\mathbf{grad}}(\beta)$ and $\vec{\mathbf{J}}_Q$ (in view of the definition of σ), to conclude.

With Fourier's law (5) as constitutive relation, we obtain

$$\begin{aligned} d_t S(t) &= \int_{\partial\Omega} \beta(t, \gamma) \left(\bar{\lambda}(\gamma) \cdot \overrightarrow{\mathbf{grad}}(T(t, \gamma)) \right) \cdot \vec{\mathbf{n}}(\gamma) \, d\gamma \\ &\quad + \int_{\Omega} \beta(t, \mathbf{x})^2 \overrightarrow{\mathbf{grad}}(T(t, \mathbf{x})) \cdot \bar{\lambda}(\mathbf{x}) \cdot \overrightarrow{\mathbf{grad}}(T(t, \mathbf{x})) \, d\mathbf{x}. \end{aligned}$$

So that $\int_{\Omega} \sigma$ is indeed positive, since $\bar{\lambda}$ is a positive symmetric tensor.

Moreover, the latter power balance suggests one possible definition for the boundary ports of the pHs in terms of the Dirichlet trace of the reciprocal temperature β , and the normal trace of the heat flux $\vec{\mathbf{J}}_Q$ at the boundary $\partial\Omega$ of the domain.

Define $f_u := \partial_t u$ as the first flow, associated to the energy variable u . By definition of the co-energy variable, the dual effort is $e_u := \beta$. Since the relation $\rho f_u = -\operatorname{div} \vec{\mathbf{J}}_Q$ must be fulfilled, we also define the effort $\vec{\mathbf{e}}_Q := \vec{\mathbf{J}}_Q$. Thus, with the following definition $\vec{\mathbf{f}}_Q := -\overrightarrow{\mathbf{grad}}(\beta)$, this leads to

$$\left(\frac{\rho f_u}{\vec{\mathbf{f}}_Q} \right) = \begin{pmatrix} 0 & -\operatorname{div} \\ -\overrightarrow{\mathbf{grad}} & 0 \end{pmatrix} \left(\frac{e_u}{\vec{\mathbf{e}}_Q} \right). \quad (8)$$

Remark that no additional hypothesis is needed at this stage. Flows and efforts are defined in order to make a link between the quantities through a skew-symmetric operator. In particular, the equality $\vec{\mathbf{f}}_Q = -\overrightarrow{\mathbf{grad}}(e_u)$ (which in turn is only algebraic and not dynamic) will not help solve the system without resorting to an extra constitutive relation linking $\vec{\mathbf{f}}_Q$ and $\vec{\mathbf{e}}_Q$ (such as Fourier's law (5) for instance). At first glance, this could seem a bit redundant, even unnecessarily complicated, but it leads to the powerful structure (1) described in the introduction.

A technical point to discuss is why f_u is defined by $f_u := \partial_t u$, and not by $f_u := \rho \partial_t u$? Indeed, the latter definition seems more straightforward, in view of (1). However, we work in L^2_{ρ} to define e_u . Thus $f_u := \partial_t u$ indeed, but in $L^2_{\rho}(\Omega)$, roughly speaking, and so (1) is true in appropriate functional spaces. The multiplication of the flow f_u by ρ is then done, so as to work back in the $L^2(\Omega)$ space, which will be more practical in the discretization process.

Concerning the choice of boundary ports, we refer to Le Gorrec et al. (2005) for a full characterization of all the possible boundary ports for 1D linear systems. Here in n -D, there are at least two straightforward choices, although more general ones could be investigated. For the first choice, $\mathcal{B}\vec{\mathbf{e}} := e_u|_{\partial\Omega}$, and $\mathcal{C}\vec{\mathbf{e}} := -(\vec{\mathbf{e}}_Q \cdot \vec{\mathbf{n}})|_{\partial\Omega}$, *i.e.* the boundary control is the reciprocal temperature, and the boundary observation is the heat flux. For the second choice, $\mathcal{B}\vec{\mathbf{e}} := -(\vec{\mathbf{e}}_Q \cdot \vec{\mathbf{n}})|_{\partial\Omega}$, and $\mathcal{C}\vec{\mathbf{e}} := e_u|_{\partial\Omega}$, *i.e.* the boundary control is the heat flux, and the boundary observation is the reciprocal temperature. Note that the choice of the signs is a convention (control or observe the inward flux).

With these notations at hand, we get the power balance in terms of the pHs variables

$$\begin{aligned} d_t S(t) &= \int_{\partial\Omega} v_{\partial}(t, \gamma) y_{\partial}(t, \gamma) \, d\gamma \\ &\quad - \int_{\Omega} \vec{\mathbf{f}}_Q(t, \mathbf{x}) \cdot \vec{\mathbf{e}}_Q(t, \mathbf{x}) \, d\mathbf{x}. \quad (9) \end{aligned}$$

With $-\int_{\Omega} \vec{f}_Q(t, \mathbf{x}) \cdot \vec{e}_Q(t, \mathbf{x}) d\mathbf{x} = \int_{\Omega} \sigma \geq 0$, the closed system is anti-dissipative, i.e. $d_t S(t) \geq 0$, and the open system is accrescent, i.e. $d_t S(t) \geq (v_{\partial}(t), y_{\partial}(t))_{L^2(\partial\Omega)} = -\int_{\partial\Omega} e_{u|_{\partial\Omega}} (\vec{e}_Q \cdot \vec{n})_{|\partial\Omega} d\gamma$.

4. ENERGY FORMULATION

Now, let us see the internal energy density u as a function of the entropy density s , and define the internal energy of the system as Hamiltonian functional, i.e.

$$U(t) := \int_{\Omega} \rho(\mathbf{x}) u(s(t, \mathbf{x})) d\mathbf{x}, \quad (10)$$

for all $t \geq 0$, with s as energy variable. The same strategy as in the previous section is now being applied.

The co-energy variable is given by the variational derivative of U w.r.t. s :

$$\delta_s U = \frac{du}{ds} = T.$$

Hence, from Gibbs formula (3) and (2), one computes

$$\begin{aligned} d_t U(t) &= \int_{\Omega} \rho(\mathbf{x}) \partial_t s(t, \mathbf{x}) T(t, \mathbf{x}) d\mathbf{x}, \\ &= \int_{\Omega} \rho(\mathbf{x}) \partial_t u(t, \mathbf{x}) d\mathbf{x}, \\ &= - \int_{\Omega} \operatorname{div} (\vec{\mathbf{J}}_Q(t, \mathbf{x})) d\mathbf{x}, \\ &= - \int_{\partial\Omega} \vec{\mathbf{J}}_Q(t, \gamma) \cdot \vec{n}(\gamma) d\gamma, \\ &= - \int_{\partial\Omega} T(t, \gamma) \vec{\mathbf{J}}_S(t, \gamma) \cdot \vec{n}(\gamma) d\gamma. \end{aligned}$$

This latter power balance suggests to define the boundary ports of the pHs in terms of the Dirichlet trace of the temperature T , and the normal trace of the entropy flux $\vec{\mathbf{J}}_S$ at the boundary $\partial\Omega$ of the domain.

Define $f_s := \partial_t s$ as the first flow, associated to the energy variable s . By definition of the co-energy variable, the dual effort is $e_s := T$. Since $\rho f_s = -\operatorname{div} \vec{\mathbf{J}}_S + \sigma$ must be fulfilled, we also define the effort $\vec{e}_S := \vec{\mathbf{J}}_S$. Now, defining $\vec{f}_S := -\overrightarrow{\operatorname{grad}}(T)$ leads to:

$$\begin{pmatrix} \rho f_s \\ \vec{f}_S \end{pmatrix} = \begin{pmatrix} 0 & -\operatorname{div} \\ -\overrightarrow{\operatorname{grad}} & 0 \end{pmatrix} \begin{pmatrix} e_s \\ \vec{e}_S \end{pmatrix} + \begin{pmatrix} \sigma \\ 0 \end{pmatrix}.$$

In this formulation though, σ appears as a right-hand side, and seems to be disconnected from the physical system itself, whereas it should be intimately linked to it, since $\sigma := \overrightarrow{\operatorname{grad}}(\beta) \cdot \vec{\mathbf{J}}_Q$. Hence, following Zhou et al. (2017); Zhou (2015), the system can be extended by introducing a new effort variable $e_{\sigma} := -\sigma$ and its related flow $f_{\sigma} := T$, in order to obtain

$$\begin{pmatrix} \rho f_s \\ \vec{f}_S \\ f_{\sigma} \end{pmatrix} = \begin{pmatrix} 0 & -\operatorname{div} & -1 \\ -\overrightarrow{\operatorname{grad}} & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} e_s \\ \vec{e}_S \\ e_{\sigma} \end{pmatrix}. \quad (11)$$

Note again that no additional hypothesis is needed at this stage, but only the definition of flows and efforts fitting into the pHs framework. Obviously, the \mathcal{J} operator obtained in (11) is formally skew-symmetric.

Concerning the possible definition of the boundary ports, here again there are at least two choices, even though more

general ones could be investigated. Either $\mathcal{B}\vec{e} := e_{s|_{\partial\Omega}}$, and $\mathcal{C}\vec{e} := -(\vec{e}_S \cdot \vec{n})_{|\partial\Omega}$, i.e. we control the temperature and observe the entropy flux. Or $\mathcal{B}\vec{e} := -(\vec{e}_S \cdot \vec{n})_{|\partial\Omega}$, and $\mathcal{C}\vec{e} := e_{s|_{\partial\Omega}}$, i.e. we control the entropy flux and observe the temperature.

Proposition 1. Extended system (11) with the boundary ports $v_{\partial} = \mathcal{B}\vec{e}$ and $y_{\partial} = \mathcal{C}\vec{e}$ in the above definitions gives rise to a Stokes-Dirac structure.

The proof is quite lengthy, but it closely follows (Zhou et al., 2017, Prop. 4.2), so it is not being reproduced here.

Proposition 1 implies that

$$\int_{\Omega} \rho f_s e_s + \vec{f}_S \cdot \vec{e}_S + f_{\sigma} e_{\sigma} d\mathbf{x} = \int_{\partial\Omega} v_{\partial} y_{\partial} d\gamma.$$

System (11) has one dynamical equation, and two algebraic equations. In order to solve them, one initial condition and two closure equations are needed. Indeed, the definition of σ translates into the first closure equation:

$$\vec{f}_S \cdot \vec{e}_S + f_{\sigma} e_{\sigma} = 0. \quad (12)$$

Moreover, Fourier's law gives a second closure equation:

$$e_s \vec{e}_S = \bar{\lambda} \cdot \vec{f}_S.$$

For a thorough thermodynamically oriented interpretation of these two closure equations, see the enlightening remark (Zhou et al., 2017, Rem. 1), which does also apply to our context.

With these notations at hand, we get the following power balance in terms of the pHs variables:

$$d_t U(t) = \int_{\partial\Omega} v_{\partial}(t, \gamma) y_{\partial}(t, \gamma) d\gamma. \quad (13)$$

Note that, according to the first law of thermodynamics, the internal energy of the isolated system is constant, the closed system is conservative, i.e. $d_t U(t) = 0$, while the open system is lossless, i.e. $d_t U(t) = (v_{\partial}(t), y_{\partial}(t))_{L^2(\partial\Omega)} = -\int_{\partial\Omega} e_{s|_{\partial\Omega}} (\vec{e}_S \cdot \vec{n})_{|\partial\Omega} d\gamma$.

5. LYAPUNOV FORMULATION

This last section is certainly less accurate from a thermodynamical point of view. But still, it does give some interesting features, widely used and known in the applied mathematics community. It has already been used, e.g. in Macchelli et al. (2004), for the heat equation in the pHs formalism, though in the restrictive case of constant coefficients and 1D geometry. The more general n -D case with space varying coefficients is presented here, allowing to recover easily (6). This third formulation deserves some interest in its own right, and will be most useful at the numerical stage also.

Let $\mathcal{H}(t) := \frac{1}{2} \int_{\Omega} \rho(\mathbf{x}) \frac{(u(t, \mathbf{x}))^2}{C_V(t, \mathbf{x})} d\mathbf{x}$ be the Hamiltonian and u the energy variable. The co-energy variable is $\delta_u \mathcal{H} = \frac{u}{C_V}$.

One easily computes from (2)

$$\begin{aligned}
d_t \mathcal{H}(t) &= \int_{\Omega} \rho(\mathbf{x}) \partial_t u(t, \mathbf{x}) \frac{u(t, \mathbf{x})}{C_V(t, \mathbf{x})} d\mathbf{x}, \\
&\quad - \frac{1}{2} \int_{\Omega} \rho(\mathbf{x}) \partial_t C_V(t, \mathbf{x}) \frac{(u(t, \mathbf{x}))^2}{(C_V(t, \mathbf{x}))^2} d\mathbf{x}, \\
&= - \int_{\Omega} \operatorname{div} (\vec{\mathbf{J}}_Q(t, \mathbf{x})) \frac{u(t, \mathbf{x})}{C_V(t, \mathbf{x})} d\mathbf{x}, \\
&\quad - \frac{1}{2} \int_{\Omega} \rho(\mathbf{x}) \partial_t C_V(t, \mathbf{x}) \frac{(u(t, \mathbf{x}))^2}{(C_V(t, \mathbf{x}))^2} d\mathbf{x}, \\
&= \int_{\Omega} \vec{\mathbf{J}}_Q(t, \mathbf{x}) \cdot \overrightarrow{\operatorname{grad}} \left(\frac{u(t, \mathbf{x})}{C_V(t, \mathbf{x})} \right) d\mathbf{x} \\
&\quad - \int_{\partial\Omega} \frac{u(t, \gamma)}{C_V(t, \gamma)} \vec{\mathbf{J}}_Q(t, \gamma) \cdot \vec{\mathbf{n}}(\gamma) d\gamma \\
&\quad - \frac{1}{2} \int_{\Omega} \rho(\mathbf{x}) \partial_t C_V(t, \mathbf{x}) \frac{(u(t, \mathbf{x}))^2}{(C_V(t, \mathbf{x}))^2} d\mathbf{x}.
\end{aligned}$$

Now let us define $f_u := \partial_t u$, $e_u := \frac{u}{C_V}$ and $\vec{\mathbf{e}}_Q := \vec{\mathbf{J}}_Q$. Then, using the same strategy as for the first two formulations, we also define $\vec{\mathbf{f}}_Q := -\overrightarrow{\operatorname{grad}} \left(\frac{u}{C_V} \right)$. As in the entropy formulation, we get:

$$\left(\begin{array}{c} \rho f_u \\ \vec{\mathbf{f}}_Q \end{array} \right) = \left(\begin{array}{cc} 0 & -\operatorname{div} \\ -\overrightarrow{\operatorname{grad}} & 0 \end{array} \right) \left(\begin{array}{c} e_u \\ \vec{\mathbf{e}}_Q \end{array} \right). \quad (14)$$

For the boundary ports, either $\mathcal{B}\vec{\mathbf{e}} := e_u|_{\partial\Omega}$ and $\mathcal{C}\vec{\mathbf{e}} := -(\vec{\mathbf{e}}_Q \cdot \vec{\mathbf{n}})|_{\partial\Omega}$, or $\mathcal{B}\vec{\mathbf{e}} := -(\vec{\mathbf{e}}_Q \cdot \vec{\mathbf{n}})|_{\partial\Omega}$ and $\mathcal{C}\vec{\mathbf{e}} := e_u|_{\partial\Omega}$.

Hence, the power balance is

$$\begin{aligned}
d_t \mathcal{H}(t) &= - \int_{\Omega} \vec{\mathbf{e}}_Q(t, \mathbf{x}) \cdot \vec{\mathbf{f}}_Q(t, \mathbf{x}) d\mathbf{x} \\
&\quad + \int_{\partial\Omega} v_{\partial}(t, \gamma) y_{\partial}(t, \gamma) d\gamma \\
&\quad - \frac{1}{2} \int_{\Omega} \rho(\mathbf{x}) \partial_t C_V(t, \mathbf{x}) (e_u(t, \mathbf{x}))^2 d\mathbf{x}. \quad (15)
\end{aligned}$$

At this stage however, to the best of our knowledge, we do not know any dynamic for C_V , and the boundary value of $\frac{u}{C_V}$ is of no use in practice.

With Dulong-Petit model, *i.e.* assuming that $u(t, \mathbf{x}) = C_V(\mathbf{x}) T(t, \mathbf{x})$, one immediately gets from (15)

$$\begin{aligned}
d_t \mathcal{H}(t) &= \int_{\Omega} \vec{\mathbf{J}}_Q(t, \mathbf{x}) \cdot \overrightarrow{\operatorname{grad}}(T(t, \mathbf{x})) d\mathbf{x} \\
&\quad - \int_{\partial\Omega} T(t, \gamma) \vec{\mathbf{J}}_Q(t, \gamma) \cdot \vec{\mathbf{n}}(\gamma) d\gamma.
\end{aligned}$$

Here, the control and the observation can be chosen to be the boundary temperature and the boundary flux (or the other way), giving useful physical meanings to both these boundary ports for control purpose.

Finally, adding Fourier's law (5) as one needed constitutive relation, the power balance becomes in terms of the pHs variables

$$\begin{aligned}
d_t \mathcal{H}(t) &= - \int_{\Omega} \vec{\mathbf{f}}_Q(t, \mathbf{x}) \cdot \bar{\lambda}(\mathbf{x}) \cdot \vec{\mathbf{f}}_Q(t, \mathbf{x}) d\mathbf{x} \\
&\quad + \int_{\partial\Omega} v_{\partial}(t, \gamma) y_{\partial}(t, \gamma) d\gamma. \quad (16)
\end{aligned}$$

Since $\bar{\lambda}$ is a positive symmetric tensor, the closed system is dissipative, *i.e.* $d_t \mathcal{H}(t) \leq 0$, while the open system is lossy, *i.e.* $d_t \mathcal{H}(t) \leq (v_{\partial}(t), y_{\partial}(t))_{L^2(\partial\Omega)} = - \int_{\partial\Omega} e_u|_{\partial\Omega} (\vec{\mathbf{e}}_Q \cdot \vec{\mathbf{n}})|_{\partial\Omega} d\gamma$.

6. CONCLUSION AND PERSPECTIVES

We saw three ways to describe the heat equation through the pHs formalism. We intend now to draw the pros and cons about these formulations.

This first important point to note is that the Lyapunov approach is theoretic, and not thermodynamically founded since the physical units of this Hamiltonian are $J \cdot K$, which is not meaningful. Furthermore, it requires a demanding and restrictive constitutive relation – the Dulong-Petit model – to achieve its main purpose: obtaining the temperature and the heat flux as boundary control and observation. But still, this kind of boundary control and observation seems to be more accurate in practice, and this justifies to some extent the presentation of this formulation in this work.

The other two choices of Hamiltonians, thermodynamically founded, lead to a practical drawback: one of the boundary port seems, to the best of our knowledge, more difficult to realize in the experiments. More precisely, we do not know if there exist actuators and sensors to deal with the boundary reciprocal temperature or the boundary entropy flux.

Finally, we would point out that with the energy formulation, since we introduced a new flux/effort couple related to the irreversible entropy production σ , one could think of the need for an additional constitutive relation to solve the system. However, this closure equation is directly obtained by definition of σ , which leads to (12). Consequently, this leads to two algebraic equations for the final system. This is indeed another difficulty, but still this formulation has its own advantages: the Hamiltonian is an energy, and we compute directly one more variable, namely σ , not reachable without extra efforts in the other two formulations.

The immediate perspective of this theoretical work is to present a structure-preserving numerical method adapted to the three formulations of the heat equation, which is the main topic of the companion paper Serhani et al. (2019a).

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