

# A GEOMETRIC MODEL FOR THE THERMODYNAMICS OF SIMPLE MATERIALS

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## Abstract

A geometric model for the thermodynamics of continuous media is constructed, providing a clearer meaning to the commonly used concept of ‘processes’ and ‘transformations’. The aim is to elucidate a clear ground suited to analyse thermodynamic transformations outside equilibrium. The model is applied to the thermodynamics of simple materials and explicit expressions for the existence of an entropy function are obtained.

*Keywords:* fibre bundle, thermodynamic, simple materials.

## 1. The Fibre Bundle of Thermodynamic Transformations

We consider a material element ([1]) and following [2] we suppose that an unambiguous definition of its state space can be given. The intuitive idea is that when a material element is given in a concrete physical situation, it is given in a definite state; the state determines everything about the element: its configuration, its stress and the response of the element in every possible test. Then we define the state space at time  $t$  as the set  $B_t$  of the state variables which ‘fit’ the configuration of the element at time  $t$  and we assume that  $B_t$  has the structure of a finite dimensional manifold. The ‘total state space’ is then given by the disjoint union.

$$\mathcal{B} = \bigcup_t \{t\} \times B_t \quad (1)$$

with the given natural structure of a fibre bundle over the real line  $\mathbb{R}$  where time flows [3, 4]. We call it the *thermodynamic bundle*. If the instantaneous state space  $B_t$  does not vary in time (i.e. there is an abstract ‘universal state space’  $B$  such that  $B_t \simeq B$  for all instants of time  $t$ ), when  $\mathcal{B}$  is trivial, i.e. it is the Cartesian product

$$\mathcal{B} \simeq \mathbb{R} \times B. \quad (2)$$

In the sequel we shall assume for the sake of simplicity that this holds, although our treatment extends with simple modifications to the general case.

Now we consider the abstract space of processes which, according to [2], consists of a set  $\Pi$  of functions

$$P_t^i : [0, t] \rightarrow \mathcal{G}, \quad (3)$$

where  $[0, t]$  is any time interval,<sup>1</sup> the space  $\mathcal{G}$  is a suitable target space suggested by the model (usually a vector space),  $i$  is a label ranging in an unspecified index set for all allowed processes and  $t \in \mathbb{R}$  is called the *duration* of the process  $P_t^i$ . For the given state space  $B$  we suppose that the set  $\Pi$  is such that the following hold:

1.  $\exists D : \Pi \rightarrow \mathcal{P}(B)$ , where  $\mathcal{P}(B)$  is the set of all subsets of  $B$ ;  $D$  is the *domain function* and  $D_t^i \equiv D(P_t^i)$  is called the domain of the  $i$ -th process (of duration  $t$ );
2.  $\exists R : \Pi \rightarrow \mathcal{P}(B)$ ;  $R$  is the *range function* and  $R_t^i \equiv R(P_t^i)$  is called the range of the  $i$ -th process (of duration  $t$ );
3. considering the restrictions

$$P_\tau^i = P_t^i|_{[0, \tau]} \quad (\tau \leq t) \quad (4)$$

new processes are obtained ('restricted processes') and they satisfy the following:<sup>2</sup>

$$\forall \tau < t \quad D(P_\tau^i) \subseteq D(P_t^i). \quad (5)$$

Incidentally, this implies that

$$\bigcap_{\tau=0}^t D(P_\tau^i) = D(P_t^i), \quad (6)$$

where  $t$  is the maximal duration. If it is not necessary to specify the duration, we shall simply write  $D^i$  in place of  $D(P_t^i) = D_t^i$ . Analogously, the abbreviated notation  $R^i$  will be used for the *range* of the  $i$ -th process.

A new function is then defined

$$\rho : \Pi \rightarrow C^0(B, B) \quad (7)$$

so that  $\forall t$  and  $\forall P_t^i \in \Pi$  a continuous mapping is obtained

$$\rho_t^i \equiv \rho(P_t^i) : D_t^i \rightarrow R_t^i \quad (8)$$

called the *transformation induced* by the process  $P_t^i$ . For any given initial state  $b \in D^i$  the transformed final state  $\rho_t^i(b) \in R^i$  will be called, by an abuse of notation, the *value* of the process (at time  $t$ ). We define now a function of time in the following way:

$$\lambda_b^i(\tau) = \begin{cases} b & \text{if } \tau = 0 \\ \rho_t^i b & \text{if } \tau \in ]0, t], \end{cases} \quad \text{with } b \in D^i, \quad (9)$$

<sup>1</sup>We explicitly consider the duration interval to be closed. Some authors (see e.g. [5], [6]) consider instead a semi-closed interval, to allow more sophisticated limiting situations.

<sup>2</sup>This requirement expresses the intuitive physical idea that restricting the time interval allows a larger set of possible initial states.

so that we have

$$\lambda_b^i(t) = \rho_t^i(b) = \Phi^i(t, b) \quad (10)$$

with

$$\Phi^i(t, b) : \mathbb{R} \times B \rightarrow B. \quad (11)$$

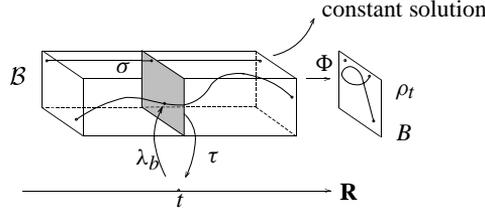


Fig. 1. Thermodynamic bundle with the transformation for the system

The transformation for the system is a function

$$\sigma : \mathbb{R} \rightarrow \mathbb{R} \times B \quad (12)$$

such that for every local trivialization of the thermodynamic bundle one has

$$\sigma : t \rightarrow (t, \lambda_b(t)). \quad (13)$$

With these positions the transformation is interpreted as a curve in the union of all the state spaces such that it intersects the instantaneous state space just once, i.e.  $\sigma$  is a section of the thermodynamic bundle ([3],[4]). Following [5] and [7] we define a composition law among processes based on the definition of *continuation* given by NOLL ([7]). If  $P_t^i$  and  $P_s^j$  are two (time dependent) processes a new process is given by:

$$(P_t^i \circ P_s^j)(\tau) = \begin{cases} P_t^i(\tau) & \text{if } \tau \in [0, t], \\ P_s^j(\tau - t) & \text{if } \tau \in ]t, t + s], \end{cases} \quad (14)$$

with  $s \in \mathbb{R}$ . On the set

$$\tilde{P} = \left\{ (P_s^j, P_t^i) \in \Pi \times \Pi : D^j \cap R^i \neq \emptyset \right\} \quad (15)$$

consisting of all the pairs  $(P_s^j, P_t^i)$  such that the range of  $\rho_t^i$  intersects the domain of  $\rho_s^j$ , the  $\Pi$ -valued functions are such that  $D(P_s^j \circ P_t^i) = (\rho_t^i)^{-1}(D^j \cap R^i)$ . Accordingly, for each  $b \in D(P_s^j \circ P_t^i)$ , the composition among transformations can be defined by:

$$\rho_{t+s}^{i,j} b = \rho_s^j[\rho_t^i(b)]. \quad (16)$$

This, in turn, allows us to define the ‘action’ of  $\Pi$  on the state space  $B$  as mapping

$$\tilde{\rho} : \Pi \times B \rightarrow B \quad (17)$$

such that the following hold:

- $\tilde{\rho}[P_t^i, b] = \rho_t^i(b)$  if  $b \in D^i$
- $\tilde{\rho}(1, b) = b \forall b \in B$
- $\tilde{\rho}[P_s^j, \tilde{\rho}(P_t^i, b)] = \tilde{\rho}(P_{t+s}^{i,j}, b)$

If the particular model chosen allows us to give the structure of a pseudogroup (or, even better, of a Lie group) to the set  $\Pi$  of all processes then  $\tilde{\rho}$  is an action in the standard sense ([3], [4]). Moreover, whenever a process  $P^i$  admits an inverse in  $\Pi$  (e.g. when  $P^i$  is reversible or  $\Pi$  is a pseudogroup) then we have the following:<sup>3</sup>

$$\mathcal{D}(P^{-1}) = \mathcal{R}(P), \quad (18)$$

$$\mathcal{R}(P^{-1}) = \mathcal{D}(P), \quad (19)$$

being, of course,

$$\rho_{P^{-1}}[\rho_P(b)] = \tilde{\rho}[P^{-1}, \tilde{\rho}(P, b)] = \quad (20)$$

$$\tilde{\rho}(P^{-1}P, b) = \tilde{\rho}(1, b) = b \quad (21)$$

and so:

$$\rho(P^{-1}) = \rho_P^{-1}. \quad (22)$$

In the product  $B \times \Pi$  we can now define a suitable subbundle  $\Pi(B)$ , called the *process bundle*, in the following way. The base manifold is given by the manifold of the state variables  $B$ . The fibre at the point  $b \in B$  is the set of the values of all the processes whose induced transformations start from that given configuration for the body element:

$$\Pi_b = \{P \in \Pi \mid b \in D^i(P)\}. \quad (23)$$

If a vector field  $X$  can be given on the state manifold in a way that its integral curves are the transformations given by the function of time ( $\lambda_b$ ) appearing in *Eqs.* (13), then the vector field determines a section of the bundle  $\Pi(B) = \bigcup_{b \in B} \Pi_b$  so constructed. We indicate with  $\tilde{X}$  the application:  $\tilde{X} : b \rightarrow b_t$  where  $b_t \in \Pi_b$  is the value of the state variable obtained through the transformation at time  $t$ .

## 2. An Application to Simple Materials

For simple materials [8], [9] the state space can be given by the *deformation gradient*  $\mathbf{F}$ , the *internal energy*  $e$  and the vector  $\beta = -\frac{1}{\mu} \text{grad} \frac{1}{\theta}$ , where  $\mu$  is the *mass density* and  $\theta$  is the *temperature*. We have then:

$$B = \text{Lin}(\mathcal{V}) \oplus \mathbb{R} \oplus \mathcal{V}, \quad (24)$$

where  $\mathcal{V}$  is the translation space of  $\mathbb{R}$ . The general process  $P_t$  is a piecewise continuous function whose values are

$$P_t(\tau) = [\mathbf{L}(\tau), h(\tau), \gamma(\tau)], \quad (25)$$

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<sup>3</sup>For the sake of simplicity an obvious short notation without indices is adopted.

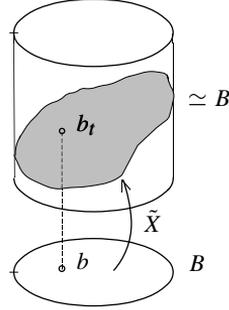


Fig. 2. Process bundle with the vector field on the state variables determining the section

where  $\mathbf{L}$  is the instantaneous value of the *velocity gradient*,  $\tau = \dot{\beta}$  and  $h = -\frac{1}{\mu} \operatorname{div} \mathbf{q}$ ,  $\mathbf{q}$  being the *heat flux vector* given as a stationary vertical field on the bundle:

$$\mathbf{q} : \mathbb{R} \times B \rightarrow \mathcal{V} \quad (26)$$

(we are not considering radiation for the sake of simplicity).

With these positions the target space turns out to be

$$\mathcal{G} = \operatorname{Lin}(\mathcal{V}) \oplus \mathbb{R} \oplus \mathcal{V} \simeq B \quad (27)$$

so that

$$B \times \mathcal{G} \simeq TB \quad (28)$$

and the process maps an interval of the real line into the fibre  $\mathcal{G}$  of the bundle

$$P : [0, t] \rightarrow \mathcal{G}. \quad (29)$$

We introduce a further stationary field on the thermodynamic bundle  $\mathbb{R} \times B$ , i.e. the *stress field*:

$$\mathbf{T} : \mathbb{R} \times B \rightarrow \operatorname{Sym}(\mathcal{V}) \quad (30)$$

so that a response functional on the state space is given by

$$\tilde{\mathbf{T}} = T \circ \rho_t : B \rightarrow \operatorname{Sym}(\mathcal{V}), \quad (31)$$

which is the stress determined by the process starting at  $b$ . Another stationary field is introduced as the *temperature field*

$$\theta : \mathbb{R} \times B \rightarrow \mathbb{R}^{++}, \quad (32)$$

$\mathbb{R}^{++}$  being the set of real positive numbers.

The system of dynamic equations considered in [5], i.e.

$$\begin{cases} \dot{\mathbf{F}}(\tau) = \mathbf{L}(\tau)\mathbf{F}(\tau), \\ \dot{e}(\tau) = \mathbf{T}(\mathbf{b}) \cdot \mathbf{L}(\tau) + h(\tau), \\ \dot{\beta}(\tau) = \tau(\tau) \end{cases} \quad (33)$$

determines in fact a linear bundle morphism  $\mathbf{G} : TB \rightarrow TB$

$$\mathbf{G} : (\mathbf{F}, e, \beta, \mathbf{L}, h, \tau) \rightarrow (\mathbf{F}, e, \beta, \dot{\mathbf{F}}, \dot{e}, \dot{\beta}), \quad (34)$$

which, in a matricial form, is given by:

$$(\mathbf{F}, e, \beta, \dot{\mathbf{F}}, \dot{e}, \dot{\beta})^T = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{A} \end{pmatrix} (\mathbf{F}, e, \beta, \mathbf{L}, h, \gamma)^T \quad (35)$$

with

$$\mathbf{A} = \begin{pmatrix} \mathbf{F} & 0 & 0 \\ \mathbf{T} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (36)$$

If we denote by  $X$  the vector field corresponding to the system of ordinary differential equations (33), according to our previous discussion the vector field  $X$  generates a section of the process bundle  $\Pi(B)$ , so that every differentiable curve  $\lambda_b$  on the base manifold is transformed into a differentiable curve  $X \circ \lambda_b$  in the section, called the  $X$ -lift and denoted by the symbol  $\hat{\phantom{x}}$  in the sequel.

The lift of the induced transformation must satisfy the following conditions

1.  $[\tau_B \circ X \circ \lambda_b]^\wedge = X \circ \lambda_b$ ,
2.  $\forall$  local trivialization  $TB \equiv B \times \mathcal{G}$ ,  $X \circ \lambda_0 = [\tau_B \circ X \circ \lambda_b, \mathbf{A} \cdot P_t]$ ,
3.  $\lambda_b(0) = \lambda_0$ ,

where  $\mathbf{A}$  is the linear transformation (36) and  $\tau_B$  is the natural projection of  $TB$ . One can notice that the latter relations on the lifted transformation hold in the case of the general model and not only for simple materials. This allows us to analyse more general systems in which  $\mathcal{G} \neq B$  and the bundle constructed does not therefore coincide with the tangent bundle of the state variables. In this way the model allows, for example, to take into account the action of internal variables (see, e.g. [10, 11]) and this will be the subject of future investigations.

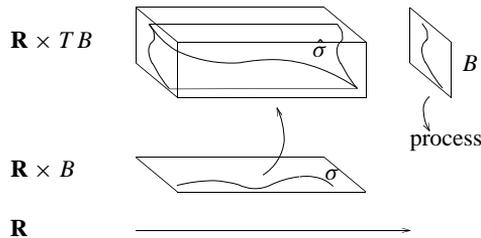


Fig. 3. State space with the time variable and related tangent space with the process for the system

Following [5], a real function called the ‘entropy function’ is defined on  $\mathbb{R} \times TB$  by:

$$s(\rho_t, b, t) = \int_0^t \frac{h(\tau)}{\theta[b(\tau)]} d\tau + \int_0^t \mathbf{q}[b(\tau)] \cdot \beta(\tau) d\tau, \quad (37)$$

so that in the thermodynamic bundle  $\mathbb{R} \times B$  a 1-form  $\Omega_\omega$  is also defined, called the ‘entropy 1-form’, whose integral along the solution curve gives exactly  $s$ , i.e.:

$$\int_\sigma \Omega_\omega = \int_0^t \frac{h(\tau)}{\theta[b(\tau)]} d\tau + \int_0^t \mathbf{q}[b(\tau)] \cdot \beta(\tau) d\tau. \quad (38)$$

In components one can write

$$\Omega_\omega = \omega_\mu dq^\mu + \omega_0 dt \equiv \omega_A da^A, \quad (39)$$

where  $q^\mu$  are the variables in  $B$  and  $q^0 = t$ , so that

$$\int_\sigma \Omega_\omega \equiv \int_0^t \omega_A[t, \lambda_b(\tau)] \dot{\lambda}_b^A d\tau. \quad (40)$$

Using Eq. (40) together with the relations  $\mathbf{L} = \mathbf{F}^{-1}\dot{\mathbf{F}}$  and  $h = \dot{e} - \mathbf{TL}$  which follow from (33), we get:

$$\Omega_\omega = -\frac{\mathbf{TF}^{-1}}{\theta} d\mathbf{F} + \frac{1}{\theta} de + \mathbf{q} \cdot \beta dt. \quad (41)$$

By differentiation a 2-form is then obtained:

$$d\Omega_\omega = [\partial_A \omega_B] dq^A \wedge dq^B \quad (42)$$

and by using the natural properties of the exterior differential one easily obtains

$$\begin{aligned} d\Omega_\omega &= d\omega_\lambda \wedge dq^\lambda + \omega_0 \wedge dt = \\ &= (\partial_0 \omega_0) dt \wedge dq^\lambda + (\partial_\mu \omega_\lambda) dq^\mu \wedge dq^\lambda + (\partial_\lambda \omega_0) dq^\lambda \wedge dt, \end{aligned} \quad (43)$$

which can be written as

$$d\Omega_\omega = (\partial_0 \omega_\lambda - \partial_\lambda \omega_0) dt \wedge dq^\lambda + \frac{1}{2} (\partial_\mu \omega_\lambda - \partial_\lambda \omega_\mu) dq^\mu \wedge dq^\lambda. \quad (44)$$

Let us now denote by  $A_{\lambda\mu}$  and  $E_\lambda$  the coefficients of the 2-form  $d\Omega_\omega$ , i.e.:

$$A_{\mu\lambda} = \partial_\mu \omega_\lambda - \partial_\lambda \omega_\mu \quad (45)$$

and

$$E_\lambda = \partial_0 \omega_\lambda - \partial_\lambda \omega_0. \quad (46)$$

Eq. (44) becomes then:

$$d\Omega_\omega = \frac{1}{2} A_{\mu\lambda} dq^\mu \wedge dq^\lambda + E_\lambda dt \wedge dq^\lambda. \quad (47)$$

By using relations (44) and (45) we obtain the following explicit expressions:

$$\partial_{\mathbf{F}} \left[ \frac{1}{\theta} \right] = \partial_e \left[ \frac{-\mathbf{TF}^{-1}}{\theta} \right], \quad (48)$$

$$0 = \partial_\beta \left[ \frac{-\mathbf{TF}^{-1}}{\theta} \right], \quad (49)$$

$$0 = \partial_\beta \left[ \frac{1}{\theta} \right], \quad (50)$$

$$\partial_t \left[ \frac{-\mathbf{TF}^{-1}}{\theta} \right] = \partial_{\mathbf{F}}[\mathbf{q} \cdot \beta], \quad (51)$$

$$\partial_t \left[ \frac{1}{\theta} \right] = \partial_e[\mathbf{q} \cdot \beta], \quad (52)$$

$$0 = \partial_\beta[\mathbf{q} \cdot \beta]. \quad (53)$$

Relations (48)–(53) give necessary conditions for the existence of the entropy function during the analysed process. While Eqs. (48), (51) and (52) express a sort of ‘irrotationality’ of the entropy 1-form  $\Omega_\omega$  and condition (50) is trivially satisfied because of the initial hypothesis, relations (49), (50) and (53) express the physical requirement that the quantities considered cannot depend on the gradient of temperature. In particular, Eq. (53) tells us that the projection of the heat flux field along the direction of the gradient of temperature is constant with respect to the same gradient.

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