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First Principle of Thermodynamics and Virtual Thermal-Work Theorem

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Duality in Mathematical physics

Continuum Mechanics

- *Dual objects: velocity fields and force systems;*
- *Axiom of dynamical equilibrium (Johann Bernoulli 1717);*
- *Theorem of virtual work: existence of a Cauchy's stress field in a continuous body subject to a force system in equilibrium;*

Cauchy, A.L., 1823. Reserches sur l'équilibre et le movement intérieur des corps solides ou fluides, élastiques ou non élastiques. Bull. Soc. Philomath., 9-13 = Euvres (2) 2, 300-304.

Cauchy, A.L., 1827. De la pression ou tension dans un corps solide. Ex. de Mathematique 2, 42-56= Euvres (2) 7, 60-78.

Cauchy, A.L., 1828. Sur les équations qui expriment les conditions d'èquilibre ou les lois du movement intérieur d'un corps solide, élastiques ou non élastiques. Ex. de Mathematique 3, 160-187= Euvres (2) 8, 195-226.

Piola's approach (Lagrange multiplier method)

Piola, G., 1833. La meccanica dei corpi naturalmente estesi trattata col calcolo delle variazioni. In: Opuscoli Matematici e Fisici di Diversi Autori Giusti, Milano, pp. 201-236.

Continuum Mechanics

Virtual work Theorem:

The following statements are equivalent:

- *Axiom of dynamical equilibrium (Johann Bernoulli 1717):*

$$\langle \ell, \mathbf{v} \rangle = 0 , \quad \forall\, \mathbf{v} \in \mathrm{C{\scriptsize ONF}} \cap \mathrm{R{\scriptsize IG}} \,.$$

- *Virtual work principle:*

$$\langle \ell, \mathbf{v} \rangle = \int_{\mathrm{P{\scriptsize AT}}(\boldsymbol{\varphi}(\mathbb{B}))} \langle \mathbf{T}, \mathrm{sym}\, \nabla \mathbf{v} \rangle_{\mathbf{g}}\, \boldsymbol{\mu} \,, \quad \forall\, \mathbf{v} \in \mathrm{C{\scriptsize ONF}} \,.$$

Romano G., Diaco M.: A Functional Framework for Applied Continuum Mechanics, New Trends in Mathematical Physics, World Scientific, pp.193-204, Singapore (2004).

IDEA

The First Principle of Thermodynamics is re-formulated as a variational condition: the Axiom of thermal equilibrium.

- *Dual objects: virtual temperature fields and thermal forces;*
- *Axiom of thermal equilibrium*
- *Theorem of virtual thermal-work:existence of a cold flow vector field in a body fulfilling the Axiom of thermal equilibrium.*

The First Principle of Thermodynamics

The principle states that given a body $\mathcal{B}$ at a placement Ω

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

for any sub-body $\mathcal{P} \subseteq \Omega$, in which

$\dot{\mathcal{E}}(\mathcal{P})$ *is the time-rate of change of the internal energy;*

$\mathcal{M}(\mathcal{P})$ *is the mechanical power;*

$\mathcal{Q}(\mathcal{P})$ *is the heat power supplied to the sub-body.*

Caratheodory, C., 1909. Untersuchungen über die Grundlagen der Thermodynamik. Math. Ann. 67.

Fermi, E., 1936. Thermodynamics. Dover Publications, New York.

Truesdell, C., 1984. Rational Thermodynamics, 2^{th} ed. Springer Verlag, New York.

It is convenient to define the energy-rate gap

$$\mathcal{G}(\mathcal{P}) := \mathcal{M}(\mathcal{P}) + \mathcal{Q}(\mathcal{P}) - \dot{\mathcal{E}}(\mathcal{P})$$

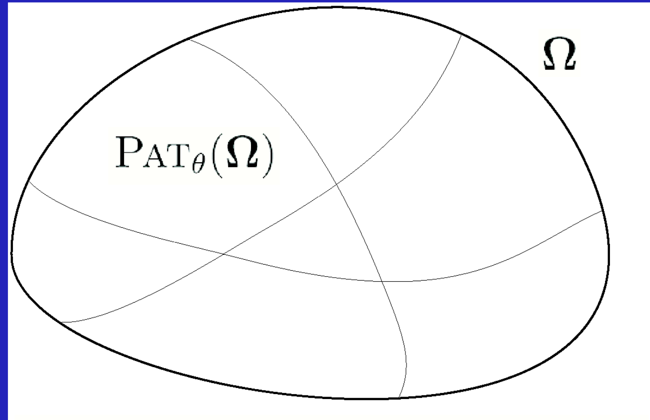
and to write the First Principle of Thermodynamics as $\mathcal{G}(\mathcal{P}) = 0$

Virtual temperatures

The linear space $\mathrm{T{\scriptsize EMP}}$ *of virtual temperatures is composed by Green regular scalar fields, i.e. square integrable fields* $\theta \in \mathrm{S{\scriptsize QIF}}(\boldsymbol{\Omega})$ *whose distributional derivates are piecewise square integrable in* $\boldsymbol{\Omega}$ *according to a regularity patchwork* $\mathrm{P{\scriptsize AT}}_\theta(\boldsymbol{\Omega})$*, i.e.* $\nabla\theta \in \mathrm{S{\scriptsize QIV}}(\mathrm{P{\scriptsize AT}}_\theta(\boldsymbol{\Omega}))$.

$\mathrm{T{\scriptsize EMP}}$ *is a pre-Hilbert space when endowed with the inner product given by:*

$$(\theta_1, \theta_2)_{\mathrm{T{\scriptsize EMP}}} := \int_{\boldsymbol{\Omega}} \theta_1\, \theta_2\, \boldsymbol{\mu} + \int_{\mathrm{P{\scriptsize AT}}_{\theta_{12}}(\boldsymbol{\Omega})} \mathbf{g}(\nabla\theta_1, \nabla\theta_2)\, \boldsymbol{\mu}$$



$\mathrm{C{\scriptsize ONF}} \subset \mathrm{T{\scriptsize EMP}}$ *is a closed linear subspace of conforming virtual temperatures such that all of its vector fields have a common regularity patchwork.*

$\mathrm{C{\scriptsize ONF}}$ *is a Hilbert space for the topology induced by* $\mathrm{T{\scriptsize EMP}}$.

Since $\mathrm{C{\scriptsize ONF}}$ *is a linear space, this definition includes any linear or affine kinematical constraint.*

Variational form of the First Principle

For any $\theta \in \textrm{TEMP}$, we consider the characteristic functions of the elements $\mathcal{P}$ of the patchwork $\textrm{PAT}_\theta(\boldsymbol{\Omega})$

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

and define the functionals:

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

Performing an extension by linearity, we consider the functionals $\mathcal{F}_{\dot{\mathcal{E}}}$, $\mathcal{F}_{\mathcal{M}}$ and $\mathcal{F}_{\mathcal{Q}}$ on the linear subspace of piecewise constant virtual temperature fields.

By Hahn's extension theorem these bounded linear functionals can be extended (non-univocally) to bounded linear functionals on $\textrm{TEMP}$ without increasing their norm

Yosida, K., 1974. Functional Analysis. 4^{th} Springer Verlag, New York.

The First Principle of Thermodynamics can then be reformulated in variational terms as:

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

Axiom of thermal equilibrium

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

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

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

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

This condition, analogous to the axiom of dynamical equilibrium in mechanics, can be stated as: the virtual-thermal work of the thermal force must vanish for any piecewise constant virtual temperature field.

The restriction of a thermal force to conforming virtual temperatures will be called a thermal load.

The closed range property of the regular part of the distributional gradient $\nabla \in BL(\mathrm{C{\scriptstyle ONF}}\,;\mathrm{S{\scriptstyle QIV}})$ leads to the following existence result.

Virtual thermal-work theorem

The First Principle of Thermodynamics:

$$\langle \mathcal{F}_{\mathcal{G}}, \theta \rangle = 0 \,, \quad \forall\, \theta \in \ker \nabla \cap \textsc{Conf}$$

is equivalent to the existence of a square integrable vector field $\mathbf{q} \in \textsc{Sqiv}$ *, the cold-flow vector field, which performs, for the regular part of the distributional gradient of a conforming virtual temperature field, a virtual thermal-work equal to the one performed by the thermal load for the conforming virtual temperature field:*

$$\langle \mathcal{F}_{\mathcal{G}}, \theta \rangle = \int_{\textsc{Pat}(\mathbf{\Omega})} \mathbf{g}(\mathbf{q} \,, \nabla\theta)\, \boldsymbol{\mu} \,, \quad \forall\, \theta \in \textsc{Conf}$$

Boundary value problem

Basic property of boundary value problems → $\ker(\mathrm{VAL}) \subseteq \mathrm{CONF}$

$\ker(\mathrm{VAL})$ *is the linear subspace of test fields in* TEMP *with vanishing boundary values on a fixed patchwork.*

The bounded linear functionals $\mathcal{F}_{\dot{\varepsilon}}$ *,* $\mathcal{F}_{\mathcal{M}}$ *and* $\mathcal{F}_{\mathcal{Q}}$ *may then be univocally defined on the whole space* TEMP *by setting:*

$$\begin{aligned} \langle \mathcal{F}_{\dot{\varepsilon}}, \theta \rangle &:= \int_{\mathbf{\Omega}} \rho_t \, \dot{\varepsilon} \, \theta \, \boldsymbol{\mu} \,, \\ \langle \mathcal{F}_{\mathcal{M}}, \theta \rangle &:= \int_{\mathbf{\Omega}} \langle \mathbf{T}, \mathrm{sym} \, \nabla \mathbf{v} \rangle \, \theta \, \boldsymbol{\mu} \,, \\ \langle \mathcal{F}_{\mathcal{Q}}, \theta \rangle &:= \int_{\mathbf{\Omega}} \rho_t \, q \, \theta \, \boldsymbol{\mu} + \int_{\partial \mathrm{PAT}_\theta(\mathbf{\Omega})} \langle \partial q, \mathrm{VAL} \, \theta \rangle \, \partial \boldsymbol{\mu} \,, \end{aligned}$$

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

$$p := -\rho_t \, \dot{\varepsilon} + \langle \mathbf{T}, \mathrm{sym} \, \nabla \mathbf{v} \rangle + \rho_t \, q \,,$$

the energy-rate gap $\mathcal{F}_{\mathcal{G}} \in \mathrm{CONF}^*$ *is given by:*

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

Localization

In a boundary value problem, a cold flow vector field $\mathbf{q}$ *in thermal equilibrium with a thermal load* $\mathcal{F}_{\mathcal{G}}$ *, i.e. fulfilling the identity in the virtual thermal-work theorem:*

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

has a distributional divergence $\mathrm{DIV}\, \mathbf{q}$ *whose restriction to each element* $\mathcal{P} \in \mathrm{PAT}_{\infty}(\mathbf{\Omega})$ *of the patchwork is g-square integrable with*

$$-\mathrm{DIV}\, \mathbf{q} = p \,, \quad \text{in} \quad \mathrm{PAT}_{\infty}(\mathbf{\Omega}) \,,$$

and the jump $[[\mathbf{g}(\mathbf{q}, \mathbf{n})]]$ *of the flux across the boundary of the domain* $\mathbf{\Omega}$ *and across the interfaces of the patchwork* $\mathrm{PAT}_{\infty}(\mathbf{\Omega})$ *fulfills the conditions:*

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

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

Conclusions

The First Principle of Thermodynamics has been reformulated, by a simple but tricky reasoning, as a variational condition in which the test fields are piecewise constant virtual temperatures.

An application of the Lagrange multipliers theorem yields the virtual thermal-work theorem which provides the existence of a cold flow vector field in the body.

In all classical treatments the existence of a heat flow vector field is instead assumed as a separate axiom of continuum thermodynamics.

In boundary value problems, thermal forces have a well-defined expression and Green's formula, by localization procedure, leads to differential and boundary conditions.

Related results

A similar treatment may be applied to any balance law in continuum physics.

As a significant example, the Principle of Mass Conservation leads to a variational principle in which the lagrangian multipliers are vector fields describing the mass flow through a control volume:

Romano, G., Barretta, R., 2008. On the variational formulation of balance laws. University of Naples Federico II, Naples, Italy. Preprint.