The Double Bracket Structure:

A methodology to build variational integrators for continuum thermodynamics.

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1. Variational integrators through the example of a rotating mass-spring system

2. Review of variational principles for continuum thermodynamics

3. Presentation of the Double Bracket Structure

4. The example of a Generalised Standard Material, small strains, unidimensional

5. The example of large strains thermo-visco-elastodynamics

6. An example of discretisation of the linear thermo-elastodynamics problem

Table of Contents

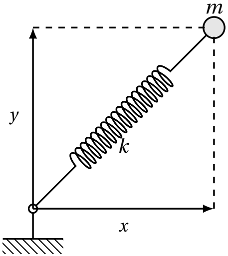
The example of the rotating mass-spring system

Consider a mass m, attached to a spring of stiffness k to a reference frame. Hamilton's principle reads

$$\forall \delta \boldsymbol{q} | \delta \boldsymbol{q}(t_0) = \delta \boldsymbol{q}(t_1) = 0, \delta \mathscr{A}[\boldsymbol{q}] = \delta \int_{t_0}^{t_1} l(\boldsymbol{q}, \dot{\boldsymbol{q}}) \, \mathrm{d}t = 0$$

For this problem, the Lagrangian is

$$l(x, y, \dot{x}, \dot{y}) = \frac{1}{2} m(\dot{x}^2 + \dot{y}^2) + \frac{1}{2} k \left(\sqrt{x^2 + y^2} - l_0 \right)^2$$

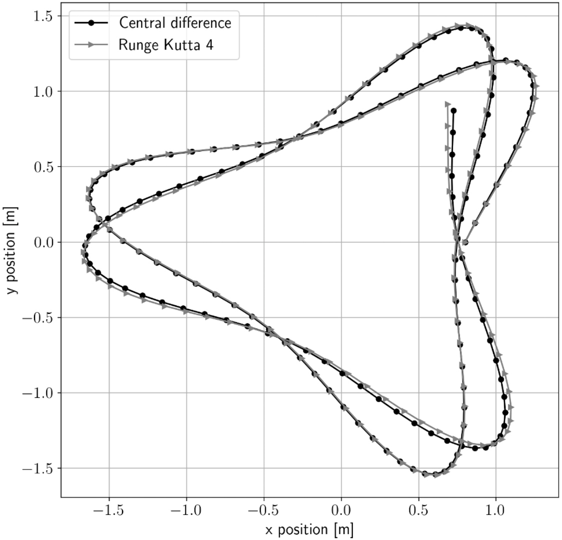


Euler-Lagrange equations are

$$m\ddot{x} + kx \left(1 - \frac{l_0}{\sqrt{x^2 + y^2}} \right) = 0$$

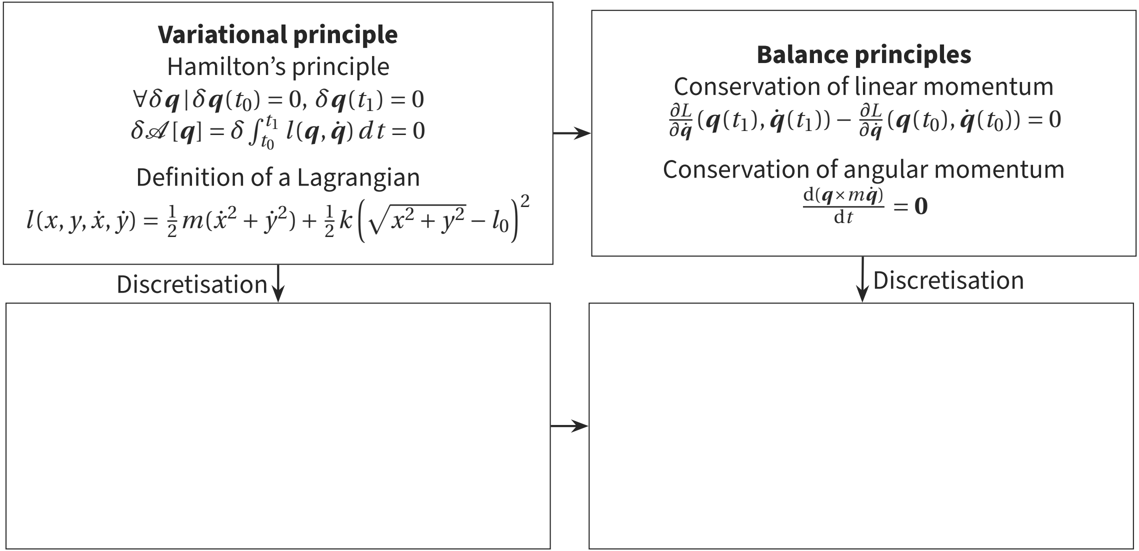
$$m\ddot{y} + ky \left(1 - \frac{l_0}{\sqrt{x^2 + y^2}} \right) = 0$$

The example of the rotating mass-spring system



1. Variational integrators through the example of a rotating mass-spring system

The example of the rotating mass-spring system



Variational principle

Hamilton's principle

$$\forall \delta \boldsymbol{q} \,|\, \delta \boldsymbol{q}(t_0) = 0,\ \delta \boldsymbol{q}(t_1) = 0$$

$$\delta \mathscr{A}[\boldsymbol{q}] = \delta \int_{t_0}^{t_1} l(\boldsymbol{q}, \dot{\boldsymbol{q}})\, dt = 0$$

Definition of a Lagrangian

$$l(x, y, \dot{x}, \dot{y}) = \tfrac{1}{2} m(\dot{x}^2 + \dot{y}^2) + \tfrac{1}{2} k \left(\sqrt{x^2 + y^2} - l_0\right)^2$$

Balance principles

Conservation of linear momentum

$$\frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}(t_1), \dot{\boldsymbol{q}}(t_1)) - \frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}(t_0), \dot{\boldsymbol{q}}(t_0)) = 0$$

Conservation of angular momentum

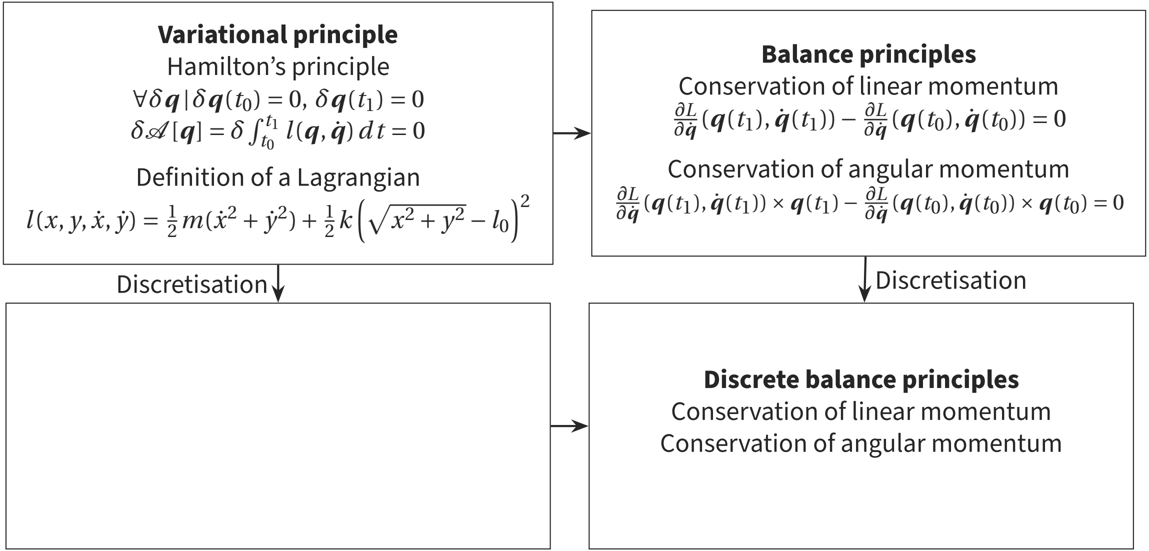
$$\frac{\mathrm{d}(\boldsymbol{q} \times m \dot{\boldsymbol{q}})}{\mathrm{d}t} = \boldsymbol{0}$$

Discretisation

Discretisation

1. Variational integrators through the example of a rotating mass-spring system

The example of the rotating mass-spring system



Variational principle

Hamilton's principle

$$\forall \delta \boldsymbol{q} \,|\, \delta \boldsymbol{q}(t_0) = 0,\ \delta \boldsymbol{q}(t_1) = 0$$

$$\delta \mathscr{A}[\boldsymbol{q}] = \delta \int_{t_0}^{t_1} l(\boldsymbol{q}, \dot{\boldsymbol{q}})\, d t = 0$$

Definition of a Lagrangian

$$l(x, y, \dot{x}, \dot{y}) = \frac{1}{2} m(\dot{x}^2 + \dot{y}^2) + \frac{1}{2} k \left(\sqrt{x^2 + y^2} - l_0\right)^2$$

Balance principles

Conservation of linear momentum

$$\frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}(t_1), \dot{\boldsymbol{q}}(t_1)) - \frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}(t_0), \dot{\boldsymbol{q}}(t_0)) = 0$$

Conservation of angular momentum

$$\frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}(t_1), \dot{\boldsymbol{q}}(t_1)) \times \boldsymbol{q}(t_1) - \frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}(t_0), \dot{\boldsymbol{q}}(t_0)) \times \boldsymbol{q}(t_0) = 0$$

Discretisation

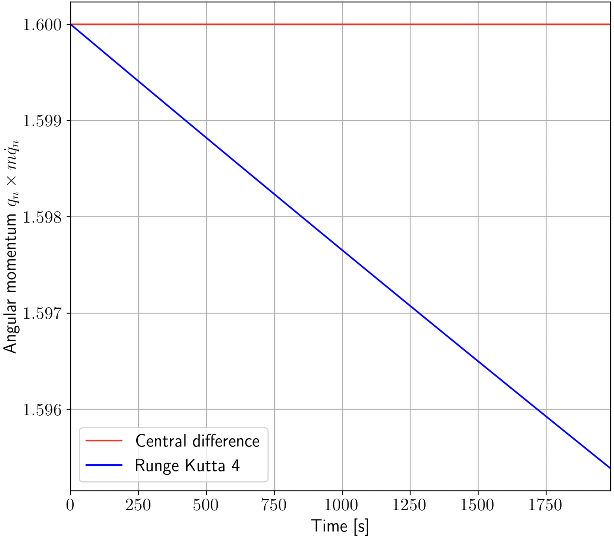
Discretisation

Discrete balance principles

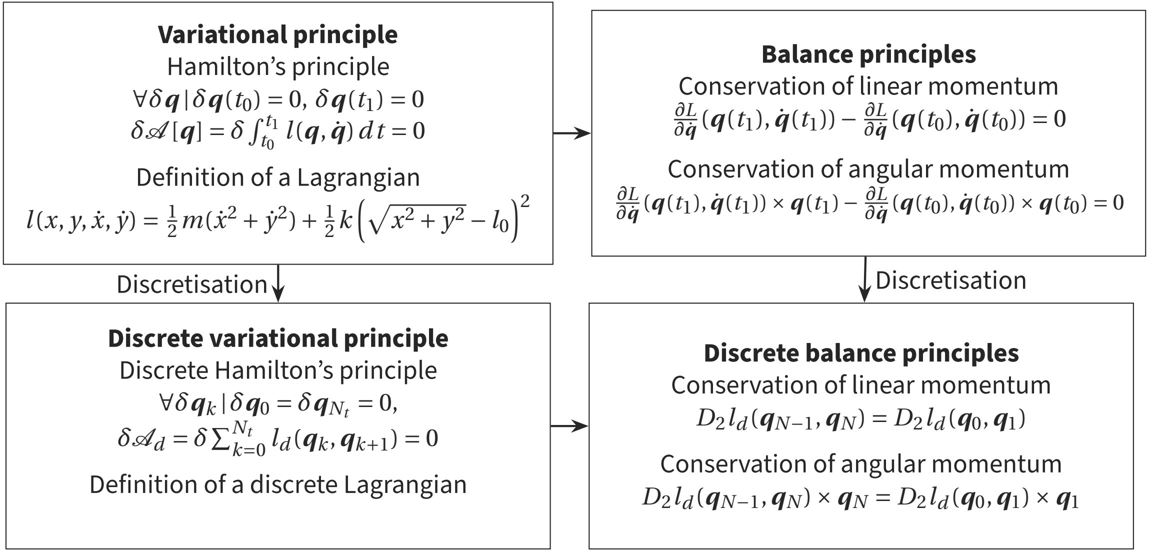
Conservation of linear momentum

Conservation of angular momentum

The example of the rotating mass-spring system



The example of the rotating mass-spring system



Variational principle

Hamilton's principle

$$\forall \delta \boldsymbol{q} \,|\, \delta \boldsymbol{q}(t_0) = 0,\ \delta \boldsymbol{q}(t_1) = 0$$

$$\delta \mathscr{A}[\boldsymbol{q}] = \delta \int_{t_0}^{t_1} l(\boldsymbol{q}, \dot{\boldsymbol{q}})\, dt = 0$$

Definition of a Lagrangian

$$l(x, y, \dot{x}, \dot{y}) = \frac{1}{2} m(\dot{x}^2 + \dot{y}^2) + \frac{1}{2} k \left(\sqrt{x^2 + y^2} - l_0 \right)^2$$

Balance principles

Conservation of linear momentum

$$\frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}(t_1), \dot{\boldsymbol{q}}(t_1)) - \frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}(t_0), \dot{\boldsymbol{q}}(t_0)) = 0$$

Conservation of angular momentum

$$\frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}(t_1), \dot{\boldsymbol{q}}(t_1)) \times \boldsymbol{q}(t_1) - \frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}(t_0), \dot{\boldsymbol{q}}(t_0)) \times \boldsymbol{q}(t_0) = 0$$

Discretisation

Discretisation

Discrete variational principle

Discrete Hamilton's principle

$$\forall \delta \boldsymbol{q}_k \,|\, \delta \boldsymbol{q}_0 = \delta \boldsymbol{q}_{N_t} = 0,$$

$$\delta \mathscr{A}_d = \delta \sum_{k=0}^{N_t} l_d(\boldsymbol{q}_k, \boldsymbol{q}_{k+1}) = 0$$

Definition of a discrete Lagrangian

Discrete balance principles

Conservation of linear momentum

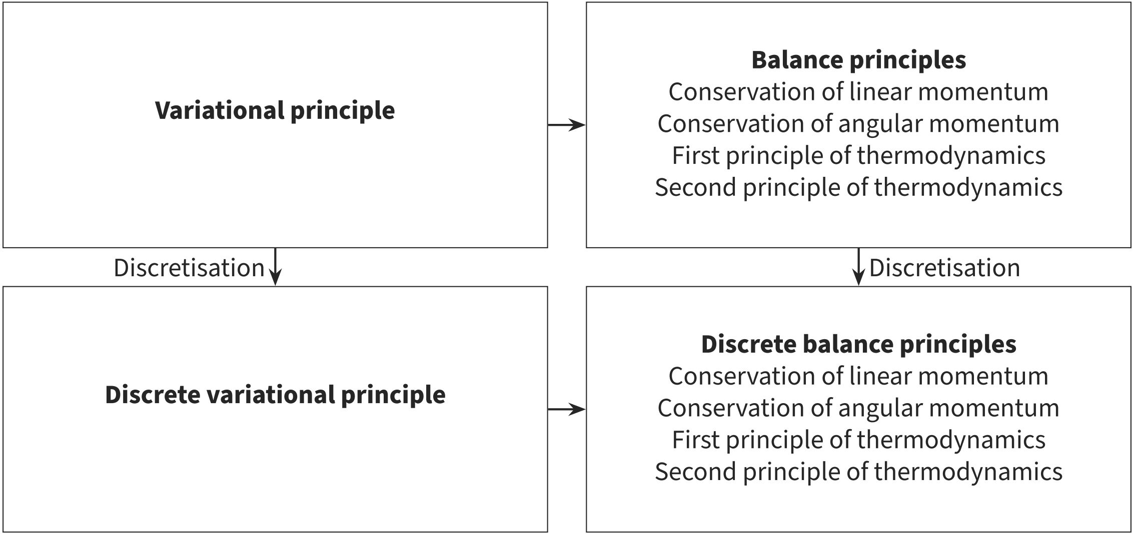
$$D_2 l_d(\boldsymbol{q}_{N-1}, \boldsymbol{q}_N) = D_2 l_d(\boldsymbol{q}_0, \boldsymbol{q}_1)$$

Conservation of angular momentum

$$D_2 l_d(\boldsymbol{q}_{N-1}, \boldsymbol{q}_N) \times \boldsymbol{q}_N = D_2 l_d(\boldsymbol{q}_0, \boldsymbol{q}_1) \times \boldsymbol{q}_1$$

1. Variational integrators through the example of a rotating mass-spring system

A variational integrator for continuum thermodynamics



Variational principle

Balance principles
Conservation of linear momentum
Conservation of angular momentum
First principle of thermodynamics
Second principle of thermodynamics

Discretisation

Discretisation

Discrete variational principle

Discrete balance principles
Conservation of linear momentum
Conservation of angular momentum
First principle of thermodynamics
Second principle of thermodynamics

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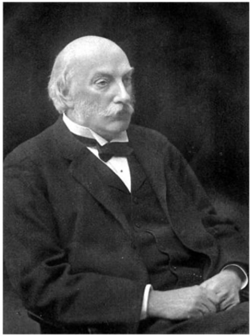
1. Variational integrators through the example of a rotating mass-spring system

Table of Contents

Variational principles - continuous

The first variational principles for continuum thermodynamics/thermodynamics of irreversible processes aimed at **stating the entropy production into a variational form.**



John William Strutt,
Lord Rayleigh

Lars Onsager

Maurice Anthony Biot

Ilya Prigogine

Variational principles - continuous

- John William Strutt. The Theory of Sound. Cambridge university press., 1877.
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- Lars Onsager. ‘Reciprocal Relations in Irreversible Processes. II.’ Physical Review 38, no. 2265 (1931).
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- Maurice Anthony Biot. ‘Variational Principles in Irreversible Thermodynamics with Application to Viscoelasticity’. Physical Review 97, no. 6 (15 March 1955): 1463–69.
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Variational principles - continuous

Brezis-Ekeland-Nayroles principle

Haïm Brezis

Ivar Ekeland

Bernard Nayroles

Variational principles - continuous

Brezis-Ekeland-Nayroles principle

- Haïm Brezis, and Ivar Ekeland. Un principe variationnel associé à certaines équations paraboliques. I. Le cas indépendant du temps. CR Acad Sci Paris Sér A-B 1976; 282: 971–974.
- Haïm Brezis, and Ivar Ekeland. Un principe variationnel associé à certaines équations paraboliques. II. Le cas dépendant du temps. CR Acad Sci Paris Sér A-B 1976; 282: 1197–1198.
- B. Nayroles. Deux théorèmes de minimum pour certains systèmes dissipatifs. CR Acad Sci Paris Sér A-B 1976; 282: A1035– A1038
- Marius Buliga, and Géry De Saxcé. 'A Symplectic Brezis–Ekeland–Nayroles Principle'. Mathematics and Mechanics of Solids 22, no. 6 (June 2017): 1288–1302.

Variational principles - continuous

Bracket formulations.
The idea is to generalise the Poisson bracket (coming from *[Dirac 1950]*) to dissipative systems. Two families of bracket formulations :

Single generator bracket formulations
(total energy)

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \{f, l^\star\} + [f, l^\star]$$

Double generators bracket formulations
(total energy and entropy)

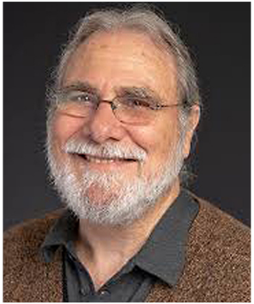
$$\frac{\mathrm{d}f}{\mathrm{d}t} = \{f, l^\star\} + (f, s)$$

Variational principles - continuous

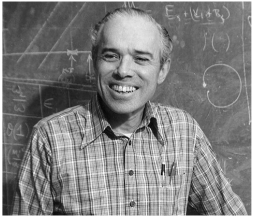
Bracket formulations.
The idea is to generalise the Poisson bracket (coming from *[Dirac 1950]*) to dissipative systems. Two families of bracket formulations

Single generator bracket formulations
(total energy)

Double generators bracket formulations
(total energy and entropy)



Philip J. Morrison



Allan Nathan Kaufman

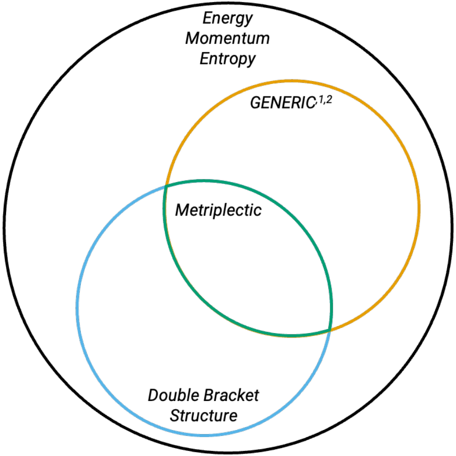
Miroslav Grmela

Hans Christian Öttinger

Variational principles - continuous

- Philip J. Morrison J. ‘Bracket Formulation for Irreversible Classical Fields’. Physics Letters A 100, no. 8 (February 1984): 423–27.
- Allan N. Kaufman. ‘Dissipative Hamiltonian Systems: A Unifying Principle’. Physics Letters A 100, no. 8 (February 1984): 419–22.
- Miroslav Grmela. ‘Bracket Formulation of Dissipative Fluid Mechanics Equations’. Physics Letters A 102, no. 8 (June 1984): 355–58.
- Hans Christian Öttinger. Beyond Equilibrium Thermodynamics. 1st ed. Wiley, 2005.
- Christopher Eldred, and François Gay-Balmaz. ‘Single and Double Generator Bracket Formulations of Multicomponent Fluids with Irreversible Processes’. Journal of Physics A: Mathematical and Theoretical 53, no. 39 (2 October 2020): 395701.

Variational principles - discrete



- Ignacio Romero. ‘Algorithms for Coupled Problems That Preserve Symmetries and the Laws of Thermodynamics’. Computer Methods in Applied Mechanics and Engineering 199, no. 25–28 (May 2010): 1841–58.
- Mark Schiebl, and Peter Betsch. ‘Structure-preserving Space-time Discretization of Large-strain Thermo-viscoelasticity in the Framework of GENERIC’. International Journal for Numerical Methods in Engineering 122, no. 14 (30 July 2021): 3448–88.

Table of Contents

General presentation

Introduce a state vector $\boldsymbol{z}$ *[Maugin and Muschik 1994]*, such that *[Buliga and De Saxcé 2017]*

$$\dot{\boldsymbol{z}} = \dot{\boldsymbol{z}}_{\text{rev}} + \dot{\boldsymbol{z}}_{\text{irr}}$$

Define a functional dependent on the state vector

$$\mathscr{F} : \ M \to \mathbb{R}, \boldsymbol{z} \mapsto \mathscr{F}[\boldsymbol{z}] = \int_{\omega_X} f(\boldsymbol{z}, d\boldsymbol{z}) \, \mathrm{d}\omega_X$$

The Double Bracket Structure reads

$$\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} = \int_{\omega_X} \left(\frac{\partial f}{\partial \boldsymbol{z}}^{\mathsf{T}} \left(\frac{\partial \boldsymbol{z}}{\partial t} \right)_{\text{rev}} + \frac{\partial f}{\partial \boldsymbol{z}}^{\mathsf{T}} \left(\frac{\partial \boldsymbol{z}}{\partial t} \right)_{\text{irr}} \right) \mathrm{d}\omega_X = \left\{ \mathscr{F}, \hat{\mathscr{E}}_{\text{tot}} \right\} + \left(\mathscr{F}, \mathscr{S} \right) + \text{boundary terms}$$

where

- $\left\{ \mathscr{F}, \hat{\mathscr{E}}_{\text{tot}} \right\}$ is a **skrew-symmetric** bracket, representing the **reversible evolution** of the system;
- $\left(\mathscr{F}, \mathscr{S} \right)$ is a **positive, symmetric** bracket, representing the **dissipative evolution** of the system.

Recovering the balance principles

We will recover the balance principles by setting different values for $\mathscr{F}$.
In particular, we obtain the **first law of thermodynamics** through

$$\mathscr{F} = \hat{\mathscr{E}}_{\text{tot}} \Rightarrow \frac{\mathrm{d}\hat{\mathscr{E}}_{\text{tot}}}{\mathrm{d}t} = \underbrace{\left\{\hat{\mathscr{E}}_{\text{tot}}, \hat{\mathscr{E}}_{\text{tot}}\right\}}_{=0} + \left(\hat{\mathscr{E}}_{\text{tot}}, \mathscr{S}\right) + \text{boundary terms}$$

and the **second law of thermodynamics** by

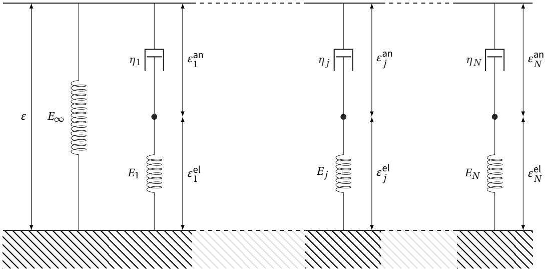
$$\mathscr{F} = \mathscr{S} \Rightarrow \frac{d\mathscr{S}}{dt} = \left\{\mathscr{S}, \hat{\mathscr{E}}_{\text{tot}}\right\} + \underbrace{\left(\mathscr{S}, \mathscr{S}\right)}_{\geq 0} + \text{boundary terms}$$

Table of Contents

What is a Generalised Standard Material?

“Nous appelons matériau standard généralisé un matériau élastoviscoplastique et élastoplastique à déformation plastique instantanée pour lequel il existe une famille de paramètres internes α telle que si A_j désigne la force associée par la relation $A_j = -\partial\phi/\partial\alpha_j$, l’hypothèse de dissipativité normale soit vérifiée pour $A = (R, A)$ [avec R la vitesse associée au gradient de la vitesse de la transformation plastique].”*[Halphen and Nguyen 1975]*

Hypothèse de dissipativité normale “Il existe un potentiel ϕ convexe, semi-continu inférieur, tel que, dans un processus thermodynamique réel, la vitesse thermodynamique α_j associée à la force thermodynamique A_J est un sous gradient de ϕ, c’est-à-dire$\alpha_j \in \partial A_j$”



4. The example of a Generalised Standard Material, small strains, unidimensional

Choice of the state vector

The state vector for the problem is **chosen** as

$$\boldsymbol{z} = \begin{pmatrix} u & p & \varepsilon & T & \boldsymbol{\alpha} \end{pmatrix}$$

where

- u is the displacement;
- p is the linear momentum;
- ε is the symmetric part of the gradient of displacement, here $\varepsilon = \partial u / \partial X$;
- T is the absolute temperature;
- $\boldsymbol{\alpha}$ is a set of internal dissipative variables.

Next, we take the time derivative of a functional $\mathscr{F}$ dependent of the state vector

$$\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} = \int_{\omega_X} \left(\frac{\partial f}{\partial u} \frac{\partial u}{\partial t} + \frac{\partial f}{\partial p} \frac{\partial p}{\partial t} + \frac{\partial f}{\partial \varepsilon} \frac{\partial \varepsilon}{\partial t} + \frac{\partial f}{\partial T} \frac{\partial T}{\partial t} + \left(\frac{\partial f}{\partial \boldsymbol{\alpha}} \right)^{\mathsf{T}} \frac{\partial \boldsymbol{\alpha}}{\partial t} \right) \mathrm{d}\omega_X$$

The state laws of thermodynamics

The Double Bracket Structure is obtained from

$$\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} = \int_{\omega_X} \left(\frac{\partial f}{\partial u}\frac{\partial u}{\partial t} + \frac{\partial f}{\partial p}\frac{\partial p}{\partial t} + \frac{\partial f}{\partial \varepsilon}\frac{\partial \varepsilon}{\partial t} + \frac{\partial f}{\partial T}\frac{\partial T}{\partial t} + \left(\frac{\partial f}{\partial \boldsymbol{\alpha}}\right)^{\mathsf{T}} \frac{\partial \boldsymbol{\alpha}}{\partial t} \right) \mathrm{d}\omega_X$$

$$\frac{\partial u}{\partial t} = \frac{\partial \hat{E}_{\text{tot}}}{\partial p}$$

First Legendre transformation

$$\frac{\partial p}{\partial t} = \frac{\partial \hat{E}_{\text{tot}}}{\partial u} + \frac{\partial}{\partial X}\left(\frac{\partial \hat{E}_{\text{tot}}}{\partial \varepsilon} - \left(\frac{\partial \hat{E}_{\text{tot}}}{\partial T}\right)\left(\frac{\partial s}{\partial T}\right)^{-1}\frac{\partial s}{\partial \varepsilon} \right)$$

Conservation of linear momentum

$$\frac{\partial \varepsilon}{\partial t} = \frac{\partial}{\partial X}\left(\frac{\partial \hat{E}_{\text{tot}}}{\partial p}\right)$$

Compatibility equation

$$\frac{\partial T}{\partial t} = \frac{1}{\rho c}\frac{\partial}{\partial X}\left(K\frac{\partial T}{\partial X}\right) - \frac{1}{c}\left(\frac{\partial \hat{E}_{\text{int}}}{\partial \boldsymbol{\alpha}}\right)^{\mathsf{T}}\frac{\partial \boldsymbol{\alpha}}{\partial t} - \left(\frac{\partial s}{\partial T}\right)^{-1}\frac{\partial s}{\partial \varepsilon}\frac{\partial}{\partial X}\left(\frac{\partial \hat{E}_{\text{tot}}}{\partial p}\right)$$

Gibbs' law

$$\frac{\partial \boldsymbol{\alpha}}{\partial t} = -\frac{1}{c} T \boldsymbol{V}^{-1}\frac{\partial \hat{E}_{\text{int}}}{\partial \boldsymbol{\alpha}}\frac{\partial s}{\partial T} + T\boldsymbol{V}^{-1}\frac{\partial s}{\partial \boldsymbol{\alpha}}$$

Internal dissipative laws

The state laws of thermodynamics

The Double Bracket Structure is obtained from

$$\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} = \int_{\omega_X} \left(\frac{\partial f}{\partial u}\frac{\partial u}{\partial t} + \frac{\partial f}{\partial p}\frac{\partial p}{\partial t} + \frac{\partial f}{\partial \varepsilon}\frac{\partial \varepsilon}{\partial t} + \frac{\partial f}{\partial T}\frac{\partial T}{\partial t} + \left(\frac{\partial f}{\partial \boldsymbol{\alpha}}\right)^{\mathsf{T}} \frac{\partial \boldsymbol{\alpha}}{\partial t} \right) \mathrm{d}\omega_X$$

$$\frac{\partial u}{\partial t} = \frac{\partial \hat{E}_{\text{tot}}}{\partial p}$$

$$\frac{\partial p}{\partial t} = \frac{\partial \hat{E}_{\text{tot}}}{\partial u} + \frac{\partial}{\partial X}\left(\frac{\partial \hat{E}_{\text{tot}}}{\partial \varepsilon} - \left(\frac{\partial \hat{E}_{\text{tot}}}{\partial T}\right)\left(\frac{\partial s}{\partial T}\right)^{-1} \frac{\partial s}{\partial \varepsilon} \right)$$

$$\frac{\partial \varepsilon}{\partial t} = \frac{\partial}{\partial X}\left(\frac{\partial \hat{E}_{\text{tot}}}{\partial p}\right)$$

$$\frac{\partial T}{\partial t} = \frac{1}{\rho c}\frac{\partial}{\partial X}\left(K \frac{\partial T}{\partial X}\right) - \frac{1}{c}\left(\frac{\partial \hat{E}_{\text{int}}}{\partial \boldsymbol{\alpha}}\right)^{\mathsf{T}} \frac{\partial \boldsymbol{\alpha}}{\partial t} - \left(\frac{\partial s}{\partial T}\right)^{-1} \frac{\partial s}{\partial \varepsilon}\frac{\partial}{\partial X}\left(\frac{\partial \hat{E}_{\text{tot}}}{\partial p}\right)$$

$$\frac{\partial \boldsymbol{\alpha}}{\partial t} = -\frac{1}{c} T \boldsymbol{V}^{-1} \frac{\partial \hat{E}_{\text{int}}}{\partial \boldsymbol{\alpha}}\frac{\partial s}{\partial T} + T\boldsymbol{V}^{-1}\frac{\partial s}{\partial \boldsymbol{\alpha}}$$

We observe a split of the **evolution of the temperature** into a **reversible** and an **irreversible** contribution.

A unidimensional Generalised Standard Material

The Double Bracket Structure **emerges from the evolution laws**

$$
\begin{aligned}
\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} =& \left\{\mathscr{F}, \hat{\mathscr{E}}_{\mathrm{tot}}\right\} + (\mathscr{F}, \mathscr{S}) + \\
&+ \int_{\partial\omega_X} \frac{\partial f}{\partial \varepsilon}\frac{\partial u}{\partial t}\,\mathrm{d}(\partial\omega_X) - \int_{\partial\omega_X} \frac{\partial f}{\partial p}\left(\frac{\partial s}{\partial T}\right)^{-1}\frac{\partial s}{\partial \varepsilon}\frac{\partial \hat{E}_{\mathrm{tot}}}{\partial T}\,\mathrm{d}(\partial\omega_X) - \int_{\partial\omega_X} \frac{1}{\rho}\frac{\partial f}{\partial T} K \frac{T^2}{c^2}\frac{\partial}{\partial X}\left(\frac{\partial s}{\partial T}\right)\mathrm{d}(\partial\omega_X)
\end{aligned}
$$

where

$$
\begin{aligned}
\left\{\mathscr{F}, \hat{\mathscr{E}}_{\mathrm{tot}}\right\} = \int_{\omega_X} \Bigg[& \left(\frac{\partial f}{\partial u} - \frac{\partial}{\partial X}\left(\frac{\partial f}{\partial \varepsilon}\right)\right)\frac{\partial \hat{E}_{\mathrm{tot}}}{\partial p} - \frac{\partial f}{\partial p}\left(\frac{\partial \hat{E}_{\mathrm{tot}}}{\partial u} - \frac{\partial}{\partial X}\left(\frac{\partial \hat{E}_{\mathrm{tot}}}{\partial \varepsilon}\right)\right) + \\
&+ \left(\frac{\partial s}{\partial T}\right)^{-1}\frac{\partial s}{\partial \varepsilon}\left(\frac{\partial \hat{E}_{\mathrm{tot}}}{\partial T}\frac{\partial}{\partial X}\left(\frac{\partial f}{\partial p}\right) - \frac{\partial f}{\partial T}\frac{\partial}{\partial X}\left(\frac{\partial \hat{E}_{\mathrm{tot}}}{\partial p}\right)\right)\Bigg]\mathrm{d}\omega_X
\end{aligned}
$$

$$
\begin{aligned}
(\mathscr{F}, \mathscr{S}) = \int_{\omega_X} \Bigg(& \frac{1}{\rho}\frac{\partial}{\partial X}\left(\frac{\partial f}{\partial T}\right) K \frac{T^2}{c^2}\frac{\partial}{\partial X}\left(\frac{\partial s}{\partial T}\right) + \frac{\partial f}{\partial T}\frac{1}{c}\frac{T}{c}\left(\frac{\partial \hat{E}_{\mathrm{int}}}{\partial \boldsymbol{\alpha}}\right)^{\mathsf{T}} \boldsymbol{V}^{-1}\frac{\partial \hat{E}_{\mathrm{int}}}{\partial \boldsymbol{\alpha}}\frac{\partial s}{\partial T} + \\
& - \frac{\partial f}{\partial T}\frac{T}{c}\left(\frac{\partial \hat{E}_{\mathrm{int}}}{\partial \boldsymbol{\alpha}}\right)^{\mathsf{T}} \boldsymbol{V}^{-1}\frac{\partial s}{\partial \boldsymbol{\alpha}} - \frac{T}{c}\left(\frac{\partial f}{\partial \boldsymbol{\alpha}}\right)^{\mathsf{T}} \boldsymbol{V}^{-1}\frac{\partial \hat{E}_{\mathrm{int}}}{\partial \boldsymbol{\alpha}}\frac{\partial s}{\partial T} + T\left(\frac{\partial f}{\partial \boldsymbol{\alpha}}\right)^{\mathsf{T}} \boldsymbol{V}^{-1}\frac{\partial s}{\partial \boldsymbol{\alpha}}\Bigg)\mathrm{d}\omega_X
\end{aligned}
$$

A unidimensional Generalised Standard Material

In details, we have the **reversible bracket**

$$\{\mathscr{F},\hat{\mathscr{E}}_{\mathrm{tot}}\} = \int_{\omega_X} \Bigg[\left(\frac{\partial f}{\partial u} - \frac{\partial}{\partial X}\left(\frac{\partial f}{\partial \varepsilon}\right)\right)\frac{\partial \hat{E}_{\mathrm{tot}}}{\partial p} - \frac{\partial f}{\partial p}\left(\frac{\partial \hat{E}_{\mathrm{tot}}}{\partial u} - \frac{\partial}{\partial X}\left(\frac{\partial \hat{E}_{\mathrm{tot}}}{\partial \varepsilon}\right)\right) +$$

$$+ \left(\frac{\partial s}{\partial T}\right)^{-1}\frac{\partial s}{\partial \varepsilon}\left(\frac{\partial \hat{E}_{\mathrm{tot}}}{\partial T}\frac{\partial}{\partial X}\left(\frac{\partial f}{\partial p}\right) - \frac{\partial f}{\partial T}\frac{\partial}{\partial X}\left(\frac{\partial \hat{E}_{\mathrm{tot}}}{\partial p}\right)\right)\Bigg] \mathrm{d}\omega_X = \int_{\omega_X} \left(\frac{\partial f}{\partial \boldsymbol{z}}\right)^{\mathsf{T}} \boldsymbol{L}(\boldsymbol{z}) \frac{\partial \hat{E}_{\mathrm{tot}}}{\partial \boldsymbol{z}} \,\mathrm{d}\omega_X$$

where we define the **skrew-symmetric** matrix

$$\boldsymbol{L}(\boldsymbol{z}) = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ -1 & 0 & \left(\frac{\partial s}{\partial T}\right)^{-1}\frac{\partial s}{\partial \varepsilon}\frac{\partial \square_{\mathrm{left}}}{\partial X} & \vdots & & \vdots \\ 0 & -\left(\frac{\partial s}{\partial T}\right)^{-1}\frac{\partial s}{\partial \varepsilon}\frac{\partial \square_{\mathrm{right}}}{\partial X} & 0 & \vdots & & \vdots \\ 0 & \cdots & \cdots & 0 & \cdots & 0 \\ \vdots & & & \vdots & & \vdots \\ 0 & \cdots & \cdots & 0 & \cdots & 0 \end{pmatrix}$$

A unidimensional Generalised Standard Material

In details, we have the **dissipative bracket**

$$
\begin{aligned}
(\mathscr{F},\mathscr{S}) = \int_{\omega_X} \Bigg(& \frac{1}{\rho}\frac{\partial}{\partial X}\left(\frac{\partial f}{\partial T}\right) K \frac{T^2}{c^2}\frac{\partial}{\partial X}\left(\frac{\partial s}{\partial T}\right) + \frac{\partial f}{\partial T}\frac{1}{c}\frac{T}{c}\left(\frac{\partial \hat{E}_{\text{int}}}{\partial \boldsymbol{\alpha}}\right)^{\mathsf{T}} \boldsymbol{V}^{-1}\frac{\partial \hat{E}_{\text{int}}}{\partial \boldsymbol{\alpha}}\frac{\partial s}{\partial T} + \\
& - \frac{\partial f}{\partial T}\frac{T}{c}\left(\frac{\partial \hat{E}_{\text{int}}}{\partial \boldsymbol{\alpha}}\right)^{\mathsf{T}} \boldsymbol{V}^{-1}\frac{\partial s}{\partial \boldsymbol{\alpha}} - \frac{T}{c}\left(\frac{\partial f}{\partial \boldsymbol{\alpha}}\right)^{\mathsf{T}} \boldsymbol{V}^{-1}\frac{\partial \hat{E}_{\text{int}}}{\partial \boldsymbol{\alpha}}\frac{\partial s}{\partial T} + T\left(\frac{\partial f}{\partial \boldsymbol{\alpha}}\right)^{\mathsf{T}} \boldsymbol{V}^{-1}\frac{\partial s}{\partial \boldsymbol{\alpha}}\Bigg)\,\mathrm{d}\omega_X = \int_{\omega_X}\left(\frac{\partial f}{\partial \boldsymbol{z}}\right)^{\mathsf{T}} \boldsymbol{M}(\boldsymbol{z})\frac{\partial s}{\partial \boldsymbol{z}}\,\mathrm{d}\omega_X
\end{aligned}
$$

where we define the **symmetric, positive** matrix

$$
\boldsymbol{M}(\boldsymbol{z}) = \begin{pmatrix}
0 & 0 & 0 & 0 & \mathbf{0}^{\mathsf{T}} \\
0 & 0 & 0 & 0 & \mathbf{0}^{\mathsf{T}} \\
0 & 0 & 0 & 0 & \mathbf{0}^{\mathsf{T}} \\
0 & 0 & 0 & \dfrac{1}{\rho}\dfrac{\partial \square_{\text{left}}}{\partial X} K\left(\dfrac{T}{c}\right)^2 \dfrac{\partial \square_{\text{right}}}{\partial X} + \dfrac{T}{c^2}\dfrac{\partial \hat{E}_{\text{int}}}{\partial \boldsymbol{\alpha}}^{\mathsf{T}} \boldsymbol{V}^{-1}\dfrac{\partial \hat{E}_{\text{int}}}{\partial \boldsymbol{\alpha}} & -\dfrac{T}{c}\left(\dfrac{\partial \hat{E}_{\text{int}}}{\partial \boldsymbol{\alpha}}\right)^{\mathsf{T}} \boldsymbol{V}^{-1} \\
\mathbf{0} & \mathbf{0} & \mathbf{0} & -\dfrac{T}{c}\boldsymbol{V}^{-1}\dfrac{\partial \hat{E}_{\text{int}}}{\partial \boldsymbol{\alpha}} & T\boldsymbol{V}^{-1}
\end{pmatrix}
$$

Remarks on the boundary terms

The Double Bracket Structure is given by

$$\begin{aligned}\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} =& \left\{\mathscr{F}, \hat{\mathscr{E}}_{\text{tot}}\right\} + (\mathscr{F}, \mathscr{S}) + \\ &+ \int_{\partial\omega_X} \frac{\partial f}{\partial \varepsilon} \frac{\partial u}{\partial t} \mathrm{d}(\partial\omega_X) - \int_{\partial\omega_X} \frac{\partial f}{\partial p} \left(\frac{\partial s}{\partial T}\right)^{-1} \frac{\partial s}{\partial \varepsilon} \frac{\partial \hat{E}_{\text{tot}}}{\partial T} \mathrm{d}(\partial\omega_X) - \int_{\partial\omega_X} \frac{1}{\rho} \frac{\partial f}{\partial T} K \frac{T^2}{c^2} \frac{\partial}{\partial X} \left(\frac{\partial s}{\partial T}\right) \mathrm{d}(\partial\omega_X)\end{aligned}$$

- **Boundary terms** appear within the calculus, which are often **neglected or cancelled** *[Romero 2010; Hütter and Svendsen 2012; Schiebl and Betsch 2021]*. However, they are necessary to be able to recover balance principles without additional information.

How to recover the balance principles from the structure?

The **conservation of linear momentum** can be obtained through

$$\mathscr{F} = \int_{\omega_X} p \,\mathrm{d}\omega_X \Rightarrow (\ldots) \Rightarrow \boxed{\frac{\partial p}{\partial t} = -\frac{\partial \hat{E}_{\text{tot}}}{\partial u} + \mathrm{div}(\sigma)}$$

The **conservation of angular momentum** does not make sense in the unidimensional problem.
The **first principle of thermodynamics** reads

$$\mathscr{F} = \hat{\mathscr{E}}_{\text{tot}} = \int_{\omega_X} \left(\frac{1}{2} p \frac{1}{\rho} p + \rho \hat{E}_{\text{int}}\left(\varepsilon, T, \alpha_i\right)\right) \mathrm{d}\omega_X \Rightarrow (\cdots) \Rightarrow \boxed{\rho \frac{\partial \hat{E}_{\text{int}}}{\partial t} = \frac{\partial \varepsilon}{\partial t} \sigma - \frac{\partial q}{\partial X}}$$

Finally, the **second principle of thermodynamics** is

$$\mathscr{F} = \mathscr{S} = \int_{\omega_X} s \,\mathrm{d}\omega_X, \Rightarrow (\ldots) \Rightarrow \boxed{\rho \frac{\partial s}{\partial t} + \frac{\partial}{\partial X}\left(\frac{q}{T}\right) \geq 0 \Leftrightarrow \frac{1}{\rho T}\left[-\frac{1}{T} q \frac{\partial T}{\partial X} - \rho \left(\frac{\partial w}{\partial \boldsymbol{\alpha}}\right)^{\mathsf{T}} \frac{\partial \boldsymbol{\alpha}}{\partial t}\right] \geq 0}$$

Table of Contents

Choice of the state vector

Small strains example

$$\boldsymbol{z} = \begin{pmatrix} u & p & \varepsilon & T & \boldsymbol{\alpha} \end{pmatrix}$$

where

- u is the displacement;
- p is the linear momentum;
- ε is the symmetric part of the gradient of displacement, here $\varepsilon = \partial u / \partial X$;
- T is the absolute temperature;
- $\boldsymbol{\alpha}$ is a set of internal dissipative variables.

Large strains thermo-visco-elastodynamics

$$\boldsymbol{z} = \begin{pmatrix} \underline{\chi} & \underline{p} & \underline{\underline{\Pi}} & T & \underline{\underline{C}}_{\mathrm{i}}^{-1} \end{pmatrix}$$

where

- $\underline{\chi}$ is the configuration;
- $\underline{p}$ is the linear momentum;
- $\underline{\underline{\Pi}}$ is the first Piola Kirchhoff stress tensor;
- T is the absolute temperature;
- $\underline{\underline{C}}_{\mathrm{i}}^{-1}$ is the inverse of the inelastic Cauchy-Green tensor.

Finite visco-elasticity - multisymplectic Hamiltonian

Thermo-**visco**-elastodynamics: Sidoroff's decomposition of the gradient of transformation *[Lee 1969; Sidoroff 1974; Govindjee and Reese 1997]*

$$\underline{\underline{F}} = \underline{\underline{F}}_{\mathrm{e}} \cdot \underline{\underline{F}}_{\mathrm{i}}$$

We hold ourselves to have the **total energy and the entropy defined in terms of the first Piola Kirchhoff stress tensor**

$$l^{\star}(\underline{\chi}, \underline{p}, \underline{\underline{\Pi}}, T, \underline{\underline{C}}_{\mathrm{i}}^{-1}) = \underline{p} \cdot \frac{\partial \underline{\chi}}{\partial t} - \underline{\underline{\Pi}} : \underline{\underline{F}} - l\left(\underline{\chi}, \frac{\partial \underline{\chi}}{\partial t}, \underline{\underline{F}}, T, \underline{\underline{C}}_{\mathrm{i}}^{-1}\right), \underline{p} = \frac{\partial l}{\partial\left(\frac{\partial \underline{\chi}}{\partial t}\right)}, \underline{\underline{\Pi}} = -\frac{\partial l}{\partial \underline{\underline{F}}}$$

$$\rho w^{*}(T, \underline{\underline{\Pi}}, \underline{\underline{C}}_{\mathrm{i}}^{-1}) = \underline{\underline{\Pi}} : \underline{\underline{F}} - \rho w(T, \underline{\underline{F}}, \underline{\underline{C}}_{\mathrm{i}}^{-1}) = \underbrace{\underline{\underline{\Pi}} : \underline{\underline{F}} + \rho T s(T, \underline{\underline{F}}, \underline{\underline{C}}_{\mathrm{i}}^{-1})}_{\rho T s^{*}(T, \underline{\underline{\Pi}}), \underline{\underline{C}}_{\mathrm{i}}^{-1}} - \rho \hat{E}_{\mathrm{int}}(T, \underline{\underline{F}}, \underline{\underline{C}}_{\mathrm{i}}^{-1})$$

Expression of the Double Bracket Structure

After “some” calculus, we obtain

$$
\begin{aligned}
\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} =& \int_{\omega_X} \left(\frac{\partial f}{\partial \underline{\chi}} \cdot \frac{\partial \underline{\chi}}{\partial t} + \frac{\partial f}{\partial \underline{p}} \cdot \frac{\partial \underline{p}}{\partial t} - \frac{\partial f}{\partial \underline{\underline{F}}} : \dot{\underline{\underline{F}}} + \frac{\partial f}{\partial T} \left(\left(\frac{\partial T}{\partial t} \right)_{\text{rev}} + \left(\frac{\partial T}{\partial t} \right)_{\text{irr}} \right) + \frac{\partial f}{\partial \underline{\underline{C}}_{\text{i}}^{-1}} : \frac{\partial \underline{\underline{C}}_{\text{i}}^{-1}}{\partial t} \right) \\
=& \left\{ \mathscr{F}, \hat{\mathscr{E}}^{*}_{\text{tot}} \right\} + \left(\mathscr{F}, \mathscr{S}^{*} \right) + \\
& + \int_{\partial\omega_X} \frac{\partial f}{\partial \underline{p}} \cdot (\underline{\underline{\Pi}} \cdot \underline{N})\, \mathrm{d}(\partial\omega_X) - \int_{\partial\omega_X} \frac{1}{\rho} \frac{\partial f}{\partial T} \underline{\underline{K}} \left(\frac{T}{c} \right)^2 \cdot \frac{\partial}{\partial \underline{X}} \left(\frac{\partial s^*}{\partial T} \right) \cdot \underline{N}\, \mathrm{d}(\partial\omega_X)
\end{aligned}
$$

- **boundary terms** already present before appear through the calculus;
- use of the **Lie derivative**, or of time derivatives on Lagrangian quantities to derive the reversible bracket;
- remark a derivative of f in terms of the gradient of transformations, which appears naturally within the calculus, through transformations using

$$\underline{\underline{\Pi}} = \underline{\underline{F}} \cdot \underline{\underline{S}}$$

where $\underline{\underline{S}}$ is the second Piola Kirchhoff stress tensor.

Details of the brackets

The **reversible bracket** is given by

$$\{\mathscr{F}, \hat{\mathscr{E}}^*_{\text{tot}}\} = \int_{\omega_X} \left(\frac{\partial f}{\partial \underline{\chi}} \cdot \frac{\partial \hat{E}^*_{\text{tot}}}{\partial \underline{p}} - \frac{\partial f}{\partial \underline{p}} \cdot \frac{\partial \hat{E}^*_{\text{tot}}}{\partial \underline{\chi}} + \underline{\underline{\nabla}}_{\underline{X}} \frac{\partial f}{\partial \underline{p}} : \frac{\partial \hat{E}^*_{\text{tot}}}{\partial \underline{\underline{\Pi}}} \underline{\underline{S}} - \frac{\partial f}{\partial \underline{\underline{\Pi}}} : \underline{\underline{\nabla}}_{\underline{X}} \frac{\partial \hat{E}^*_{\text{tot}}}{\partial \underline{p}} \underline{\underline{S}} + \right.$$
$$\left. - \frac{\partial \hat{E}^*_{\text{tot}}}{\partial T} \left(\frac{\partial s^*}{\partial T} \right)^{-1} \underline{\underline{\nabla}}_{\underline{X}} \frac{\partial f}{\partial \underline{p}} : \frac{\partial s^*}{\partial \underline{\underline{\Pi}}} \underline{\underline{S}} + \frac{\partial f}{\partial T} \left(\frac{\partial s^*}{\partial T} \right)^{-1} \frac{\partial s^*}{\partial \underline{\underline{\Pi}}} : \underline{\underline{\nabla}}_{\underline{X}} \frac{\partial \hat{E}^*_{\text{tot}}}{\partial \underline{p}} \underline{\underline{S}} \right) \mathrm{d}\omega_X$$

- The bracket is skrew-symmetric if the second Piola-Kirchhoff stress tensor is symmetric

$$\underline{\underline{S}} = \underline{\underline{S}}^{\mathsf{T}}$$

- Comparison with the previous reversible bracket

$$\{\mathscr{F}, \hat{\mathscr{E}}_{\text{tot}}\} = \int_{\omega_X} \left[\left(\frac{\partial f}{\partial u} - \frac{\partial}{\partial X} \left(\frac{\partial f}{\partial \varepsilon} \right) \right) \frac{\partial \hat{E}_{\text{tot}}}{\partial p} - \frac{\partial f}{\partial p} \left(\frac{\partial \hat{E}_{\text{tot}}}{\partial u} - \frac{\partial}{\partial X} \left(\frac{\partial \hat{E}_{\text{tot}}}{\partial \varepsilon} \right) \right) + \right.$$
$$\left. + \left(\frac{\partial s}{\partial T} \right)^{-1} \frac{\partial s}{\partial \varepsilon} \left(\frac{\partial \hat{E}_{\text{tot}}}{\partial T} \frac{\partial}{\partial X} \left(\frac{\partial f}{\partial p} \right) - \frac{\partial f}{\partial T} \frac{\partial}{\partial X} \left(\frac{\partial \hat{E}_{\text{tot}}}{\partial p} \right) \right) \right] \mathrm{d}\omega_X$$

Details of the brackets

The **dissipative bracket** is given by

$$
\begin{aligned}
(\mathscr{F}, \mathscr{S}^*) = \int_{\omega_X} \Bigg[& \frac{1}{\rho} \frac{\partial}{\partial \underline{X}} \left(\frac{\partial f}{\partial T} \right) \cdot \underline{\underline{K}} \left(\frac{T}{c} \right)^2 \cdot \frac{\partial}{\partial \underline{X}} \left(\frac{\partial s^*}{\partial T} \right) + \frac{\partial f}{\partial T} \frac{4}{c^2} \left(\frac{\partial \hat{E}^*_{\mathrm{int}}}{\partial \underline{\underline{C}}_{\mathrm{i}}^{-1}} \cdot \underline{\underline{C}}_{\mathrm{i}}^{-1} \right) : T \underline{\underline{\underline{\underline{N}}}} : \left(\frac{\partial \hat{E}^*_{\mathrm{int}}}{\partial \underline{\underline{C}}_{\mathrm{i}}^{-1}} \cdot \underline{\underline{C}}_{\mathrm{i}}^{-1} \right) \frac{\partial s^*}{\partial T} + \\
& - \frac{\partial f}{\partial T} \frac{4}{c} \left(\frac{\partial s^*}{\partial \underline{\underline{C}}_{\mathrm{i}}^{-1}} \cdot \underline{\underline{C}}_{\mathrm{i}}^{-1} \right) : T \underline{\underline{\underline{\underline{N}}}} : \left(\frac{\partial \hat{E}^*_{\mathrm{int}}}{\partial \underline{\underline{C}}_{\mathrm{i}}^{-1}} \cdot \underline{\underline{C}}_{\mathrm{i}}^{-1} \right) - \frac{\partial s^*}{\partial T} \frac{4}{c} \left(\frac{\partial \hat{E}^*_{\mathrm{int}}}{\partial \underline{\underline{C}}_{\mathrm{i}}^{-1}} \cdot \underline{\underline{C}}_{\mathrm{i}}^{-1} \right) : T \underline{\underline{\underline{\underline{N}}}} : \left(\frac{\partial f}{\partial \underline{\underline{C}}_{\mathrm{i}}^{-1}} \cdot \underline{\underline{C}}_{\mathrm{i}}^{-1} \right) + \\
& + 4 \left(\frac{\partial s^*}{\partial \underline{\underline{C}}_{\mathrm{i}}^{-1}} \cdot \underline{\underline{C}}_{\mathrm{i}}^{-1} \right) : T \underline{\underline{\underline{\underline{N}}}} : \left(\frac{\partial f}{\partial \underline{\underline{C}}_{\mathrm{i}}^{-1}} \cdot \underline{\underline{C}}_{\mathrm{i}}^{-1} \right) \Bigg] \mathrm{d}\omega_X
\end{aligned}
$$

The bracket is symmetric if the conduction operator $\underline{\underline{K}}$ and the viscous operator $\underline{\underline{\underline{\underline{N}}}}$ are both symmetric

$$\underline{\underline{K}}^{\mathsf{T}} = \underline{\underline{K}} \qquad\qquad \underline{\underline{\underline{\underline{N}}}}^{\mathsf{T}} = \underline{\underline{\underline{\underline{N}}}} \qquad (\Leftrightarrow N_{ABCD} = N_{BADC})$$

The bracket is positive if $\underline{\underline{K}}$, $\underline{\underline{\underline{\underline{N}}}}$ and the temperature are positive

$$\underline{a} \cdot \underline{\underline{K}} \cdot \underline{a} \geq 0 \quad \forall \underline{a} \qquad\qquad \underline{\underline{A}} : \underline{\underline{\underline{\underline{N}}}} : \underline{\underline{A}} \geq 0 \quad \forall \underline{\underline{A}}$$

Recover the balance principles

The **conservation of linear momentum** can be obtained through

$$\mathscr{F} = \int_{\omega_X} \underline{p}\,\mathrm{d}\omega_X \Rightarrow (\cdots) \Rightarrow \boxed{\frac{\partial \underline{p}}{\partial t} = -\frac{\partial \hat{E}^*_{\text{tot}}}{\partial \underline{\chi}} + \mathrm{DIV}_{\underline{X}}\,\underline{\underline{\Pi}}}$$

The **conservation of angular momentum** yields

$$\mathscr{F} = \int_{\omega_X} (\underline{\chi} \times \underline{p})\,\mathrm{d}\omega_X \Rightarrow (\cdots) \Rightarrow \boxed{\underline{\underline{S}} = \underline{\underline{S}}^{\mathsf{T}} \,(\Leftrightarrow \underline{\underline{\Pi}} \cdot \underline{\underline{F}}^{\mathsf{T}} = \underline{\underline{F}} \cdot \underline{\underline{\Pi}}^{\mathsf{T}})}$$

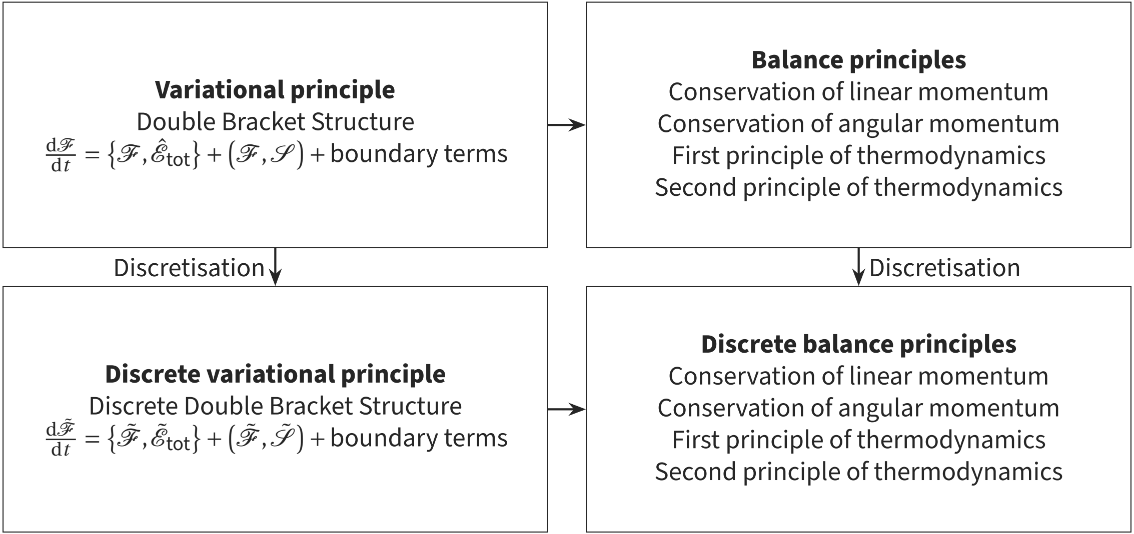
The **first principle of thermodynamics** reads

$$\mathscr{F} = \hat{\mathscr{E}}^*_{\text{tot}} = \int_{\omega_X} \left(\frac{1}{2}\frac{1}{\rho}\underline{p} \cdot \underline{p} + \rho \hat{E}^*_{\text{int}}\right) \mathrm{d}\omega_X \Rightarrow (\cdots) \Rightarrow \boxed{\rho \frac{\partial \hat{E}^*_{\text{int}}}{\partial t} = \frac{\partial \underline{\underline{F}}}{\partial t} : \underline{\underline{\Pi}} - \mathrm{DIV}_{\underline{X}}\,\underline{Q}}$$

Finally, the **second principle of thermodynamics** is

$$\mathscr{F} = \mathscr{S}^* = \int_{\omega_X} s^*\,\mathrm{d}\omega_X \Rightarrow (\cdots) \Rightarrow \boxed{\rho \frac{\partial s^*}{\partial t} + \mathrm{DIV}_{\underline{X}}\left(\frac{\underline{Q}}{T}\right) \geq 0 \Leftrightarrow -\frac{1}{T}\underline{Q} \cdot \frac{\partial T}{\partial \underline{X}} - \rho \frac{\partial w}{\partial \underline{\underline{C}}_{\text{i}}^{-1}} : \frac{\partial \underline{\underline{C}}_{\text{i}}^{-1}}{\partial t} \geq 0}$$

A variational integrator for continuum thermodynamics



Variational principle

Double Bracket Structure

$$\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} = \left\{\mathscr{F}, \hat{\mathscr{E}}_{\text{tot}}\right\} + \left(\mathscr{F}, \mathscr{S}\right) + \text{boundary terms}$$

Balance principles

Conservation of linear momentum
Conservation of angular momentum
First principle of thermodynamics
Second principle of thermodynamics

Discretisation

Discretisation

Discrete variational principle

Discrete Double Bracket Structure

$$\frac{\mathrm{d}\tilde{\mathscr{F}}}{\mathrm{d}t} = \left\{\tilde{\mathscr{F}}, \tilde{\mathscr{E}}_{\text{tot}}\right\} + \left(\tilde{\mathscr{F}}, \tilde{\mathscr{S}}\right) + \text{boundary terms}$$

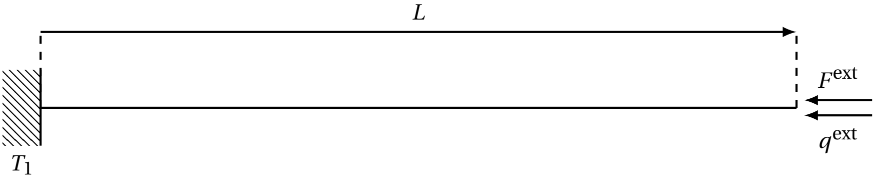
Discrete balance principles

Conservation of linear momentum
Conservation of angular momentum
First principle of thermodynamics
Second principle of thermodynamics

Table of Contents

Statement of the problem

Consider the following problem



We have the following boundary conditions

$\sigma(X = L, t) = F^{\text{ext}}/S$	for $X = L$	Mechanical Neumann condition
$u(X = 0, t) = 0$	for $X = 0$	Mechanical Dirichlet condition
$q(X = L, t) = q^{\text{ext}}$	for $X = L$	Thermic Neumann condition
$T(X = 0, t) = T_1$	for $X = 0$	Thermic Dirichlet condition

Statement of the problem

The Double Bracket Structure is given by

$$
\begin{aligned}
\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} = \int_0^L & \left(\left(\frac{\partial f}{\partial u} - \frac{\partial}{\partial X}\left(\frac{\partial f}{\partial \varepsilon}\right)\right) \frac{\partial \hat{E}_{\text{tot}}}{\partial p} - \frac{\partial f}{\partial p}\left(\frac{\partial \hat{E}_{\text{tot}}}{\partial u} - \frac{\partial}{\partial X}\left(\frac{\partial \hat{E}_{\text{tot}}}{\partial \varepsilon}\right)\right) + \right. \\
& \left. + \left(\frac{\partial s}{\partial T}\right)^{-1} \frac{\partial s}{\partial \varepsilon}\left(\frac{\partial \hat{E}_{\text{tot}}}{\partial T}\frac{\partial}{\partial X}\left(\frac{\partial f}{\partial p}\right) - \frac{\partial f}{\partial T}\frac{\partial}{\partial X}\left(\frac{\partial \hat{E}_{\text{tot}}}{\partial p}\right)\right)\right) \mathrm{d}X + \\
& + \int_0^L \left(\frac{1}{\rho}\frac{\partial}{\partial X}\left(\frac{\partial f}{\partial T}\right) K \frac{T^2}{c^2}\frac{\partial}{\partial X}\left(\frac{\partial s}{\partial T}\right)\right) \mathrm{d}X + \\
& + \left[\frac{\partial f}{\partial \varepsilon}\frac{\partial u}{\partial t}\right]_0^L - \left[\frac{\partial f}{\partial p}\left(\frac{\partial s}{\partial T}\right)^{-1}\frac{\partial s}{\partial \varepsilon}\frac{\partial \hat{E}_{\text{tot}}}{\partial T}\right]_0^L - \left[\frac{1}{\rho}\frac{\partial f}{\partial T} K \frac{T^2}{c^2}\frac{\partial}{\partial X}\left(\frac{\partial s}{\partial T}\right)\right]_0^L
\end{aligned}
$$

The equations of linear thermo-elasticity

Consider the potentials of linear thermo-elasticty, for **small perturbations, small variations of temperature**

$$\begin{aligned}
\rho w\left(\frac{\partial u}{\partial X}, T\right) &= \frac{1}{2}\frac{\partial u}{\partial X}(\lambda+2\mu)\frac{\partial u}{\partial X} - (T-T_0)k\frac{\partial u}{\partial X} - \frac{1}{2}\frac{\rho c}{T_0}(T-T_0)^2 \\
\rho s\left(\frac{\partial u}{\partial X}, T\right) &= k\frac{\partial u}{\partial X} + \frac{\rho c}{T_0}(T-T_0) \\
\hat{E}_{\text{tot}}\left(u, p, \frac{\partial u}{\partial X}, T\right) &= \frac{1}{2}p\frac{1}{\rho}p + \frac{1}{2}\frac{\partial u}{\partial X}(\lambda+2\mu)\frac{\partial u}{\partial X} + T_0 k\frac{\partial u}{\partial X} + \frac{1}{2}\frac{\rho c}{T_0}(T^2 - T_0^2)
\end{aligned}$$

Consider the expression of

$$f = \delta u^*(X)u(X,t) + \delta p^*(X)p(X,t) + \delta T^*(X)T(X,t)$$

where $\delta u^*(X), \delta p^*(X), \delta T^*(X)$ are test fields.

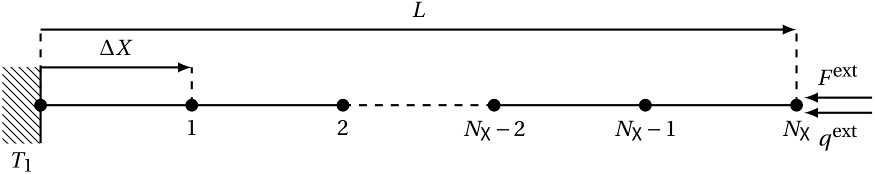
The equations of linear thermo-elasticity

We obtain the equations of linear thermo-elasticity *[Day 1985; Lemaitre and Chaboche 2001]*

$$
\begin{aligned}
&\rho \frac{\partial u}{\partial t} = p \\
&\frac{\partial p}{\partial t} = \frac{1}{S} F_{\text{ext}} + \frac{\partial}{\partial X}\left((\lambda + 2\mu) \frac{\partial u}{\partial X} - k(T - T_0) \right) \\
&\rho c \frac{\partial T}{\partial t} + k T_0 \frac{\partial}{\partial X}\left(\frac{1}{\rho} p \right) = K \frac{\partial^2 T}{\partial X^2} - q^{\text{ext}}
\end{aligned}
$$

A semi-discretised Double Bracket Structure

Consider the following discretisation of the problem



Consider a **finite element discretisation** of the fields (and their corresponding test fields)

$$u(X,t)=\sum_a \mathsf{N}^u_a(X)\mathsf{u}^a(t), \qquad \delta u^*(X)=\sum_a \mathsf{N}^u_a(X)\mathsf{du}^a$$

$$p(X,t)=\sum_a \mathsf{N}^p_a(X)\mathsf{p}^a(t), \qquad \delta p^*(X)=\sum_a \mathsf{N}^p_a(X)\mathsf{dp}^a$$

$$T(X,t)=\sum_a \mathsf{N}^T_a(X)\mathsf{T}^a(t), \qquad \delta T^*(X)=\sum_a \mathsf{N}^T_a(X)\mathsf{dT}^a$$

A semi-discretised Double Bracket Structure

We have a **weak formulation of the Double Bracket Structure**

$$
\begin{aligned}
&\int_0^L \left(\delta u^* \frac{\partial u}{\partial t} + \delta p^* \frac{\partial p}{\partial t} + \delta T^* \frac{\partial T}{\partial t}\right) \mathrm{d}X \\
&\quad = \int_0^L \left[\delta u^* \frac{1}{\rho} p - \frac{\partial \delta p^*}{\partial X} (\lambda + 2\mu) \frac{\partial u}{\partial X} + \frac{\partial \delta p^*}{\partial X} kT - \delta T^* \frac{T_0}{\rho c} \frac{\partial}{\partial X}\left(\frac{1}{\rho} p\right) + \frac{\partial \delta T^*}{\partial X} \frac{K}{\rho c} \frac{\partial T}{\partial X}\right] \mathrm{d}X \\
&\qquad - \delta T^* (X = L) \frac{q^{\text{ext}}}{\rho c} + \delta p^* (X = L) \frac{F^{\text{ext}}}{S} - \delta p^* (X = L) T_0 k
\end{aligned}
$$

which gives the following expression of a **semi-discretised Double Bracket Structure**

$$
\begin{pmatrix} \boldsymbol{I}^{uu} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{I}^{pp} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \boldsymbol{I}^{TT} \end{pmatrix}
\begin{pmatrix} \dot{\mathbf{u}} \\ \dot{\mathbf{p}} \\ \dot{\mathbf{T}} \end{pmatrix}
=
\begin{pmatrix} \mathbf{0} & {\boldsymbol{M}^{-\mathbf{1}}}^{up} & \mathbf{0} \\ -\boldsymbol{H}^{p'u'} & \mathbf{0} & \boldsymbol{L}^{p'T} \\ \mathbf{0} & -\frac{T_0}{\rho c}\frac{1}{\rho}\boldsymbol{L}^{Tp'} & \mathbf{0} \end{pmatrix}
\begin{pmatrix} \mathbf{u} \\ \mathbf{p} \\ \mathbf{T} \end{pmatrix}
+
\begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\frac{1}{\rho c}\boldsymbol{K}^{T'T'} \end{pmatrix}
\begin{pmatrix} \mathbf{u} \\ \mathbf{p} \\ \mathbf{T} \end{pmatrix}
+
\begin{pmatrix} \mathbf{0} \\ \mathbf{F}^{\text{ext}} \\ -\frac{1}{\rho c}\mathbf{q}^{\text{ext}} \end{pmatrix}
$$

A semi-discretised Double Bracket Structure

How to express the semi-discretised Double Bracket Structure in terms of the total energy

$$\hat{\mathscr{E}}_{\text{tot}} = \int_0^L \hat{E}_{\text{tot}}\left(u, p, \frac{\partial u}{\partial X}, T\right) \mathrm{d}X = \int_0^L \left(\frac{1}{2} p \frac{1}{\rho} p + \frac{1}{2}\frac{\partial u}{\partial X}(\lambda + 2\mu)\frac{\partial u}{\partial X} + T_0 k \frac{\partial u}{\partial X} + \frac{1}{2}\frac{\rho c}{T_0}(T^2 - T_0^2)\right) \mathrm{d}X$$

$$\tilde{\mathscr{E}}_{\text{tot}}[\mathbf{u}, \mathbf{p}, \mathbf{T}] = \frac{1}{2}\mathbf{p}^\top \boldsymbol{M}^{-\mathbf{1}^{pp}}\mathbf{p} + \frac{1}{2}\mathbf{u}^\top \boldsymbol{H}^{u'u'}\mathbf{u} + \mathbf{T}_0^\top \boldsymbol{L}^{Tu'}\mathbf{u} + \frac{1}{2}\mathbf{T}^\top \boldsymbol{I}^{TT}\mathbf{T} + \frac{1}{2}T_0^2\frac{\rho c}{T_0}$$

$$\frac{\partial \tilde{\mathscr{E}}_{\text{tot}}}{\partial \mathbf{u}} = \boldsymbol{H}^{u'u'}\mathbf{u} + \mathbf{T}_0^\top \boldsymbol{L}^{Tu'}, \quad \frac{\partial \tilde{\mathscr{E}}_{\text{tot}}}{\partial \mathbf{p}} = \boldsymbol{M}^{-1^{pp}}\mathbf{p}, \quad \frac{\partial \tilde{\mathscr{E}}_{\text{tot}}}{\partial \mathbf{T}} = \frac{\rho c}{T_0}\boldsymbol{I}^{TT}\mathbf{T}$$

We need to impose the **same test functions on the displacement and the linear momentum** to identify the energy within the previous expression.

$$\mathsf{N}_a^u = \mathsf{N}_a^p \qquad \forall a$$

Then, we identify, within the semi-discretised double bracket structure the expresion of the derivatives of the total energy.

A semi-discretised Double Bracket Structure

We obtain an expression of the **semi-discretised Double Bracket Structure in terms of the derivatives of the total energy**

$$\begin{pmatrix} \dot{\mathbf{u}} \\ \dot{\mathbf{p}} \\ \dot{\mathbf{T}} \end{pmatrix} = \begin{pmatrix} \mathbf{0} & (\boldsymbol{I}^{uu})^{-1} & \mathbf{0} \\ -(\boldsymbol{I}^{pp})^{-1} & \mathbf{0} & \frac{T_0}{\rho c}(\boldsymbol{I}^{pp})^{-1}\boldsymbol{L}^{p'T}(\boldsymbol{I}^{TT})^{-1} \\ \mathbf{0} & -\frac{T_0}{\rho c}(\boldsymbol{I}^{TT})^{-1}\boldsymbol{L}^{Tp'}(\boldsymbol{I}^{pp})^{-1} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \dfrac{\partial \tilde{\mathscr{E}}_{\text{tot}}}{\partial \mathbf{u}} \\ \dfrac{\partial \tilde{\mathscr{E}}_{\text{tot}}}{\partial \mathbf{p}} \\ \dfrac{\partial \tilde{\mathscr{E}}_{\text{tot}}}{\partial \mathbf{T}} \end{pmatrix} +$$

$$+ \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \frac{1}{\rho c}(\boldsymbol{I}^{TT})^{-1}\boldsymbol{K}^{T'T'} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{p} \\ \mathbf{T} \end{pmatrix} + \begin{pmatrix} \mathbf{0} \\ (\boldsymbol{I}^{pp})^{-1}\boldsymbol{F}^{\text{ext}} + (\boldsymbol{I}^{pp})^{-1}\mathbf{T}_0^{\mathsf{T}}\boldsymbol{L}^{Tu'} \\ -(\boldsymbol{I}^{TT})^{-1}\frac{1}{\rho c}\boldsymbol{q}^{\text{ext}} \end{pmatrix}$$

Can we identify a semi-discrete Poisson Structure?
The following developments consider **no conduction effects**.

A semi-discrete Poisson Structure?

Consider two functions dependent on semi-discretised variables

$$\tilde{\mathscr{F}} = \tilde{\mathscr{F}}[\mathbf{u}, \mathbf{p}, \mathbf{T}], \qquad \tilde{\mathscr{E}}_{\text{tot}} = \tilde{\mathscr{E}}_{\text{tot}}[\mathbf{u}, \mathbf{p}, \mathbf{T}]$$

Taking the time derivative of $\tilde{\mathscr{F}}$ yields

$$\frac{d\tilde{\mathscr{F}}}{dt} = \left(\frac{\partial \tilde{\mathscr{F}}}{\partial \mathbf{u}}\right)^{\mathsf{T}} \dot{\mathbf{u}} + \left(\frac{\partial \tilde{\mathscr{F}}}{\partial \mathbf{p}}\right)^{\mathsf{T}} \dot{\mathbf{p}} + \left(\frac{\partial \tilde{\mathscr{F}}}{\partial \mathbf{T}}\right)^{\mathsf{T}} \dot{\mathbf{T}} = \{\tilde{\mathscr{F}}, \tilde{\mathscr{E}}_{\text{tot}}\} + \left(\frac{\partial \tilde{\mathscr{F}}}{\partial \mathbf{p}}\right)^{\mathsf{T}} (\boldsymbol{I}^{pp})^{-1} \mathbf{T}_0^{\mathsf{T}} \boldsymbol{L}^{Tu'}$$

where

$$\{\tilde{\mathscr{F}}, \tilde{\mathscr{E}}_{\text{tot}}\} = \begin{pmatrix} \dfrac{\partial \tilde{\mathscr{F}}}{\partial \mathbf{u}} \\ \dfrac{\partial \tilde{\mathscr{F}}}{\partial \mathbf{p}} \\ \dfrac{\partial \tilde{\mathscr{F}}}{\partial \mathbf{T}} \end{pmatrix}^{\mathsf{T}} \underbrace{\begin{pmatrix} \mathbf{0} & (\boldsymbol{I}^{uu})^{-1} & \mathbf{0} \\ -(\boldsymbol{I}^{pp})^{-1} & \mathbf{0} & \dfrac{T_0}{\rho c} (\boldsymbol{I}^{pp})^{-1} \boldsymbol{L}^{p'T} (\boldsymbol{I}^{TT})^{-1} \\ \mathbf{0} & -\dfrac{T_0}{\rho c} (\boldsymbol{I}^{TT})^{-1} \boldsymbol{L}^{Tp'} (\boldsymbol{I}^{pp})^{-1} & \mathbf{0} \end{pmatrix}}_{\boldsymbol{B}} \begin{pmatrix} \dfrac{\partial \tilde{\mathscr{E}}_{\text{tot}}}{\partial \mathbf{u}} \\ \dfrac{\partial \tilde{\mathscr{E}}_{\text{tot}}}{\partial \mathbf{p}} \\ \dfrac{\partial \tilde{\mathscr{E}}_{\text{tot}}}{\partial \mathbf{T}} \end{pmatrix}$$

A semi-discrete Poisson Structure?

We obtain the following bracket

$$\{\tilde{\mathscr{F}}, \tilde{\mathscr{E}}_{\text{tot}}\} = \begin{pmatrix} \dfrac{\partial \tilde{\mathscr{F}}}{\partial \mathbf{u}} \\ \dfrac{\partial \tilde{\mathscr{F}}}{\partial \mathbf{p}} \\ \dfrac{\partial \tilde{\mathscr{F}}}{\partial \mathbf{T}} \end{pmatrix}^{\mathsf{T}} \underbrace{\begin{pmatrix} \mathbf{0} & (\boldsymbol{I}^{uu})^{-1} & \mathbf{0} \\ -(\boldsymbol{I}^{pp})^{-1} & \mathbf{0} & \dfrac{T_0}{\rho c}(\boldsymbol{I}^{pp})^{-1}\boldsymbol{L}^{p'T}(\boldsymbol{I}^{TT})^{-1} \\ \mathbf{0} & -\dfrac{T_0}{\rho c}(\boldsymbol{I}^{TT})^{-1}\boldsymbol{L}^{Tp'}(\boldsymbol{I}^{pp})^{-1} & \mathbf{0} \end{pmatrix}}_{\boldsymbol{B}} \begin{pmatrix} \dfrac{\partial \tilde{\mathscr{E}}_{\text{tot}}}{\partial \mathbf{u}} \\ \dfrac{\partial \tilde{\mathscr{E}}_{\text{tot}}}{\partial \mathbf{p}} \\ \dfrac{\partial \tilde{\mathscr{E}}_{\text{tot}}}{\partial \mathbf{T}} \end{pmatrix}$$

It is **skrew-symmetric** provided that

$$\boldsymbol{L}^{p'T} = (\boldsymbol{L}^{Tp'})^{\mathsf{T}}$$

If the skrew-symmetry is fulfilled, then it automatically checks **Leibniz’ and Jacobi’s identities**.

A time integration scheme

We can propose a time-integration scheme (based on the central difference scheme for the displacement-momentum part)

$$\boldsymbol{I}^{uu}\boldsymbol{u}_{n+1} = \boldsymbol{I}^{uu}\boldsymbol{u}_n + \Delta t\,\boldsymbol{M^{-1}}^{pp}\boldsymbol{p}_{n+1/2}$$

$$\boldsymbol{I}^{pp}\boldsymbol{p}_{n+3/2} = \boldsymbol{I}^{pp}\boldsymbol{p}_{n+1/2} + \Delta t\Big(\boldsymbol{F}^{\text{ext}} - \big(\boldsymbol{H}^{u'u'}\boldsymbol{u}_{n+1} - \boldsymbol{L}^{p'T}\boldsymbol{T}_{n+1}\big)\Big)$$

$$\big(\boldsymbol{I}^{TT} + \frac{1}{2}\frac{\Delta t}{\rho c}\boldsymbol{K}^{T'T'}\big)\boldsymbol{T}_{n+1} = \big(\boldsymbol{I}^{TT} - \frac{1}{2}\frac{\Delta t}{\rho c}\boldsymbol{K}^{T'T'}\big)\boldsymbol{T}_n - \Delta t\frac{T_0}{\rho c}\frac{1}{\rho}\boldsymbol{L}^{Tp'}\boldsymbol{p}_{n+1/2} + \Delta t\frac{1}{\rho c}\boldsymbol{q}^{\text{ext}}$$

This scheme is said to **preserve the Poisson structure** if *[Hairer, Lubich, and Wanner 2006]*

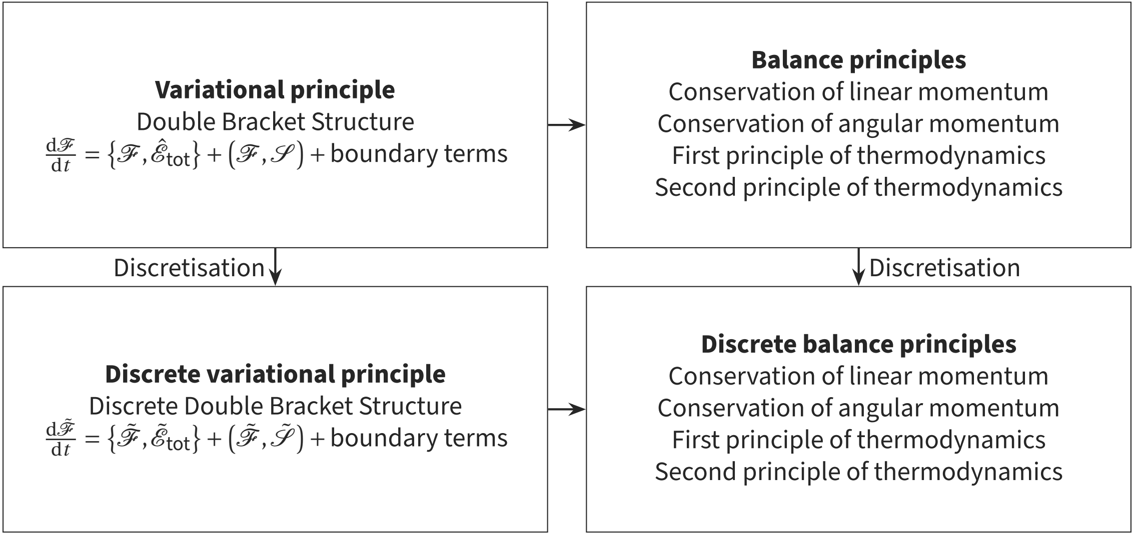
$$\Phi'(\boldsymbol{z}_n)\boldsymbol{B}(\boldsymbol{z}_n)\Phi'(\boldsymbol{z}_n)^{\mathsf{T}} = \boldsymbol{B}(\Phi(\boldsymbol{z}_n))$$

where

$$\Phi : (\boldsymbol{u}_n, \boldsymbol{p}_{n+1/2}, \boldsymbol{T}_n) \mapsto (\boldsymbol{u}_{n+1}, \boldsymbol{p}_{n+3/2}, \boldsymbol{T}_{n+1})$$

is the algorithm, Φ' is the amplification matrix (the Jacobian).

A variational integrator for continuum thermodynamics



Variational principle

Double Bracket Structure

$$\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} = \{\mathscr{F}, \hat{\mathscr{E}}_{\text{tot}}\} + (\mathscr{F}, \mathscr{S}) + \text{boundary terms}$$

Balance principles

Conservation of linear momentum

Conservation of angular momentum

First principle of thermodynamics

Second principle of thermodynamics

Discretisation

Discretisation

Discrete variational principle

Discrete Double Bracket Structure

$$\frac{\mathrm{d}\tilde{\mathscr{F}}}{\mathrm{d}t} = \{\tilde{\mathscr{F}}, \tilde{\mathscr{E}}_{\text{tot}}\} + (\tilde{\mathscr{F}}, \tilde{\mathscr{S}}) + \text{boundary terms}$$

Discrete balance principles

Conservation of linear momentum

Conservation of angular momentum

First principle of thermodynamics

Second principle of thermodynamics

The Double Bracket Structure:

A methodology to build variational integrators for continuum thermodynamics.

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