Objective time derivatives in non-equilibrium thermodynamics

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- Introduction – thermodynamics and objectivity
- Traditional objectivity - problems
    - We need 4 dimensions
- Four-dimensional kinematics
- Objective non-equilibrium thermodynamics
- Discussion

What is non-equilibrium thermodynamics?

Thermodynamics $\neq$ science of temperature

Thermodynamics $\neq$ science of macroscopic energy changes

Thermodynamics (?) $=$ general framework of any
macroscopic (?)
continuum (?)
theories

General framework:

- Second Law
- fundamental balances
- objectivity – material frame indifference

Objectivity:

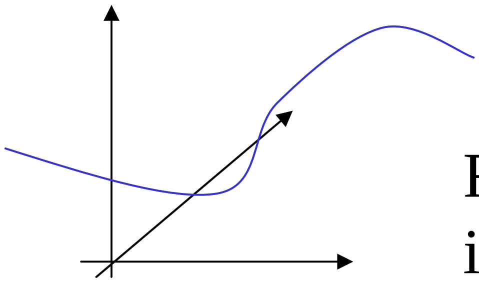
The principle of material frame-indifference:

$$\boxed{\textit{The material behaviour is independent of observers.}}$$

Its usual mathematical formulation (Noll, 1958):

The material behaviour is described by a mathematical relation having the same functional form for all observers.

Mechanics: Newton equation



Frame dependence - inertial accelerations

Second Law:

$$\dot{\mathbf{a}} + \nabla \cdot \mathbf{j}_a = \sigma_a$$ basic balances $\mathbf{a} = (\rho, \rho\mathbf{v}, e, \ldots)$

(and other constraints)

Frame independent?

– basic state: $\mathbf{a}$

– constitutive state: $C = (\mathbf{a}, \dot{\mathbf{a}}, \nabla\mathbf{a}, \ldots)$

– constitutive functions: $\mathbf{j}_\mathrm{a}(\mathrm{C})$

<u>Second law:</u>

$$\dot{s}(C) + \nabla \cdot \mathbf{J}(C) = \sigma_s \geq 0$$

$\boxed{\text{Constitutive theory}}$

Methods: Onsagerian forces and fluxes, Liu procedure, …

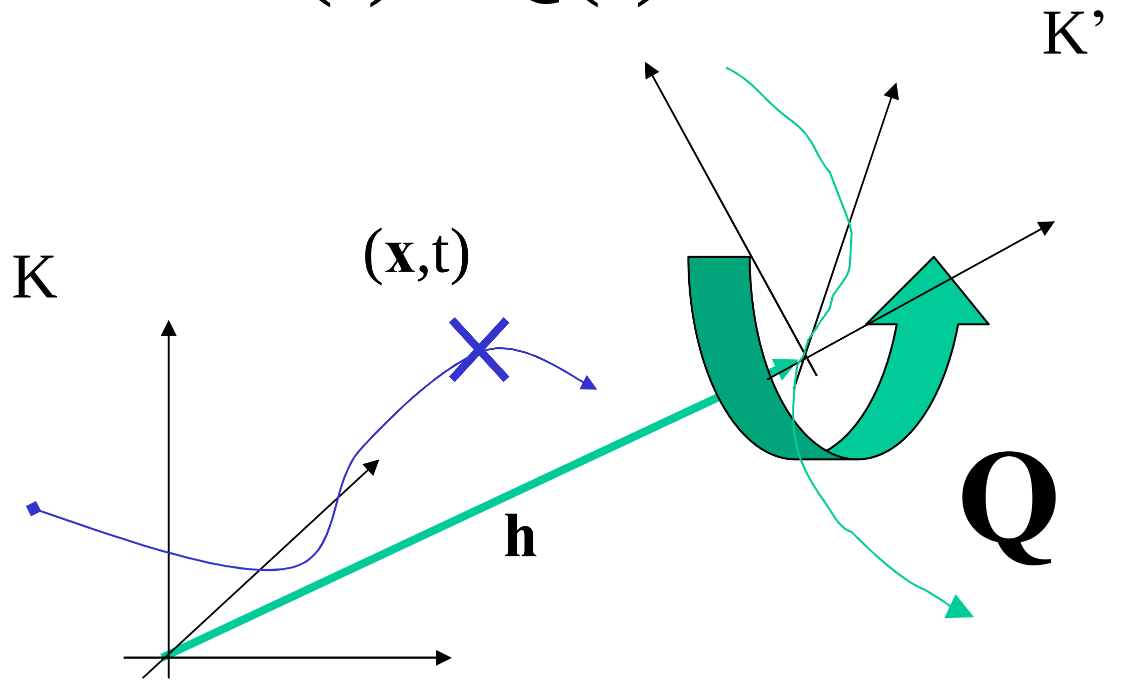
What is a vector?

– element of a vector space - mathematics

– something that transforms according to some rules - physics (observer changes, objectivity)

Rigid observers are distinguished:

$$\hat{t} = t, \qquad \hat{\mathbf{x}} = \mathbf{h}(t) + \mathbf{Q}(t)\mathbf{x}$$



Rigid rotating frames:

$$\hat{t} = t, \qquad \hat{\mathbf{x}} = \mathbf{h}(t) + \mathbf{Q}(t)\mathbf{x}$$ Noll (1958)

c is an objective vector, if

$$\hat{c}^i = \hat{J}^i{}_j c^j, \qquad \text{where} \qquad \hat{J}^i{}_j = \frac{\partial \hat{x}^i}{\partial x^j} = Q^i{}_j$$

$\Rightarrow$ velocity is not an objective vector:

motion: $\mathbf{r}(t) \quad \Rightarrow \quad \dot{\mathbf{r}} = \mathbf{v}$

derivation and transformation:

$$\hat{\mathbf{r}} = \mathbf{h} + \mathbf{Q}\mathbf{r} \quad \Rightarrow \quad \dot{\hat{\mathbf{r}}} = \hat{\mathbf{v}} = \dot{\mathbf{h}} + \dot{\mathbf{Q}}\mathbf{r} + \mathbf{Q}\dot{\mathbf{r}} \neq \mathbf{Q}\mathbf{v}$$

Material frame indifference

Noll (1958), Truesdell and Noll (1965)
Müller (1972, …) (kinetic theory)
Edelen and McLennan (1973)
Bampi and Morro (1980)
Ryskin (1985, …)
Lebon and Boukary (1988)
Massoudi (2002) (multiphase flow)
Speziale (1981, …, 1998), (turbulence)
Murdoch (1983, …, 2005) and Liu (2005)
Muschik (1977, …, 1998), Muschik and Restuccia (2002)
……..

Consequences:

usage of objective physical quantities

- symmetric part of the deformation gradient
- velocity excluded – kinetic energy?

objective time derivatives are necessary

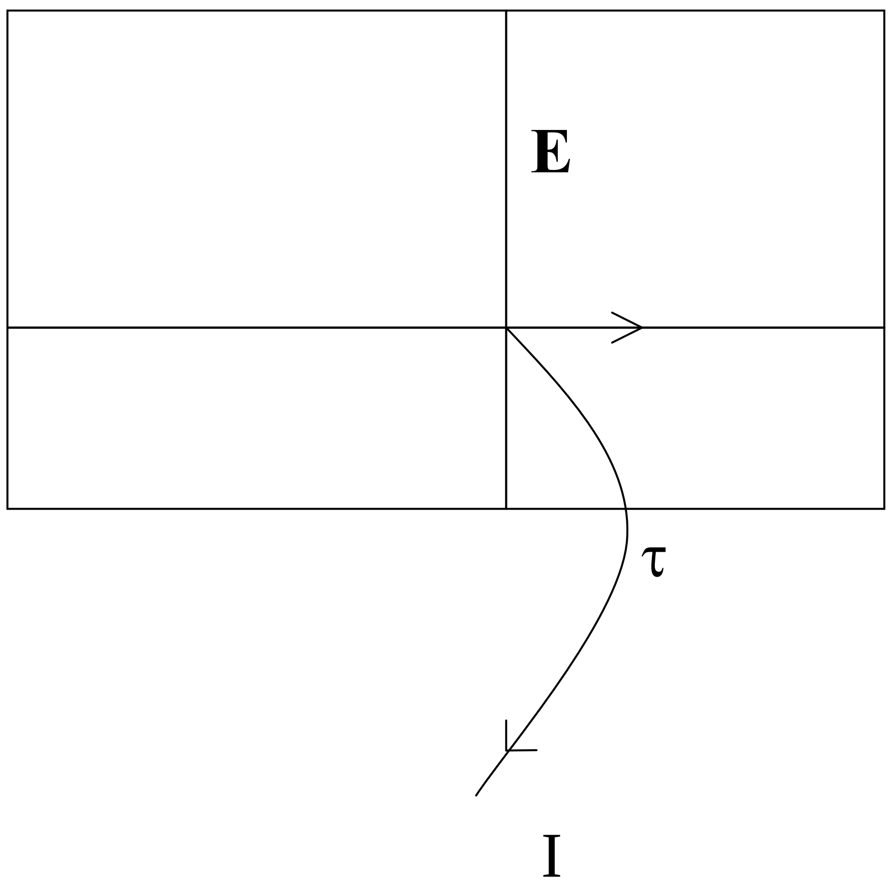
rheology – ad-hoc rules with moderate success

kinetic theory ?

Application experience:

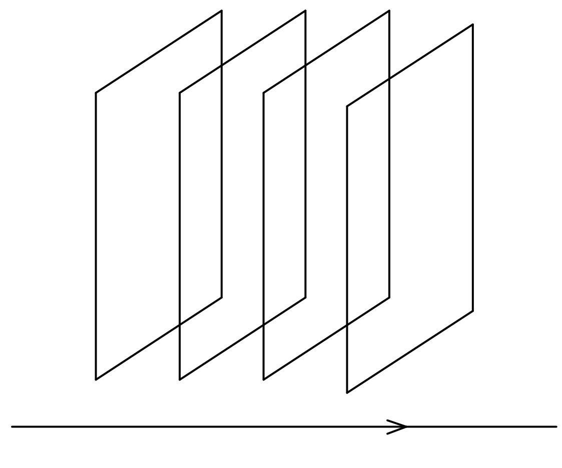
- complicated procedures – no clear evidence
- material manifold formulation works well

What is non-relativistic space-time?



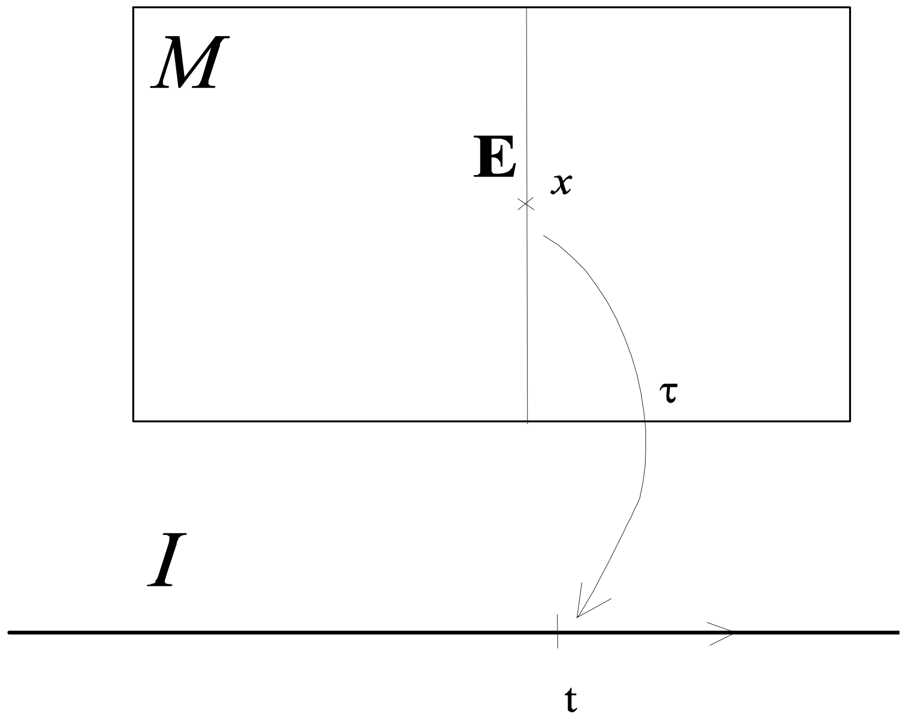
M=**E**×**I**

M=E×I



Geometry of non-relativistic space-time?

Absolute time.



Space-time M:	four dimensional affine space (over the vector space $\mathbf{M}$),
Time I:	is a one-dimensional affine space,
Time evaluation τ: $M \to I$:	is an affine surjection.
Distance:	Euclidean structure on $\mathbf{E}=\mathrm{Ker}(\tau)$

$\Rightarrow$ TIME CANNOT BE NEGLECTED!

Observers and reference frames:

$$\hat{t} = t, \qquad \hat{\mathbf{x}} = \mathbf{h}(t) + \mathbf{Q}(t)\mathbf{x}$$ Noll (1958)

$c^a = (c^0, \mathbf{c})$ is a four dimensional objective vector, if

$$\hat{c}^a = \hat{J}^a{}_b c^b, \qquad \text{where} \qquad \hat{J}^a{}_b = \frac{\partial \hat{x}^a}{\partial x^b} = \begin{pmatrix} 1 & 0 \\ \dot{\mathbf{h}} + \dot{\mathbf{Q}}\mathbf{x} & \mathbf{Q} \end{pmatrix}$$

$$\begin{pmatrix} \hat{c}^0 \\ \hat{\mathbf{c}} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \dot{\mathbf{h}} + \dot{\mathbf{Q}}\mathbf{x} & \mathbf{Q} \end{pmatrix} \begin{pmatrix} c^0 \\ \mathbf{c} \end{pmatrix} = \begin{pmatrix} c^0 \\ (\dot{\mathbf{h}} + \dot{\mathbf{Q}}\mathbf{x})c^0 + \mathbf{Q}\mathbf{c} \end{pmatrix}$$

$\Rightarrow$ four-velocity is an objective vector.

$\Rightarrow$ four-velocity is an objective vector.

four-motion: $(t, \mathbf{r}(t)) \quad \Rightarrow \quad (t, \mathbf{r}(t))\dot{} = (1, \dot{\mathbf{r}}(t))$

derivation:

$$\hat{\mathbf{r}} = \mathbf{h} + \mathbf{Q}\mathbf{r} \quad \Rightarrow \quad \dot{\hat{\mathbf{r}}} = \hat{\mathbf{v}} = \dot{\mathbf{h}} + \dot{\mathbf{Q}}\mathbf{r} + \mathbf{Q}\dot{\mathbf{r}}$$

transformation:

$$\begin{pmatrix} 1 \\ \hat{\mathbf{v}} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \dot{\mathbf{h}} + \dot{\mathbf{Q}}\mathbf{x} & \mathbf{Q} \end{pmatrix} \begin{pmatrix} 1 \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} 1 \\ \dot{\mathbf{h}} + \dot{\mathbf{Q}}\mathbf{x} + \mathbf{Q}\dot{\mathbf{v}} \end{pmatrix}$$

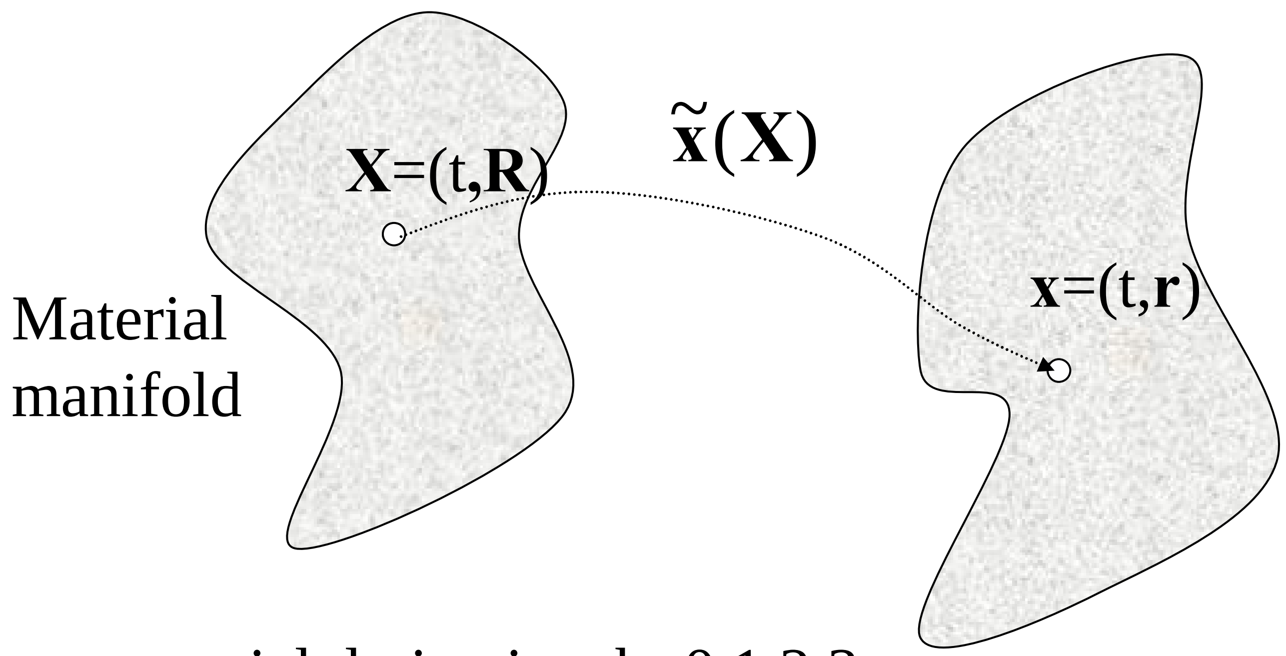
Are there four quantities in non-relativistic spacetime?

$$(\rho, \rho\mathbf{v}), \ (\rho e, \mathbf{j}_e), \ (\rho\mathbf{v}, \mathbf{P}), \ \ldots.$$

Is there anything else?

Material quantities and material manifold

A distinguished observer: material



material derivative, b=0,1,2,3

$$Y^a{}_b = \tilde{\partial}_b \tilde{x}^a = (\tilde{\partial}_t, \tilde{\partial}_j)\begin{pmatrix} t \\ \tilde{r}^i \end{pmatrix} = \begin{pmatrix} 1 & 0_j \\ \tilde{\partial}_t \tilde{r}^i & \tilde{\partial}_j \tilde{r}^i \end{pmatrix} = \begin{pmatrix} 1 & 0_j \\ \tilde{v}^i & \tilde{F}^i{}_j \end{pmatrix}$$

material quantity

$$Y^a{}_b = \tilde{\partial}_b \tilde{x}^a = (\tilde{\partial}_t, \tilde{\partial}_j)\begin{pmatrix} t \\ \tilde{r}^i \end{pmatrix} = \begin{pmatrix} 1 & 0_j \\ \tilde{\partial}_t \tilde{r}^i & \tilde{\partial}_j \tilde{r}^i \end{pmatrix} = \begin{pmatrix} 1 & 0_j \\ \tilde{v}^i & \tilde{F}^i{}_j \end{pmatrix}$$

space-time derivative

$$Z^a{}_b = \partial_b X^a = (\partial_t, \partial_j)\begin{pmatrix} t \\ R^i \end{pmatrix} = \begin{pmatrix} 1 & 0_j \\ \partial_t R^i & \partial_j R^i \end{pmatrix} = \begin{pmatrix} 1 & 0_j \\ V^i & G^i{}_j \end{pmatrix}$$

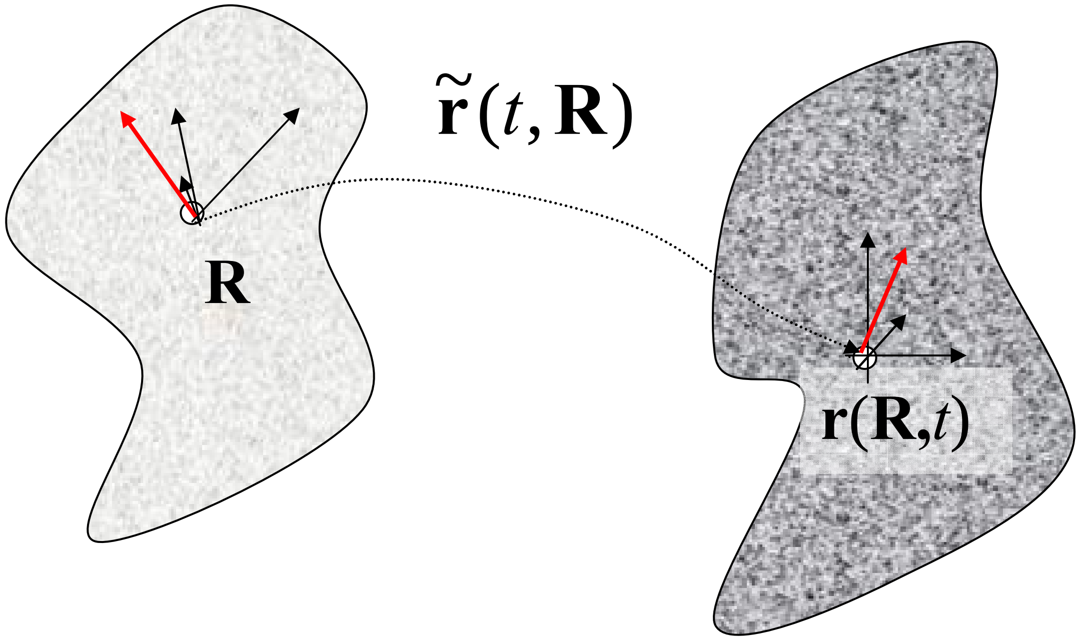
field quantity

X and **x** are inverses:

$$\begin{pmatrix} 1 & 0_k \\ V^i & G^i{}_k \end{pmatrix}\begin{pmatrix} 1 & 0_j \\ v^k & F^k{}_j \end{pmatrix} = \begin{pmatrix} 1 & 0_j \\ V^i + G^i{}_k v^k & G^i{}_k F^k{}_j \end{pmatrix} = \begin{pmatrix} 1 & 0_j \\ 0^i & \delta^i{}_j \end{pmatrix}$$

$$\boxed{\Rightarrow \quad G^i{}_k = \left(F^{-1}\right)^k{}_j, \quad V^i = -\left(F^{-1}\right)^i{}_k v^k}$$

Material form of physical quantities – spacelike



$$\mathbf{F}(\mathrm{t},\mathbf{R})\mathbf{C}(\mathrm{t},\mathbf{r}(\mathrm{t},\mathbf{R})) \longrightarrow \mathbf{c}(\mathrm{t},\mathbf{r})$$

material vector

vector field

Jacobian!

$\tilde{\mathbf{x}}(\mathbf{X}) \Rightarrow$ four-Jacobian

Material form of physical quantities – general

scalar: $\hat{f} = \tilde{f} = f \circ \tilde{\mathbf{x}}$

vector:

$$\hat{c}^a = \begin{pmatrix} \hat{c}^0 \\ \hat{c}^i \end{pmatrix} = \tilde{Z}^a{}_v \tilde{c}^a = \begin{pmatrix} 1 & 0_j \\ -G^i{}_k v^k & G^i{}_j \end{pmatrix} \begin{pmatrix} c^0 \\ c^i \end{pmatrix} = \begin{pmatrix} c^0 \\ G^i{}_j (c^j - v^j c^0) \end{pmatrix}$$

Jacobian

Galilei tansformation

covector:

$$\hat{k}_a = \left(\hat{k}_0, \hat{k}_i\right) = \tilde{Y}_a^b \tilde{k}_b = \begin{pmatrix} 1 & v^j \\ 0_i & F_i^j \end{pmatrix} \begin{pmatrix} k_0 \\ k_j \end{pmatrix} = \left(k_0 + v^j k_j \;\; F_i^j k_j\right)$$

Examples:

Force: $\begin{pmatrix} 0 & f_i \end{pmatrix} \rightarrow \begin{pmatrix} v^i f_i & f_i \end{pmatrix}$

power

Derivatives of a scalar:

$$\tilde{\partial}_a \tilde{f} = \tilde{\partial}_a f \circ \tilde{\mathbf{x}} = \left((\tilde{\partial}_t, \tilde{\partial}_j) f(t, r^i(t, \mathbf{R})) = \right) =$$

$$\partial_b \tilde{f}\, \tilde{\partial}_a \tilde{x}^b = \partial_b \tilde{f}\, \tilde{Y}^b{}_a = \begin{pmatrix} \partial_t f + v^j \partial_j f \\ \partial_j f\, F^j{}_i \end{pmatrix}$$

$$\boxed{\tilde{\partial}_t = \partial_t + v^j \partial_j \quad , \qquad \tilde{\partial}_j = \partial_j \quad F^j{}_i}$$

Material derivative??

substantial derivative of the material form of physical quantities

Material time derivative =

time derivative of a material quantity (Lie-derivative)

Spec. 1: f is a scalar field

$$f^{\lozenge} = \tilde{\partial}_t \tilde{f} = v^a \partial_a \tilde{f} = \begin{pmatrix} 1 \\ v^i \end{pmatrix} \begin{pmatrix} \partial_t & \partial_i \end{pmatrix} f = (\partial_t + v^i \partial_i) f = \dot{f}$$

The material derivative of a scalar field is the substantial derivative.

Spec. 2: $\boldsymbol{c}$ vektor

$$c^{i\lozenge} = \tilde{\partial}_t \left(\left(F^{-1}\right)^i_k c^k \right) = \mathbf{F}^{-1}\dot{\mathbf{c}} - \mathbf{F}^{-1}\dot{\mathbf{F}}\mathbf{F}^{-1}\mathbf{c} = \dot{\mathbf{c}} - \mathbf{c} \cdot \nabla \mathbf{v}$$

The material derivative of a spacelike vector field is the upper-convected derivative.

Four quantities are a necessity: $f^{\lozenge} = v^a \partial_a f \qquad v^a = (1, v^i)\,!$

Special examples:

Velocity (four or three):

$$v^{a\Diamond} = \tilde{\partial}_t\left(\begin{pmatrix} 1 & 0_j \\ -G^i{}_k v^k & G^i{}_j \end{pmatrix}\begin{pmatrix} 1 \\ v^j \end{pmatrix}\right) = \tilde{\partial}_t\begin{pmatrix} 1 \\ 0^j \end{pmatrix} = \begin{pmatrix} 0 \\ 0^j \end{pmatrix}$$

$\Rightarrow$ cannot enter in constitutive functions?

Deformation gradient (four or three):

$$\left(F^i{}_j\right)^{\Diamond} = \tilde{\partial}_t\left(\left(F^{-1}\right)^i{}_k F^k{}_l F^l{}_j\right) = \tilde{\partial}_t F^i{}_j = \dot{F}^i{}_j$$

$\Rightarrow$ pure mechanics does not change.

Non-equilibrium thermodynamics:

$$\dot{\mathbf{a}} + \nabla \cdot \mathbf{j}_a = 0 \rightarrow \tilde{\partial}_a \tilde{A}^a = 0$$

basic balances

e.g. $\tilde{\mathbf{A}} = \left(\rho_0 \mathbf{v} \;\; \mathbf{T}\right)$

balance of linear momentum

– basic state: a_0

– constitutive state: $C = (\ldots)$

– constitutive functions: $\mathbf{j}_a(C)$

Second law:

$$\dot{s}(C) + \nabla \cdot \mathbf{J}(C) = \sigma_s \geq 0$$

$\boxed{\text{Constitutive theory}}$

Where are the objective time derivatives?

$$\dot{s}(C) + \nabla \cdot \mathbf{J}(C) = \sigma_s \geq 0$$

Constitutive theory

$$\dot{s}(e, \hat{F}^i{}_j, \hat{\boldsymbol{\xi}}) = \frac{\partial s}{\partial e} e^{\Diamond} + \frac{\partial s}{\partial \hat{F}^i{}_j} \left(F^i{}_j\right)^{\Diamond} + \frac{\partial s}{\partial \hat{\boldsymbol{\xi}}} \boldsymbol{\xi}^{\Diamond} =$$

$$= \frac{\partial s}{\partial e} \dot{e} + \frac{\partial s}{\partial \hat{F}^i{}_j} \dot{F}^i{}_j + \frac{\partial s}{\partial \hat{\boldsymbol{\xi}}} \boldsymbol{\xi}^{\Diamond}$$

$$T\sigma_S = \cancel{\frac{1}{T}\mathbf{q} \cdot \nabla T} + \left(\mathbf{t} + \rho T \mathbf{F} \frac{\partial s}{\partial \mathbf{F}} \right) : \dot{\mathbf{F}}\mathbf{F}^{-1} - \rho \frac{\partial s}{\partial \boldsymbol{\xi}} : \boldsymbol{\xi}^{\Diamond} \geq 0$$

force

flux

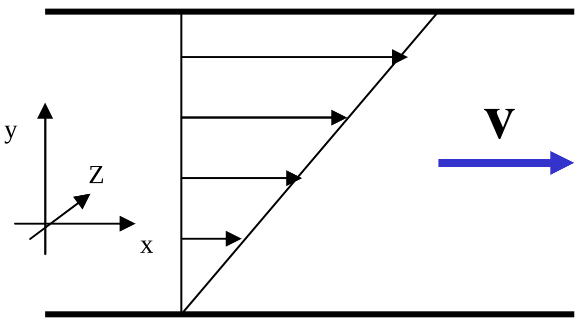
$$\boxed{\begin{aligned}\mathbf{t}^{v} &= \mathbf{L}^{1}\ \nabla\circ\mathbf{v}-\mathbf{L}^{12}\rho\,\boldsymbol{\xi},\\ \boldsymbol{\xi}^{\lozenge} &= \mathbf{L}^{21}\nabla\circ\mathbf{v}-\mathbf{L}^{2}\ \rho\,\boldsymbol{\xi}\end{aligned}}$$

Linear conductivity

Isotropy:

symmetric traceless part + scalars:

Simple shear:



$$\nabla\circ\mathbf{v}=\begin{pmatrix}0 & \boldsymbol{\kappa} & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix},\quad \mathbf{t}=\begin{pmatrix}t_{1} & t_{12} & t_{13}\\ t_{21} & t_{2} & t_{23}\\ t_{31} & t_{32} & t_{3}\end{pmatrix}$$

$$\mathbf{t}^{\lozenge}=\dot{\mathbf{t}}-\nabla\circ\mathbf{v}\cdot\mathbf{t}-\mathbf{t}\cdot\left(\nabla\circ\mathbf{v}\right)^{T}=-\kappa\begin{pmatrix}t_{12}+t_{21} & t_{2} & t_{23}\\ t_{2} & 0 & 0\\ t_{32} & 0 & 0\end{pmatrix}$$

Solution:

$$\hat{\boldsymbol{\eta}} = \frac{t_{12}}{\boldsymbol{\kappa}} = \frac{\boldsymbol{\eta}(3 + 4\boldsymbol{\kappa}^2\boldsymbol{\tau}\boldsymbol{\tau}_d)}{3 + 2\boldsymbol{\kappa}^2\boldsymbol{\tau}^2},$$

$$\Psi_1 = \frac{t_1 - t_2}{\boldsymbol{\kappa}^2} = \frac{2\boldsymbol{\eta}(3\boldsymbol{\tau} - 3\boldsymbol{\tau}_d + 2\boldsymbol{\kappa}^2\boldsymbol{\tau}^2\boldsymbol{\tau}_d)}{3 + 2\boldsymbol{\kappa}^2\boldsymbol{\tau}^2},$$

$$\Psi_2 = -\frac{t_2 - t_3}{\boldsymbol{\kappa}^2} = -2\boldsymbol{\eta}\boldsymbol{\tau}_d.$$

$$\boldsymbol{\tau} = \frac{1}{\boldsymbol{\rho} l_2}, \quad \boldsymbol{\eta} = \frac{l_1 l_2 - l_{12} l_{21}}{2 l_2}, \quad \boldsymbol{\tau}_d = \frac{l_1}{\boldsymbol{\rho}(l_1 l_2 - l_{12} l_{21})}$$

Corotational Jeffreys-Verhás:

$$\hat{\eta} = \frac{t_{12}}{\kappa} = \eta \frac{1 + \tau_t \tau_d \kappa^2}{1 + \tau_t^2 \kappa^2},$$

$$\Psi_1 = \frac{t_1 - t_2}{\kappa^2} = \frac{2\eta(\tau_t - \tau_d)}{1 + \tau_t^2 \kappa^2},$$

$$\Psi_2 = -\frac{t_2 - t_3}{\kappa^2} = \frac{\Psi_1}{2}.$$

Conclusions:

– Objectivity has to be extended to a four dimensional setting.

– Material time derivative can be defined uniquely. Its expression is different for fields of different tensorial order.

$$\text{space} + \text{time} \neq \text{spacetime}$$

Objective non-equilibrium thermodynamics:

– Material manifold and material derivatives

– Liu-procedure (mechanics!) + material frame indifference

– Traditional consequences of MFI must be checked:

better models in rheology, material inhomogeneities, etc..

References:

T. Matolcsi: *Spacetime Without Reference Frames*, Publishing House of the Hungarian Academy of Sciences, Budapest, 1993.

Matolcsi, T. and Ván, P., Can material time derivative be objective?, *Physics Letters A*, 2006, **353**, p109-112, (math-ph/0510037).

Matolcsi, T. and Ván, P., Absolute time derivatives, *Journal of Mathematical Physics* 2007, **48,** 053507, (math-ph/0608065).

Ván, P. and Bíró, T. S., Relativistic hydrodynamics - causality and stability, 2007, accepted at EPJ, (arXiv:0704.2039v2).

Ván, P., Internal energy in dissipative relativistic fluids, 2007, accepted in Journal of Mechanics of Materials and Structures, (Lecture held at TRECOP'07, arXiv:07121437)


Thank you for your attention!