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 \text{science of temperature}

- Thermodynamics \neq \text{science of macroscopic energy changes}

- \text{Thermodynamics ()?} = \text{general framework of any macroscopic (?) continuum (?) theories}

General framework:
- Second Law
- fundamental balances
- objectivity – material frame indifference
Objectivity:

The principle of material frame-indifference:

*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
Second Law:

\[ \dot{\mathbf{a}} + \nabla \cdot \mathbf{j}_a = \mathbf{\sigma}_a \]

basic balances \[ \mathbf{a} = (\rho, \rho \mathbf{v}, e, \ldots) \]

(and other constraints)

- Basic state:
- Constitutive state:
- Constitutive functions:

\[ \mathbf{a} \}
\mathbf{C} = (\mathbf{a}, \dot{\mathbf{a}}, \nabla \mathbf{a}, \ldots) \]
\[ \mathbf{j}_a (\mathbf{C}) \]

Second law:

\[ \dot{s}(\mathbf{C}) + \nabla \cdot \mathbf{J}(\mathbf{C}) = \mathbf{\sigma}_s \geq 0 \]

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:

$$\hat{t} = t, \quad \hat{x} = h(t) + Q(t)x$$
Rigid rotating frames:

\[ \hat{t} = t, \quad \hat{x} = h(t) + Q(t)x \]

Noll (1958)

c is an objective vector, if

\[ \hat{c}^i = \hat{J}^i_j c^j, \quad \text{where} \quad \hat{J}^i_j = \frac{\partial \hat{x}^i}{\partial x^j} = Q^i_j \]

⇒ velocity is not an objective vector:

motion: \[ r(t) \Rightarrow \dot{r} = v \]

derivation and transformation:

\[ \hat{r} = h + Qr \Rightarrow \dot{r} = \dot{v} = \dot{h} + \dot{Q}r + Q\dot{r} \neq Qv \]
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)
........
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?

$M = E \times I$

$M = E \times I$
Geometry of non-relativistic space-time?

Absolute time.

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

$\Rightarrow$ TIME CANNOT BE NEGLECTED!
Observers and reference frames:

\[ \hat{t} = t, \quad \hat{x} = h(t) + \dot{Q}(t)x, \quad \text{Noll (1958)} \]

\[ c^a = (c^0, c) \] is a four dimensional objective vector, if

\[ \hat{c}^a = \hat{J}^a_b c^b, \quad \text{where} \quad \hat{J}^a_b = \frac{\partial \hat{x}^a}{\partial x^b} = \begin{pmatrix} 1 & 0 \\ \dot{h} + \dot{Q}x & Q \end{pmatrix} \]

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

\[ \Rightarrow \quad \text{four-velocity is an objective vector.} \]
⇒ four-velocity is an objective vector.

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

derivation:
\[
\dot{\mathbf{r}} = \mathbf{h} + Q\mathbf{r} \quad \Rightarrow \quad \dot{\mathbf{r}} = \dot{\mathbf{v}} = \dot{\mathbf{h}} + Q\mathbf{r} + Q\dot{\mathbf{r}}
\]

transformation:
\[
\begin{pmatrix}
1 \\
\dot{\mathbf{v}}
\end{pmatrix} =
\begin{pmatrix}
1 & 0 \\
\dot{\mathbf{h}} + Q\mathbf{x} & Q
\end{pmatrix}
\begin{pmatrix}
1 \\
\mathbf{v}
\end{pmatrix} =
\begin{pmatrix}
1 \\
\dot{\mathbf{h}} + Q\mathbf{x} + Q\dot{\mathbf{v}}
\end{pmatrix}
\]

Are there four quantities in non-relativistic spacetime?

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

Is there anything else?
Material quantities and material manifold

A distinguished observer: material

\[ \dot{X} = (t, R) \]

Material manifold

\[ \tilde{x}(X) \]

Material quantity

Material derivative, \( b = 0, 1, 2, 3 \)

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

\text{space-time derivative}

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

\text{field quantity}

\(X\) and \(x\) are inverses:

\[
\begin{pmatrix} 1 & 0_k \\ V^i & G^i_k \end{pmatrix} \begin{pmatrix} 1 & 0_j \\ \nu^k & F^k{}_j \end{pmatrix} = \begin{pmatrix} 1 & 0_j \\ V^i + G^i_k \nu^k & G^i_k F^k{}_j \end{pmatrix} = \begin{pmatrix} 1 & 0_j \\ 0^i & \delta^i{}_j \end{pmatrix}
\]

\[ \Rightarrow \quad G^i{}_k = (F^{-1})^k{}_j, \quad V^i = -(F^{-1})^i_k \nu^k \]
Material form of physical quantities – spacelike

\[ \mathbf{r}(t, \mathbf{R}) \]

\[ \mathbf{c}(t, \mathbf{r}) \]

Jacobian!

\[ \mathbf{F}(t, \mathbf{R})\mathbf{C}(t, \mathbf{r}(t, \mathbf{R})) \]

vector field

\[ \mathbf{\tilde{x}}(\mathbf{X}) \Rightarrow \text{four-Jacobian} \]
Material form of physical quantities – general

scalar: \( \hat{f} = \tilde{f} = f \circ \tilde{x} \)

vector:

\[
\hat{c}^a = \begin{pmatrix} \hat{c}^0 \\ \hat{c}^i \end{pmatrix} = \tilde{Z}^a_{\nu} \tilde{\nu}^a = \begin{pmatrix} 1 & 0_j \\ -G^i_k \nu^k & G^i_j \end{pmatrix} \begin{pmatrix} c^0 \\ c^i \end{pmatrix} = \begin{pmatrix} c^0 \\ G^i_j (c^j - \nu^j c^0) \end{pmatrix}
\]

Jacobian

Galilei transformation

covector:

\[
\hat{k}_a = (\hat{k}_0, \hat{k}_i) = \tilde{Y}^b_a \tilde{\nu}^b_b = \begin{pmatrix} 1 & \nu^j \\ 0_i & F^j_i \end{pmatrix} \begin{pmatrix} k_0 \\ k_j \end{pmatrix} = \begin{pmatrix} k_0 + \nu^j k_j \\ F^j_i k_j \end{pmatrix}
\]
Examples:

Force: \( (0 \ f_i) \rightarrow \left( v^i \ f_i \ f_i \right) \)

Derivatives of a scalar:

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

\[
\partial_b \tilde{f} \tilde{\partial}_a \tilde{x}^b = \partial_b \tilde{f} \tilde{Y}^b_a = \begin{pmatrix}
\partial_t f + v^j \partial_j f \\
\partial_j f \ F^j_i
\end{pmatrix}
\]

\[
\tilde{\partial}_t = \partial_t + v^j \partial_j , \quad \tilde{\partial}_j = \partial_j \ F^j_i
\]

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

\[
f^{\diamond} = \tilde{\partial}_t \tilde{f} = v^a \partial_a \tilde{f} = \left( \frac{1}{v^i} \right) (\partial_t \partial_i) f = (\partial_t + v^i \partial_i) f = \dot{f}
\]

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

Spec. 2: \( c \) vektor

\[
c^{\diamond}_{i} = \tilde{\partial}_i \left( \left( F^{-1} \right)^k_i c^k \right) = F^{-1} \dot{c} - F^{-1} \dot{F} F^{-1} c = \dot{c} - c \cdot \nabla v
\]

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

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

$$\left( F^i_j \right)^\diamond = \tilde{\partial}_t \left( \left( F^{-1}\right)_k^i F^k_l F^l_j \right) = \tilde{\partial}_t F^i_j = \dot{F}^i_j$$

$$\Rightarrow$$ pure mechanics does not change.
Non-equilibrium thermodynamics:

\[ \dot{a} + \nabla \cdot j_a = 0 \rightarrow \tilde{\partial}_a \tilde{A}^a = 0 \]

basic balances

e.g. \[ \tilde{A} = (\rho_0 v T) \]

balance of linear momentum

- basic state:
- constitutive state:
- constitutive functions:

\[ a_0 \quad C = (...) \quad j_a (C) \]

Second law:

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

Constitutive theory
Where are the objective time derivatives?

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

Constitutive theory

\[
\dot{s}(e, \hat{F}^i_j, \hat{\xi}) = \frac{\partial s}{\partial e} \dot{e} + \frac{\partial s}{\partial \hat{F}^i_j} (\hat{F}^i_j) + \frac{\partial s}{\partial \hat{\xi}} \hat{\xi} = \\
= \frac{\partial s}{\partial e} \dot{e} + \frac{\partial s}{\partial \hat{F}^i_j} \dot{\hat{F}}^i_j + \frac{\partial s}{\partial \hat{\xi}} \hat{\xi}
\]

\[
T\sigma_s = \frac{1}{T} \mathbf{q} \cdot \nabla T + \left( \mathbf{t} + \rho \mathbf{T} \mathbf{F} \frac{\partial s}{\partial \mathbf{F}} \right) : \dot{\mathbf{F}} \mathbf{F}^{-1} - \rho \frac{\partial s}{\partial \hat{\xi}} \hat{\xi} \geq 0
\]

force

flux
Linear conductivity
Isotropy:
symmetric traceless part + scalars:

\[ t^\nu = L^1 \nabla \circ v - L^{12} \rho \xi, \]

\[ \xi \hat{\nu} = L^{21} \nabla \circ v - L^2 \rho \xi \]

Simple shear:

\[
\begin{bmatrix}
0 & \kappa & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix},
\quad
\begin{pmatrix}
t_1 \\
t_2 \\
t_3
\end{pmatrix}
\]

\[
\nabla \circ v = \begin{pmatrix}
t_{12} + t_{21} & t_2 & t_{23} \\
t_{31} & t_{32} & t_3
\end{pmatrix} = -\kappa
\begin{pmatrix}
t_1 \\
t_2 \\
t_3
\end{pmatrix}
\]
Solution:

\[ \hat{\eta} = \frac{t_{12}}{\kappa} = \frac{\eta(3 + 4\kappa^2 \tau_d)}{3 + 2\kappa^2 \tau^2}, \]

\[ \Psi_1 = \frac{t_1 - t_2}{\kappa^2} = \frac{2\eta(3\tau - 3\tau_d + 2\kappa^2 \tau^2 \tau_d)}{3 + 2\kappa^2 \tau^2}, \]

\[ \Psi_2 = -\frac{t_2 - t_3}{\kappa^2} = -2\eta \tau_d. \]

\[ \tau = \frac{1}{\rho l_2}, \quad \eta = \frac{l_1 l_2 - l_{12} l_{21}}{2l_2}, \quad \tau_d = \frac{l_1}{\rho(l_1 l_2 - l_{12} l_{21})} \]

Corotational Jeffreys-Verhás:

\[ \hat{\eta} = \frac{t_{12}}{\kappa} = \eta \left( \frac{1 + \tau_d \kappa^2}{1 + \tau_t^2 \kappa^2} \right), \]

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

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

\[
\text{space + time } \neq \text{ spacetime}
\]

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:


Thank you for your attention!