Objective thermomechanics – a spacetime approach

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Reference frame, coordinate system, initial/reference time, reference configuration: description helping auxiliary elements.

Objectivity: 'equations must have a physical content independently of these auxiliary elements' – formulation is controversial.

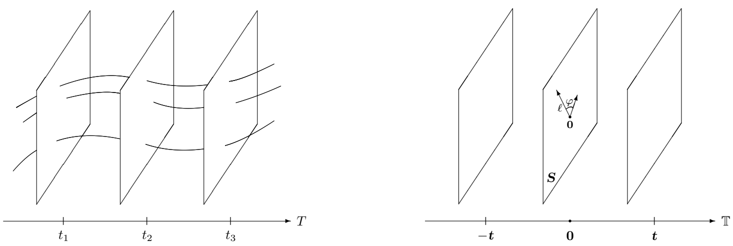
A safe solution: to use the frame free description of spacetime and of physical quantities – introduced by Weyl [1], mentioned by Arnold, elaborated by Matolcsi [2], standard in general relativity, not yet widespread elsewhere.

Even the Galilean case (hereafter) needs spacetime: $\mathbf{r}' = \mathbf{r} - \mathbf{V}t$.

Objective: can be formulated without auxiliary elements.

Kinematic quantities for solid continua

A continuum: a 3-dimensional smooth manifold $\mathcal{C}$ (material manifold). Its tangent vectors: material vectors. $\Longrightarrow$ material tensors of various type. Covectors not identified with vectors!
Hereafter, Penrose's abstract index notation, K: material index, $\hat{k}$: spacetime index, k: spacelike spacetime index.
Any material point $P \in \mathcal{C}$ exists in spacetime along a world line: at a given time t, P is at spacetime point $r(t, P)$. The partial derivatives will be denoted by overdot and ∇_K, respectively.



World lines in Galilean spacetime; Galilean spacetime vectors

World line gradient: $J^k{}_K := \nabla_K r^{\hat{k}}$, maps the Euclidean metric h_{kl} of spacelike spacetime vectors onto $\mathcal{C}$: $h_{KL} := J^k{}_K h_{kl} J^l{}_L$: *the instantaneous metric.*

$v^{\hat{k}} := \dot{r}^{\hat{k}}$: *four-velocity,* $L^k{}_L := \nabla_L v^{\hat{k}} = \dot{J}^k{}_L$: *velocity gradient.*

Solids have an additional structure: g_{KL}: *the relaxed metric.* In a relaxed state, $h_{KL} = g_{KL}$. In general: $A^K{}_L := \left(g^{-1}\right)^{KM} h_{ML}$: *elastic shape tensor.* $\{D^K{}_L\} := \frac{1}{2} \ln\{A^K{}_L\}$: *elastic deformedness.*

Thermal expansion: $g_{KL} = g_{KL}(T)$, $\quad \alpha_I{}^J := \frac{1}{2} \frac{\mathrm{d}g_{IK}}{\mathrm{d}T} \left(g^{-1}\right)^{KJ}$.

Plastic change rate tensor: $Z_I{}^J := \frac{1}{2} \left(\frac{\mathrm{d}g_{IK}}{\mathrm{d}t}\right)_{\text{plastic}} \left(g^{-1}\right)^{KJ}$.

Altogether, the kinematic state variable A^i_j evolves as

$$\dot{A}^i_j = L^i_k A^k_j + A^i_k \left(h^{-1}\right)^{kl} L_l^m h_{mj} - 2A^i_k \left(h^{-1}\right)^{kl} \left(\alpha_l{}^m \dot{T} + Z_l{}^m\right) h_{mj}.$$

From mechanics to thermodynamics: isotropic case

The customary balances for mass and linear momentum are straightforward to rewrite as frame free four-equations:

$$\dot{\varrho} = -\varrho \nabla_i v^{\hat{i}}, \qquad \varrho \dot{v}^{\hat{i}} = \nabla_j \left[\left(h^{-1}\right)^{jk} \sigma^i{}_k\right].$$

Pure elasticity: $\sigma^i{}_j = \sigma^i{}_j\left(\{A^k{}_l\}\right)$ [or of $\{D^k{}_l\}$], e.g.,
$\sigma^i{}_j = E^{\text{dev}} \left(D^{\text{dev}}\right)^i{}_j + E^{\text{sph}} \left(D^{\text{sph}}\right)^i{}_j \quad \left(E^{\text{dev}} = 2G,\ E^{\text{sph}} = 3K\right)$;
$\sigma^i{}_j$ originates from a specific elastic energy $e_{\text{el}}\left(\{D^i{}_j\}\right)$, an isotropic scalar function of $\{D^i{}_j\}$, as $\sigma^i{}_j = \varrho \frac{\mathrm{d}e_{\text{el}}}{\mathrm{d}D^j{}_i}$. As a consequence, $\varrho \dot{e}_{\text{el}} = \sigma^i{}_j \left(L^{\text{S}}\right)^j{}_i$.

Thermal effects: $e_{\text{el}} = e_{\text{el}}\left(T, \{D^i{}_j\}\right)$ in general [e.g., in the above example, $E^{\text{dev}} = E^{\text{dev}}(T)$, $E^{\text{sph}} = E^{\text{sph}}(T)$]. Also, there may be thermal expansion: $g_{KL} = g_{KL}(T)$. Third, in addition to mechanical power, a heat flux $(j_e)^i$ may also be present.
$\varrho \dot{e}_{\text{el}} = \sigma^i{}_j \left(L^{\text{S}}\right)^j{}_i$ gets generalized to the first law of thermodynamics in the form $\varrho \dot{e} = -\nabla_i (j_e)^i + \sigma^i{}_j \left(L^{\text{S}}\right)^j{}_i$.

A specific entropy $s\left(T, \{D^i{}_j\}\right)$ should also exist, with a balance $\varrho \dot{s} = -\nabla_i (j_s)^i + \pi_s$, where we assume $(j_s)^i = \frac{1}{T} (j_e)^i$.
Under the requirement that thermal expansion is reversible (i.e., gives no contribution to entropy production π_s), we find

$$e = e_{\text{th}}(T) + e_{\text{el}} + T \left(\frac{1}{\varrho} \sigma^j{}_k \left(h^{-1}\right)^{kl} \alpha_l{}^m h_{mj} - \frac{\partial e_{\text{el}}}{\partial T}\right), \tag{1}$$

$$s = s_{\text{th}}(T) + \left(\frac{1}{\varrho} \sigma^j{}_k \left(h^{-1}\right)^{kl} \alpha_l{}^m h_{mj} - \frac{\partial e_{\text{el}}}{\partial T}\right), \tag{2}$$

$$\pi_s = \left(\nabla_i \frac{1}{T}\right) (j_e)^i + \frac{1}{T} \sigma^j{}_k \left(h^{-1}\right)^{kl} Z_l{}^m h_{mj}. \tag{3}$$

$e_{\text{th}}(T)$ is related to specific heat, i.e., $c|_{D^i{}_j = 0}$.

Heat conduction: either $(j_e)^i = \lambda \left(g^{-1}\right)^{ij} \nabla_j \frac{1}{T}$ or $(j_e)^i = \lambda \left(h^{-1}\right)^{ij} \nabla_j \frac{1}{T}$. Ambiguity unseen by conventional kinematics.

A realistic plasticity model ($Z_i^j \sim \sigma^k_l$ not so realistic):

$Z_i^j = \Gamma h_{ik} \left(\dot{\sigma}^{\text{dev}}\right)^k{}_l \left(h^{-1}\right)^{lj}, \qquad$ where $\gamma > 0$,

$\Gamma = \gamma H\left(\left(\sigma^{\text{dev}}\right)^i{}_j \left(\sigma^{\text{dev}}\right)^j{}_i - \frac{2}{3} \sigma^2_{\text{yield}}\right) H\left(\left(\sigma^{\text{dev}}\right)^i{}_j \left(\dot{\sigma}^{\text{dev}}\right)^j{}_i\right)$.

The first Heaviside function H: von Mises type yield criterion.

Positive definite entropy production switches off plastic change during unloading (second Heaviside function).

Duhamel–Neumann theory, Joule–Thomson effect covered.

Thermal stress even with T independent $e_{\text{el}}\left(\{D^i{}_j\}\right)$, via $\alpha_K{}^L$.

Anisotropy

Means distinguished *material* directions (tangent vectors of $\mathcal{C}$).
E.g., $C^I{}_J{}^L{}_K$ is constant in $\sigma^I{}_J = C^I{}_J{}^L{}_K D^K{}_L$.
Constitutive properties expected to be connected to the material manifold form (while balances primarily live on spacetime).
Now $\frac{\mathrm{d}f}{\mathrm{d}D^K{}_L} \neq 2 \frac{\mathrm{d}f}{\mathrm{d}A^M{}_L} A^M{}_K \neq 2 A^L{}_N \frac{\mathrm{d}f}{\mathrm{d}A^K{}_N}$! The distinguished choice is $\sigma^J{}_K = 2\varrho \frac{\partial e_{\text{el}}}{\partial A^I{}_J} A^I{}_K$, with which (1)–(3) remain valid.

Conclusions, outlook

- Successfully applied to evaluate measurements on plastic samples [4] and in Smoothed-Particle Hydrodynamics numerics
- We could have started with an $e(s, \{h_{KL}\})$ (g_{KL}: where e has a strict minimum in h_{KL}). More abstract, less engineer-friendly, less application-friendly, harder to express Hooke's law, Duhamel–Neumann, plasticity etc.
- Finite-deformation rheology/viscoelasticity can be added (tensorial internal variable methodology [5])
- Balances can be unified: for four-energy-momentum [6, 7]
- Spacetime aspects of GENERIC and other nonequilibrium thermodynamical frameworks?

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