Non-equilibrium thermodynamics and the evolution equations of continuum physics

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Outline

1. The problem
   - Real and ideal: thermodynamics and mechanics
2. Evolution with second law
   - Thermostatics and thermodynamics
   - Thermodynamics and dynamics
   - Origin of evolution equations
3. Heat conduction

Evolution equation, equation of motion, dynamical law, governing equation, etc...

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System of ordinary or partial differential equations, that determines the time-space evolution of a physical system.

Original and extension

Fourier

$$\partial_t T - \lambda_F \partial_{xx} T = 0, \qquad \lambda_F > 0.$$

Memory extension: Maxwell-Cattaneo-Vernotte

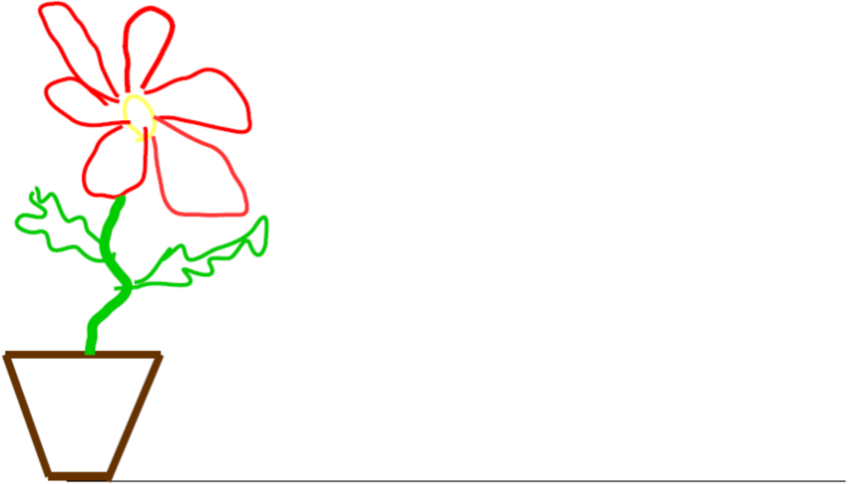
$$\tau \partial_{tt} T + \partial_t T - \lambda_F \partial_{xx} T = 0, \qquad \lambda_F, \tau > 0.$$

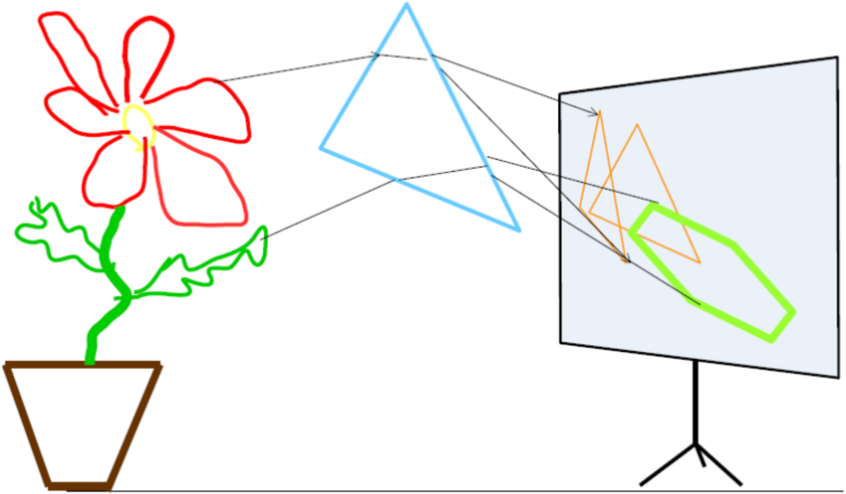
Weakly nonlocal and memory extensions: Guyer-Krumhansl

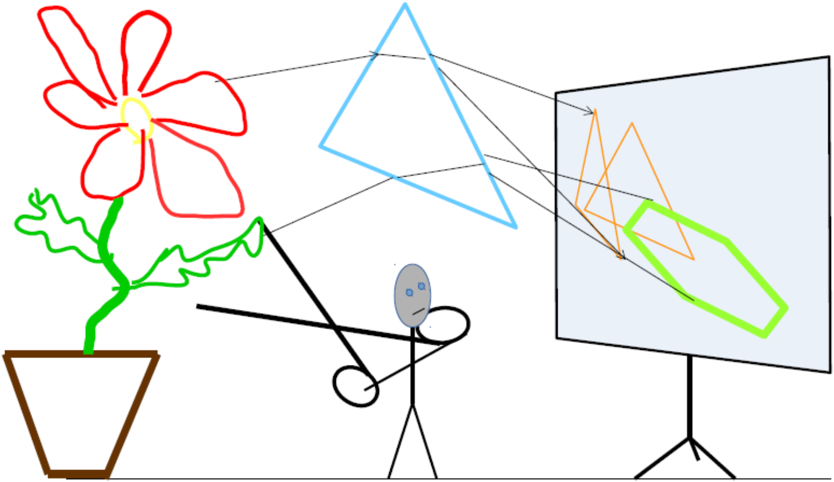
$$\tau \partial_{tt} T + \partial_t T - \lambda_F \partial_{xx} T - a \partial_{txx} T = 0, \qquad \lambda_F, \tau, a > 0.$$

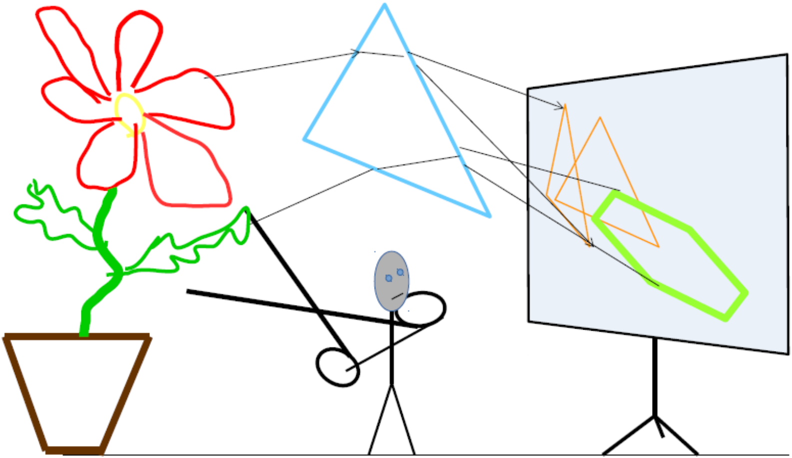
Higher grade fluids (wnl in v^i), Korteweg fluids (wnl in ρ), Cosserat solids (wnl and memory in ϵ^{ij}), rheology of solids (memory in ϵ^{ij}), internal variables, ...

Reality









Mathematics is the light.

True, unbiased and sharp vision

Mechanics: the nonexisting ideal

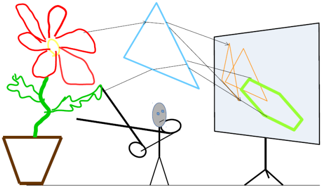
- Microscopic, ideal building blocks;
- Variational principles: dissipation is a necessary evil;

Thermodynamics: the dirty real

- Obscure empirical corrections, confusing basic concepts;
- What is the origin of the evolution equations?

Research strategy

- Mathematical clarity, logical minimum;
- Physical control: observations and experiments;
- Engineering flexibility: prediction machine.



Thermostatics and thermodynamics

Matolcsi (Akadémiai, 2005)
Berezovski-Ván (Springer, 2017)

What is entropy?

Universal and/or absolute: structure independent.
Statistical physics - statics; kinetic theory - dynamics: they are special.

Ordinary thermodynamics

- Thermodynamic bodies. Evolution by ordinary differential equations.

$$\dot{E} = Q(E, V) - p(E, F)\, F(E, V), \qquad \dot{V} = F(E, V).$$

- Second law: $S(E, V)$ is concave and increasing along the d.e.? Asymptotic stability of the equilibrium? Clear and sound physics.
- Double meanings. E.g. $dE = TdS - pdV$ versus $\dot{E} = T\dot{S} - p\dot{V}$

Thermodynamics is a theory of stability

- Interesting and simple math: bifurcations and phase transitions, generalized gradient systems, metriplectic structures, etc.
- Constructing the evolution.
- Transition to continua: Euler homogeneity.

Thermodynamics and dynamics

Ván (in Applied Wave Mechanics, Springer, 2009)
Berezovski-Ván (Springer, 2017)

The origin of dissipative evolution

Internal variables: scalar α

- Duhem (1907), Mandelstam and Leontovich (1937), Landau and Lifshitz, etc...
- Coleman and Gurtin (1967): only local evolution
- Inertial or relaxational i.e. mechanical or thermodynamical evolution?

α evolution? $\dot{\alpha} = f(\alpha, \partial_i\alpha, \partial_{ij}\alpha)$

Local: thermodynamic state variables

$$S(\alpha): \quad \dot{S}(\alpha) = \frac{dS}{d\alpha}\dot{\alpha} = \frac{dS}{d\alpha} f \geq 0 \quad \to \quad f = l\frac{dS}{d\alpha}, \quad l \geq 0$$

- Flux: f, Force: $\frac{dS}{d\alpha}$, constitutive equation.
- nonlinear, $l(\alpha)$: Lagrange theorem. General solution,
- Local and weakly nonlocal extensions: constitutive state space.

Heuristic weak nonlocality

Internal variables: scalar α

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α evolution? $\dot{\alpha} = f(\alpha, \partial_i \alpha, \partial_{ij}\alpha)$

Weakly nonlocal: α and gradients.

$$S(\alpha, \partial_i \alpha): \quad \frac{dS}{d\alpha} \rightarrow \frac{\delta S}{\delta \alpha} = \frac{\partial S}{\partial \alpha} - \partial_i \frac{\partial S}{\partial(\partial_i \alpha)}, \quad \text{therefore} \quad \boxed{\dot{\alpha} = l \frac{\delta S}{\delta \alpha}}$$

- Second order weakly nonlocal.
- Heuristic combination of mechanics and thermodynamics. Phase-field.

Linear algebra

System of constrained inequalities.

Theorem of Liu (1972) needs special affine Farkas (1918)

Let $\mathbf{a}_i \neq \mathbf{0}$ be vectors in a finite dimensional vector space $\mathbb{V}$ and α_i real numbers, $i = 1...n$ and $S_L = \{\mathbf{p} \in \mathbb{V}^* | \mathbf{p} \cdot \mathbf{a}_i = \alpha_i, i = 1...n\}$. The following statements are equivalent for a $\mathbf{b} \in \mathbb{V}$ and a real number β:
(i) $\mathbf{p} \cdot \mathbf{b} \geq \beta$, for all $\mathbf{p} \in S_L$,
(ii) There are real numbers $\lambda_1, ..., \lambda_n$ such that

$$\mathbf{b} = \sum_{i=1}^{n} \lambda_i \mathbf{a}_i, \quad \textit{and} \quad \beta \leq \sum_{i=1}^{n} \lambda_i \alpha_i.$$

$$0 \leq (\mathbf{p}\cdot\mathbf{b} - \beta) - \sum_{i=1}^{n} \lambda_i (\mathbf{p}\cdot\mathbf{a}_i - \alpha_i) = \mathbf{p}\cdot(\mathbf{b} - \sum_{i=1}^{n} \lambda_i \cdot \mathbf{a}_i) - \beta + \sum_{i=1}^{n} \lambda_i \alpha_i, \quad \forall \mathbf{p} \in \mathbb{V}^*.$$

Process directions, Liu equations, Lagrange-Farkas multipliers, dissipation inequality, ...

Internal variables: rigorous evolution

Coleman-Gurtin: with constitutive state space $(\alpha, \partial_i \alpha)$

f?, if $\dot{S}(\alpha, \partial_i \alpha) \geq 0$, whenever $\dot{\alpha} - f(\alpha, \partial_i \alpha) = 0$.

$$\dot{S}(\alpha, \partial_i \alpha) - \lambda(\dot{\alpha} - f(\alpha, \partial_i \alpha)) = \underline{(\partial_\alpha S - \lambda)}\dot{\alpha} + \underline{\partial_{\partial_i \alpha} S}\, \partial_i \dot{\alpha} + \lambda f \geq 0$$

- Process directions: $\dot{\alpha}, \partial_i \dot{\alpha}$
- Liu equations: $\partial_\alpha S - \lambda = 0, \quad \partial_{\partial_i \alpha} S = 0.$
- Dissipation inequality: $\partial_\alpha S\, f \geq 0 \quad \to \quad f = l\, \partial_\alpha S, \quad (l \geq 0)$

Where is Ginzburg-Landau?

- Higher order constitutive state space: $(\alpha, \partial_i \alpha, \partial_{ij} \alpha)$;
- Arbitrary, constitutive entropy flux;
- Gradient constraint: $\partial_i \dot{\alpha} = \partial_i f$

Weakly nonlocal internal variables

- Higher order constitutive state space: $(\alpha, \partial_i\alpha, \partial_{ij}\alpha)$;
- Arbitrary, constitutive entropy flux;
- Gradient constraint: $\partial_i\dot\alpha = \partial_i f$

Constitutive state space $(\alpha, \partial_i\alpha, \partial_{ij}\alpha)$

f?, if $\dot S(\alpha, \partial_i\alpha, \partial_{ij}\alpha) + \partial_i J^i(\alpha, \partial_i\alpha, \partial_{ij}\alpha) \geq 0$, whenever

$$\dot\alpha - f(\alpha, \partial_i\alpha, \partial_{ij}\alpha) = 0 \text{ and } \partial_i\dot\alpha - \partial_i f(\alpha, \partial_i\alpha, \partial_{ij}\alpha) = 0.$$

$$\dot S + \partial_i J^i - \lambda(\dot\alpha - f) - \Lambda^i(\partial_i\dot\alpha - \partial_i f) \geq 0$$

- Process directions: $\dot\alpha, \partial_i\dot\alpha, \partial_{ij}\dot\alpha, \partial_{ijk}\alpha$
- Liu equations: $\partial_\alpha S = \lambda, \quad \partial_{\partial_i\alpha} S = \Lambda^i, \quad \partial_{\partial_{ij}\alpha} S = 0_{ij}$
- Entropy flux: $J^i = -\partial_{\partial_i\alpha} S\, f + \hat J^i(\alpha, \partial_i\alpha)$,
- Dissipation inequality $\boxed{0 \leq f\left(\partial_\alpha S - \partial_i(\partial_{\partial_i\alpha} S)\right)} = f\frac{\delta S}{\delta\alpha}$

Diffusion. Internal variables or CIT

The constraint is a balance, the flux, j^i, is constitutive.

$$\dot{S}(\alpha, \partial_i \alpha) + \partial_i J^i(\alpha, \partial_i \alpha) \geq 0, \quad \textit{whenever} \quad \partial_t \alpha + \partial_i j^i(\alpha, \partial_i \alpha) = 0,$$

$$\dot{S} + \partial_i J^i - \lambda(\partial_t \alpha + \partial_i j^i) \geq 0$$

- Process directions: $\dot{\alpha}, \partial_i \dot{\alpha}$
- Liu equations: $\partial_\alpha S - \lambda = 0, \quad \partial_{\partial_i \alpha} S = 0, \ J^i = \partial_\alpha S j^i + \hat{J}^i(\alpha)$
- Dissipation inequality:
  $\partial^i(\partial_\alpha S)\, j^i \geq 0 \quad \rightarrow \quad \boxed{j^i = \kappa\, \partial^i(\partial_\alpha S)}, \quad (\kappa \geq 0)$

Internal variables: rigorous Cahn-Hilliard

Cahn-Hilliard equation: extended diffusion.

$$\partial_t \alpha + \partial_i j^i = 0, \quad j^i = \kappa \partial^i \left(\frac{\delta S}{\delta \alpha} \right) = \kappa \partial^i \left(\partial_\alpha S - \partial_k (\partial_{\partial_k \alpha} S) \right), \qquad \kappa > 0.$$

The problem

- The order of the constitutive state space: $(\alpha, \partial_i \alpha, \partial_{ij} \alpha, \partial_{ijk} \alpha, ...)$??
- How many gradient constraints: $\partial_i(\partial_t \alpha + \partial_i j^i) = 0$, ...?

A solution

- Fourth order constitutive state space and a single gradient constraint.
- A repeated application of the Liu conditions. Further specifications for the extra entropy flux: $\mathfrak{J}^i(3) \to \hat{\mathfrak{J}}^i(2)$.

$$J^i = \left(\partial_\alpha S - \underline{\partial_k (\partial_{\partial_i \alpha} S)} \right) j^k + (\partial_{\partial_k \alpha} S) \partial_k j^i + \hat{\mathfrak{J}}^i(\alpha, \partial_i \alpha, \partial_{ij} \alpha)$$

Dissipation inequality: $\boxed{0 \leq \partial_i \left[\partial_\alpha S - \partial_k (\partial_{\partial_k \alpha} S) \right] j^i}$

Verification : Non-Fourier heat conduction

Ván-Fülöp (AdP, 2012)
Kovács-Ván (IJHMT, 2015)
Ván et al (EPL, 2017)

Second sound, ballistic propagation

Second sound - wavelike propagation of internal energy (temperature); Ballistic propagation - temperature disturbances with the speed of the sound?

- New kind of dissipation: hierarchical balances of extended thermodynamics
- Entropy density and entropy flux: internal variables and Nyíri multipliers
- Experimental observation: low temperatures, microscopic explanation
- Universality: does heterogeneity leads to non-Fourier heat conduction?

Heuristic heat conduction

Heuristic: functions are determined along the calculations.

$$\partial_t E + \partial_i q^i = 0, \qquad dE = TdS, \quad J^i := \frac{dS}{dE} q^i = \frac{q^i}{T}$$

$$\partial_t S(E) + \partial_i J^i = \frac{1}{T}\partial_t E + \partial_i \left(\frac{q^i}{T}\right) = q^i \partial_i \left(\frac{1}{T}\right) \geq 0$$

$$q^i = \lambda \partial_i \left(\frac{1}{T}\right) = -\lambda_F \partial_i T$$

Internal (?) variables with Nyíri multipliers:

$$\partial_t S(E, q^2) + \partial_i J^i(\ldots) = \partial_t \left(S_0(E) - m\frac{q^2}{2} \right) + \partial_i (b^{ij} q_j) =$$

$$\left(b^{ij} - \frac{1}{T}\delta^{ij} \right) \partial_i q_j - (m\partial_t q^i - \partial_j b^{ij}) q_j \geq 0$$

Fluxes and forces again.

A practical tool

$$\left(b - \frac{1}{T}\right) \partial_x q - (m\partial_t q - \partial_x b) q \geq 0$$

$$\left(b - \frac{1}{T}\right) = l\partial_x q, \qquad m\partial_t q - \partial_x b = -kq, \qquad l, k \geq 0.$$

A convenient solution.

$$m\partial_t q - \partial_x \left(\frac{1}{T} + l\partial_x q\right) = kq$$

$$\boxed{\tau\partial_t q + q + \lambda_F \partial_x T - a\partial_{xx} q = 0}$$

Fourier, Maxwell-Cattaneo-Vernotte, Guyer-Krumhansl

Guyer-Krumhansl secrets

Balance + constitutive, nondimensional

$$\begin{aligned} \partial_t T + \partial_x q &= 0, \\ \tau \partial_t q + q + \lambda_F \partial_x T - a \partial_{xx} q &= 0 \end{aligned}$$

Where is the wave?

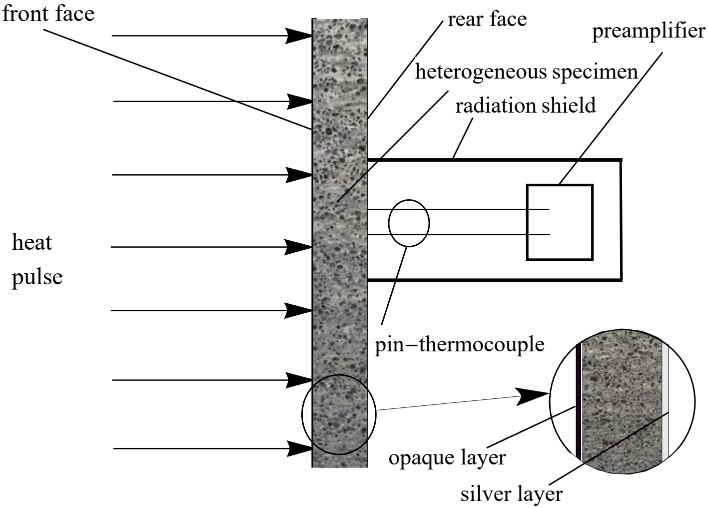
$$\tau \partial_{tt} T - \lambda_F \partial_{xx} T + \partial_t T - a \partial_{txx} T = 0$$

Hierarchy

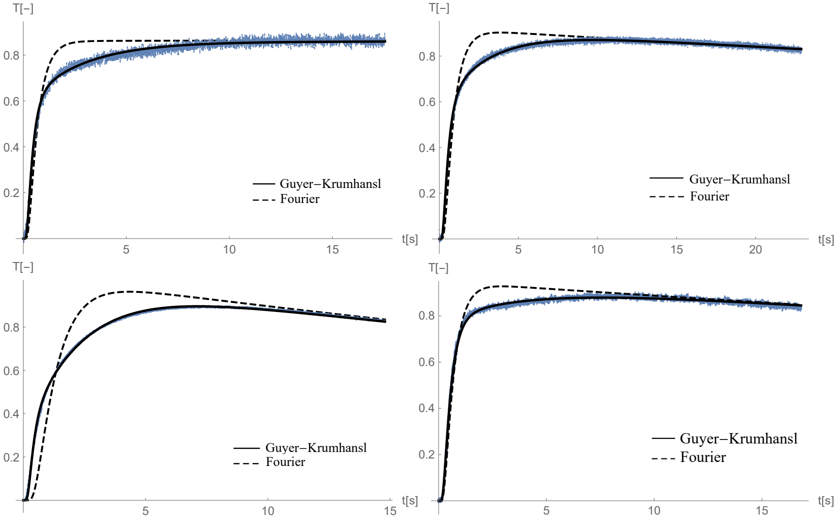
$$\tau \partial_t \left(\partial_t T - \frac{a}{\tau} \partial_{xx} T \right) + \partial_t T - \lambda \partial_{xx} T = 0$$

$\tau\lambda = a$: exact Fourier solutions!

Heat pulse experiments

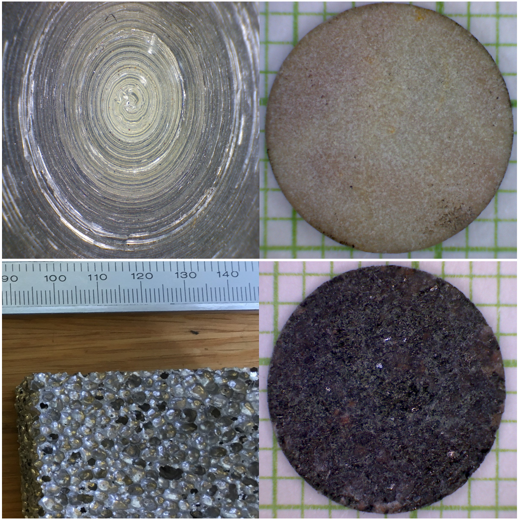


Fourier vs. Guyer-Krumhansl evaluation



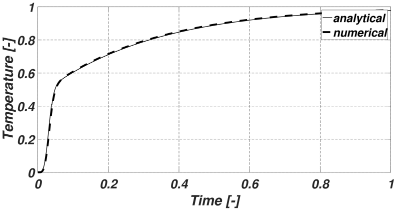
Capacitor, milesstone from Villány, metal foam, leucocratic rock

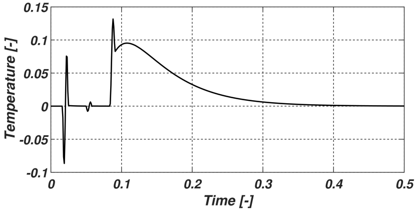
Samples



Capacitor, limestone from Villány, metal foam, leucocratic rock

- Boundary conditions: natural for heat flux,
- Explicit finite differences with stability (Jury) and convergence.
- Shifted fields, explicit and implicit schemes,
- Tested by analytical and exact solutions (Zhukovskii),
- Fast. Commercial solutions (ComSol) do not work,
- Easy to generalize: ballistic propagation, acoustics, ...





Rieth, Kovács and Fülöp, manuscript

Theoretical aspects (T. Ruggeri)

Rational extended thermodynamics

- Special structure of local balances: state space is $(F, F^i, F^{ij}, ...)$

$$\partial_t F + \partial_i F^i = 0,$$
$$\partial_t F^i + \partial_j F^{ij} = 0,$$
$$\partial_t F^{ij} + \partial_k F^{ijk} = P^{ij},$$
$$...$$

  + main field.
- Concave entropy is a generator of a gradient system: symmetry.
- Zero entropy production: hyperbolicity.

Problem 1: Energy is the trace of F^{ij}: the pressure.
Problem 2: Spacetime compatibility.
Problem 3: Experiments?
Internal variables and Nyíri multipliers can do a better job. (We think that.)

Summary

Thermodynamic compatibility of evolution

- Thermodynamics is connected to stability
- Heuristic and rigorous constructive methods: fluxes and forces vs. Liu procedure
- New and extended equations: Ginzburg-Landau and Cahn-Hilliard

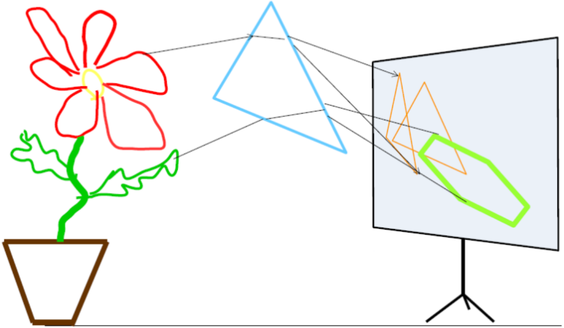
Further aspects

- Spacetime is essential: covectors and higher order tensors, ...
- Dual internal variables for mechanics, generalized entropy flux, ...
- Generalized continua, Korteweg fluids, etc...

Heat conduction: verification and prediction

- Discovery of room temperature heat conduction beyond MCV,
- Hierarchical structure,
- Numerical methods.

Thank you for your attention !



Generalizations of Fourier

Ballistic-conductive system:

$$\begin{aligned} \rho c \partial_t T + \partial_x q &= 0, \\ \tau_q \partial_t q + q + \lambda \partial_x T + \kappa \partial_x Q &= 0, \\ \tau_Q \partial_t Q + Q + \kappa \partial_x q &= 0, \to \end{aligned}$$

$$\tau_q \tau_Q \partial_{ttt} T + (\tau_q + \tau_Q) \partial_{tt} T + \partial_t T = \alpha \partial_{xx} T + (\kappa^2 + \tau_Q) \partial_{txx} T$$

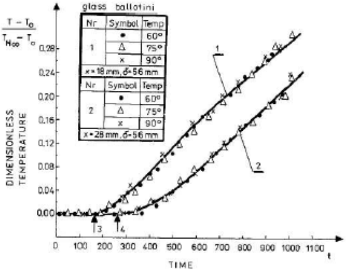
Special cases:

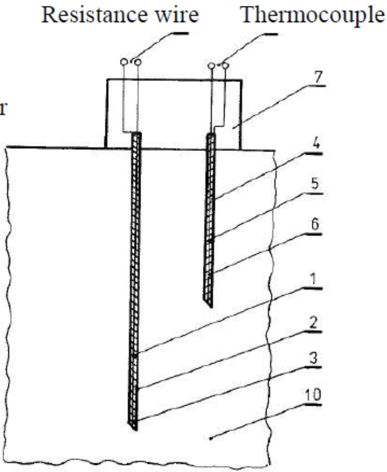
- Maxwell-Cattaneo-Vernotte: $\tau_q \partial_{tt} T + \partial_t T = \alpha \partial_{xx} T$
- **Guyer-Krumhansl** ($\tau_Q = 0$):
  $$\tau_q \partial_{tt} T + \partial_t T = \alpha \partial_{xx} T + l^2 \partial_{txx} T$$

Particulate materials:

sand, glass balottini, ion exchanger

τ = 20-60 s

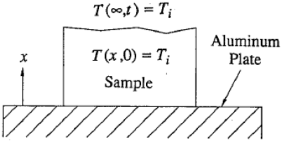


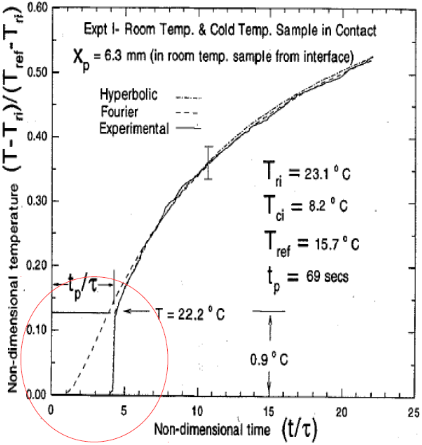


Mitra et al., 1995

Mitra-Kumar-Vedavarz-Moallemi, 1995

Processed frozen meat:
τ = 20-60 s





Korteweg fluids: $P^{ij}(\rho, \partial_i\rho, \partial_{ij}\rho, \partial_i v^j)$

Classical, istropic, polynomial Korteweg:

$$P^{ij} = [p(\rho) - \alpha\partial_k^k\rho - \beta\partial^k\rho\partial_k\rho]\delta^{ij} - \gamma\partial_{ij}\rho - \delta\partial^i\rho\partial^j\rho + \Pi^{ij}$$

A Liu based approach

- Second order constitutive state space in ρ: $(e, \partial_i e, \rho, \partial_i\rho, \partial_{ij}\rho, \partial_i v^j)$.
- Constraints: balance of mass, total energy, momentum, gradient of balance of mass, comoving frame ($(\dot{\partial_i a}) = \partial_i\dot{a} - \partial_i v^k\partial_k a$)

$$J^i = (q^i - v_j P^{ji})\frac{1}{T} + \frac{\rho}{2}\left(\partial_{\partial_i\rho}S\partial_j v^j + \partial_{\partial_k\rho}S\partial_k v^i\right) + \mathfrak{J}^i.$$

Dissipation inequality ($\mathfrak{s} = S/\rho$): $(q^i - v_j P^{ij})\partial_i\frac{1}{T} -$

$$\frac{1}{T}\left[P^{ij} - \left(p + \frac{T\rho^2}{2}\partial_k\left(\partial_{\partial_k\rho}\mathfrak{s}\right)\right)\delta^{ij} - \frac{T\rho^2}{2}\partial^j\left(\partial_{\partial_i\rho}\mathfrak{s}\right)\right]\partial_i v_j \geq 0.$$

Internal variables : various concepts

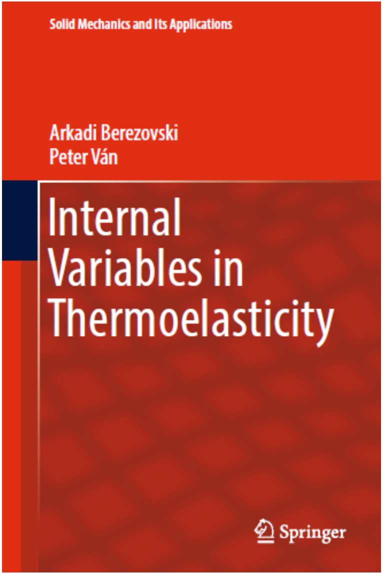
Short story : Muschik and Maugin I-II. (JNET, 1994)

- Thermodynamic state variables : local, first order ;
- Internal degrees of freedom : Lagrangian mechanics and dissipation potentials, second order in time ;
- Dynamic degrees of freedom (Verhás) : local, generalized entropy flux ;
- Weakly nonlocal ;
- Dual and weakly nonlocal : Ván-Berezovski-Engelbrecht (JNET, 2008).

- Duality : α, β ;
- Second order weakly nonlocal state space $(\alpha, \partial_i\alpha, \partial_{ij}\alpha, \beta, \partial_i\beta, \partial_{ij}\beta)$;
- Constitutive entropy flux ;
- Evolution equations are constraints :

$$\dot{e} + \partial_i q^i = 0, \qquad \dot{\alpha} = f, \qquad \dot{\beta} = g$$

$$\boxed{0 \leq \hat{q}^i \partial_i \frac{1}{T} + f\,(\partial_\alpha S - \partial_i(\partial_{\partial_i\alpha} S)) + g\,(\partial_\beta S - \partial_i(\partial_{\partial_i\beta} S))}$$


Solid Mechanics and Its Applications
Arkadi Berezovski
Peter Ván
Internal Variables in Thermoelasticity
Springer

Essential aspects

Content

1. Internal variables in thermomechanics;
2. Dispersive elastic waves in one spatial dimension;
3. Thermal effects;
4. Weakly nonlocal thermoelasticity of microstructured solids

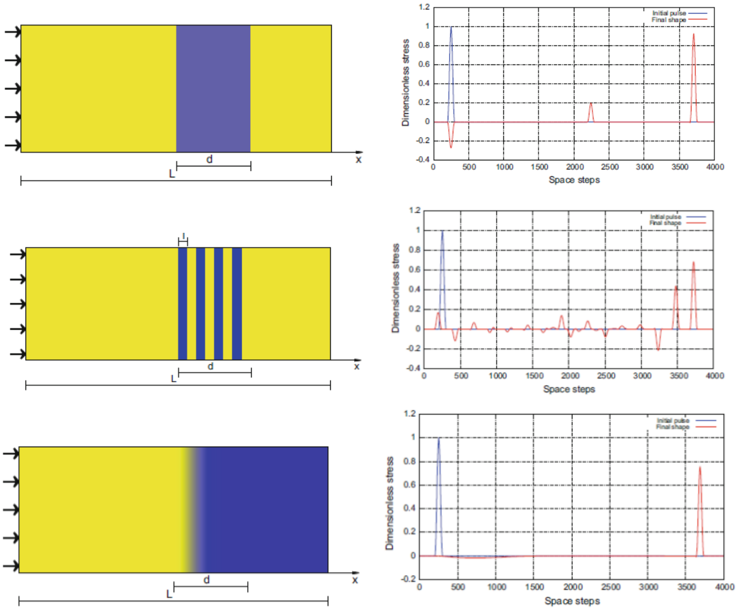
Content

- A systematic method to extend classical continuum theories;
- Mechanics and thermodynamics;
- Simple and constructive.

Perticular aspects

- Wave propagation in 1+1D;
- Material manifolds, small strains;
- Numerical algorithms;

The role of heterogeneity



Aspects of space-time

Matolcsi-Ván (PLA, 2006)
Fülöp-Ván (MMAS, 2012)
Ván (CMaT, 2017)

Objectivity and relativity

Transformation rules

- Galilei invariance
- Rigid body motion

Transformation rule of Noll (1958):

$$x'^a = \begin{pmatrix} t' \\ x'^i \end{pmatrix} = \begin{pmatrix} t \\ h^i(t) + Q^i{}_j(t)x^j \end{pmatrix},$$

where $Q^{-1} = Q^T$ is an orthogonal tensor, a is abstract index.
Jakobian:

$$J^a{}_b = \frac{\partial x'^a}{\partial x^b} = \begin{pmatrix} 1 & 0^j \\ \dot{h}^i + \dot{Q}^i{}_j x^j & Q^i{}_j \end{pmatrix}$$

Transformation rule:

$$C'^a = J^a{}_b C^b$$

Four-velocity vs. three velocity

Transformation of four-vectors (A^b) vs. three-vectors (a^i):

$$J^a{}_b A^b = \begin{pmatrix} 1 & 0^j \\ \dot{h}^i + \dot{Q}^i{}_j x^j & Q^i{}_j \end{pmatrix} \begin{pmatrix} 0 \\ a^i \end{pmatrix} = \begin{pmatrix} 0 \\ Q^i{}_j a^j \end{pmatrix}$$

Three-vector transformation rule:

$$a'^i = Q^i{}_j a^j$$

Velocity is a vector:

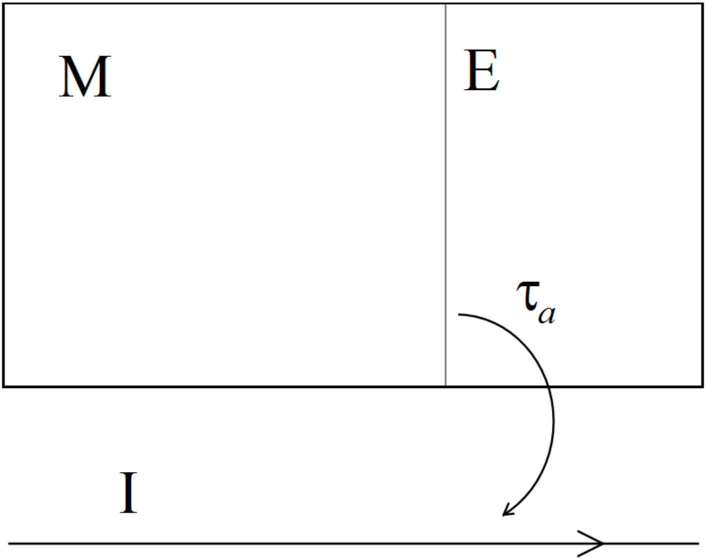
$$v^a := \dot{x}^a(t) = \begin{pmatrix} 1 \\ \dot{x}^i \end{pmatrix} = \begin{pmatrix} 1 \\ v^i \end{pmatrix}$$

$$v'^a := \dot{x}'^a = \begin{pmatrix} 1 \\ \dot{x}'^i \end{pmatrix} = \begin{pmatrix} 1 \\ \dot{h}^i + (Q^i{}_j x^j)^{\cdot} \end{pmatrix}$$

Transformation by the Jakobian:

$$v'^a = J^a{}_b v^b = \begin{pmatrix} 1 & 0^j \\ \dot{h}^i + \dot{Q}^i{}_j x^j & Q^{ij} \end{pmatrix} \begin{pmatrix} 1 \\ v^i \end{pmatrix} = \begin{pmatrix} 1 \\ \dot{h}^i + \dot{Q}^i{}_j x^j + Q^i{}_j v^j \end{pmatrix}$$

The four dimensions of Galilean relativistic space-time



Mathematical structure of Galilean relativistic space-time

1. The *space-time* $\mathbb{M}$ is an oriented four dimensional vector space of the $x^a \in \mathbb{M}$ *world points or events*. There are no Euclidean or pseudoeuclidean structures on $\mathbb{M}$: the length of a space-time vector does not exist.
2. The *time* $\mathbb{I}$ is a one dimensional oriented vector space of $t \in \mathbb{I}$ *instants*.
3. $\tau_a : \mathbb{M} \to \mathbb{I}$ is the *timing* or *time evaluation*, a linear surjection.
4. $\delta_{ij} : \mathbb{E} \times \mathbb{E} \to \mathbb{R} \otimes \mathbb{R}$ Euclidean structure is a symmetric bilinear mapping, where $\mathbb{E} := Ker(\tau) \subset \mathbb{M}$ is the three dimensional vector space of *space vectors*.

- Reference frames are global and smooth velocity fields.
- Transformation rules can be derived between any reference frames.
- Thinking in space-time: momentum balance is a constraint, density and flux, gradients are covectors,...

Thermostatics of elasticity: $S(E, \epsilon_{ij}, \rho)$

From discrete to continuum: extensivity.
$\lambda \mathbb{S}(\mathbb{E}, V, M) = \mathbb{S}(\lambda \mathbb{E}, \lambda V, \lambda M) \leftrightarrow \exists s(e, v) \leftrightarrow \mathbb{E} = T\mathbb{S} - pV + \mu M$

Gibbs relation for elasticity: specific quantities

$$de = \theta ds + \frac{\sigma_{ij}}{\rho} d\epsilon^{ij}, \qquad e = \theta s + \frac{\sigma_{ij}}{\rho}\epsilon^{ij} + \mu.$$

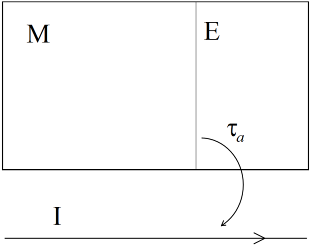
Gibbs relation for elasticity: densities

$$dE = \theta dS + \sigma_{ij} d\epsilon^{ij} + \left(\mu + \frac{\sigma_{ij}\epsilon^{ij}}{\rho}\right) d\rho, \qquad E = \theta S + \sigma_{ij}\epsilon^{ij} + \mu\rho.$$

Gibbs relation for elasticity: free energy

$$dW = -Sd\theta + \sigma_{ij} d\epsilon^{ij} + \left(\mu + \frac{\sigma_{ij}\epsilon^{ij}}{\rho}\right) d\rho, \qquad W = \sigma_{ij}\epsilon^{ij} + \mu\rho.$$

Vectors an covectors are different



$$A'^a B'_a = A^a B_a = AB + A^i B_i$$

$$\begin{pmatrix} t' \\ x'^i \end{pmatrix} = \begin{pmatrix} t \\ x^i + v^i t \end{pmatrix}$$

Vector transformations (extensives):

$$\begin{pmatrix} A' \\ A'^i \end{pmatrix} = \begin{pmatrix} A \\ A^i + v^i A \end{pmatrix}$$

Covector transformations (derivatives):

$$\begin{pmatrix} B' & B'_i \end{pmatrix} = \begin{pmatrix} B - B_k v^k & B_i \end{pmatrix}$$

Balances: absolute, local and substantial

$$\boxed{\partial_a A^a = 0} \quad \longrightarrow \quad \begin{aligned} u^a: \quad D_u A + \partial_i A^i &= d_t A + \partial_i A^i = 0, \\ u'^a: \quad D_{u'} A + \partial_i A'^i &= \partial_t A + \partial_i A'^i = 0. \end{aligned}$$

$(a,b,c \in \{0,1,2,3\})$

Transformed: $(d_t - v^i \partial_i)A + \partial_i(A^i + Av^i) = d_t A + A\partial_i v^i + \partial_i A^i = 0$

From relative to absolute fluids

Usual substantial balances

$$
\begin{aligned}
\dot{\rho} + \rho \partial_i v^i &= 0, \\
\rho \dot{v}^i + \partial_k P^{ik} &= 0^i, \\
\dot{e} + e \partial_i v^i + \partial_i q^i + P^{ij} \partial_i v_j &= 0.
\end{aligned}
$$

Energy-momentum-density does not work in Galilean relativity.

Entropy production rate

$$
\frac{1}{T}\left(P^{ij} - p\delta^{ij}\right)\partial_i v_j + q^i \partial_i \frac{1}{T} \geq 0
$$

Products of relative and absolute quantities.

Mass, energy and momentum

What kind of quantity is the energy?

- Square of the relative velocity → 2nd order tensor
- Kinetic theory: trace of a contravariant second order tensor.
- Energy density and flux: additional order

Basic field:

$$\boxed{Z^{abc} = z^{bc}u^a + z^{ibc} : \qquad \text{mass-energy-momentum density-flux tensor}}$$

$a, b, c \in \{0,1,2,3\}, \quad i, j, k \in \{1,2,3\}$

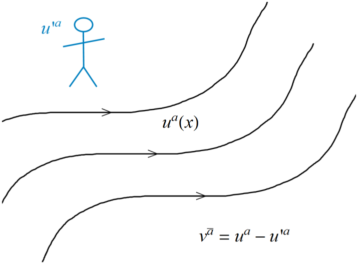
$$z^{bc} \to \begin{pmatrix} \rho & p^j \\ p^k & e^{jk} \end{pmatrix}, \qquad z^{ibc} \to \begin{pmatrix} j^i & P^{ij} \\ P^{ik} & q^{ijk} \end{pmatrix}, \qquad e = \frac{e^j{}_j}{2}$$

$$\boxed{Z'^{abc} = G^a_d G^b_e G^c_f Z^{def}}$$

$$Z^{abc} = \left(\begin{pmatrix} \rho & p^i \\ p^j & e^{ji} \end{pmatrix} \quad \begin{pmatrix} j^k & P^{ki} \\ P^{kj} & q^{kij} \end{pmatrix} \right), \qquad G^a_d = \begin{pmatrix} 1 & 0^i \\ v^j & \delta^{ji} \end{pmatrix}, \qquad e = \frac{e^i{}_i}{2}$$

Transformation rules follow:

$$\begin{aligned} \rho' &= \rho, \\ p'^i &= p^i + \rho v^i, \\ e' &= e + p^i v_i + \rho \frac{v^2}{2}, \\ j'^i &= j^i + \rho v^i, \end{aligned}$$



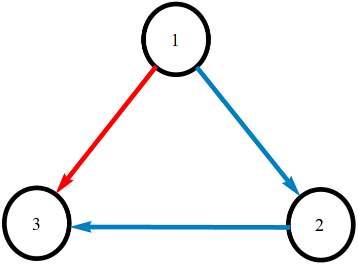
$$\begin{aligned} P'^{ij} &= P^{ij} + \rho v^i v^j + j^i v^j + p^j v^i, \\ q'^i &= q^i + e v^i + P^{ij} v_j + p^j v_j v^i + (j^i + \rho v^i) \frac{v^2}{2}. \end{aligned}$$

Galiean transformation of energy

Transitivity:

$$\left.\begin{aligned} e_2 &= e_1 + p_1 v_{12} + \rho \frac{v_{12}^2}{2} \\ e_3 &= e_2 + p_2 v_{23} + \rho \frac{v_{23}^2}{2} \end{aligned}\right\} \rightarrow e_3 = e_1 + p_1 v_{13} + \rho \frac{v_{13}^2}{2}$$

$$p_2 = p_1 + \rho v_{12}, \qquad v_{13} = v_{12} + v_{23}$$



Balance transformations

Absolute

$$\partial_a Z^{abc} = \dot{z}^{bc} + z^{bc}\partial_a u^a + \partial_a z^{ibc} = 0$$

Rest frame

$$\begin{aligned}
\dot{\rho} + \partial_i j^i &= 0, \\
\dot{p}^i + \partial_k P^{ik} &= 0^i, \\
\dot{e} + \partial_i q^i &= 0.
\end{aligned}$$

Inertial reference frame

$$\begin{aligned}
\dot{\rho} + \rho\partial_i v^i + \partial_i j^i &= 0, \\
\dot{p}^i + p^i\partial_k v^k + \partial_k P^{ik} + \rho\dot{v}^i + j^k\partial_k v^i &= 0^i, \\
\dot{e} + e\partial_i v^i + \partial_i q^i + p^i\dot{v}_i + P^{ij}\partial_i v_j &= 0.
\end{aligned}$$

Further consequences

- Fluid mechanics, thermodynamics, including entropy production, are absolute: independent of reference and flow-frames.
- Four-tensors are useful. Transformation rules can be calculated easily. For inertial frames those are the same as in RET.
- Thermodynamics of motion: four-cotensor of intensive quantities. Absolute entropy production with absolute thermodynamic fluxes and forces.
- Second law: (linear) asymptotic stability of homogeneous equilibrium.
- Key concept: flow-frame.

Verification: Generalized mechanics

Berezovski-Engelbrecht-Maugin (AAM, 2011)
Ván-Papenfuss-Berezovski (CMaT, 2014)

Thermostatics of internal variables: $S(E, \epsilon_{ij}, \rho, \alpha, \partial_i \alpha)$

Gibbs relation for elasticity: free energy

$$dW = -Sd\theta + \sigma_{ij} d\epsilon^{ij} + \left(\mu + \frac{\sigma_{ij}\epsilon^{ij}}{\rho} \right) d\rho, \qquad W = \sigma_{ij}\epsilon^{ij} + \mu\rho.$$

Gibbs relation: internal variables and gradients

$$dW = -Sd\theta + \sigma_{ij} d\epsilon^{ij} - A d\alpha - A_i^d d\partial_i \alpha + \frac{W}{\rho} d\rho,$$

$$W = \sigma_{ij}\epsilon^{ij} + \mu\rho - A\alpha - -A_i^d \partial^i \alpha,$$

$$A = -\frac{\partial W}{\partial \alpha}(S, \epsilon_{ij}, \rho, \alpha, \partial_i \alpha), \quad A_i^d = -\frac{\partial W}{\partial(\partial^i \alpha)}(S, \epsilon_{ij}, \rho, \alpha, \partial_i \alpha).$$

Dissipative Hamiltonian dynamics

Solution with free energy density W

$$\begin{pmatrix} \dot\alpha \\ \dot\beta \\ q^i - \partial_{\partial_i\alpha} W\dot\alpha - -\partial_{\partial_i\beta} W\dot\beta \end{pmatrix} = \mathbb{L} \begin{pmatrix} T\left(\partial_\alpha W - \partial_i(\partial_{\partial_i\alpha} W)\right) \\ T\left(\partial_\beta W - \partial_i(\partial_{\partial_i\beta} W)\right) \\ -\partial_i T \end{pmatrix}$$

- Linear solution $(\dot\alpha, \dot\beta, q^i)$.
- Single local variable: rheology;
- Single weakly nonlocal variable: phase field;
- Dual weakly nonlocal variables: microdeformation;
- Antisymmetry: no dissipation, Hamiltonian evolution.
- Prediction: there is no need of reciprocity.
- Coupling with temperature.

Micromorphic linear elasticity

micro displacement: $\hat{u}_i$ and micro-strain ψ_{ij}:

$$\epsilon_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i) \qquad \psi_{ij} = \frac{1}{2}(\partial_i \hat{u}_j + \partial_j \hat{u}_i)$$

Quadratic, isotropic free energy:

$$W(\epsilon_{ij}, \psi_{ij}, \partial_k \psi_{ij}) = \frac{\lambda}{2}\epsilon_{ii}^2 + \frac{\mu}{2}\epsilon_{ij}\epsilon_{ij} + \frac{b_1}{2}\psi_{ii}^2 + \frac{b_2}{2}\psi_{ij}\psi_{ij} + 14 terms$$

Macrostress, microstresses: Cauchy, relative and double stress:

$$\sigma_{ij} = \partial_{\epsilon_{ij}} W, \quad \tau_{ij} = \partial_{\psi_{ij}} W, \quad \mu_{ijk} = \partial_{\partial_k \psi_{ij}} W.$$

Evolution (e.g. variational, Mindlin)

$$\rho \ddot{u}_i = \partial_j \sigma_{ji} + f_i, \quad \hat{\rho} d_{ki}^2 \ddot{\psi}_{kj} = \partial_k \mu_{ijk} - \tau_{ij} + \Phi_{ij}$$

microinertia $\hat{\rho} d_{ki}^2$, double-force density Φ_{ij}

Mechanics and dual internal variables

Weakly nonlocal constitutive state space:

$$e, \partial_i e, \epsilon_{ij}, \partial_k \epsilon_{ij}, \psi_{ij}, \partial_k \psi_{ij}, \partial_{kl} \psi_{ij}, \beta_{ij}, \partial_k \beta_{ij}, \partial_{kl} \beta_{ij}$$

Constraints:

$$\dot{e} + \partial_k q_i = \sigma_{ij} \partial_j v_i, \quad \dot{\epsilon}_{ij} = \partial_{(j} v_{i)}, \quad \dot{\psi}_{ij} = f_{ij} \quad \dot{\beta}_{ij} = g_{ij}.$$

Entropy production, linear isotropic solution, evolution:

$$\boxed{0 \leq q_i \partial_i \frac{1}{T} + \frac{1}{T}(\sigma_{ij} + \rho_0 T \partial_{ij} s)\dot{\epsilon}_{ij} + \rho_0 A_{ij} \dot{\psi}_{ij} + \rho_0 B_{ij} \dot{\beta}_{ij}}$$

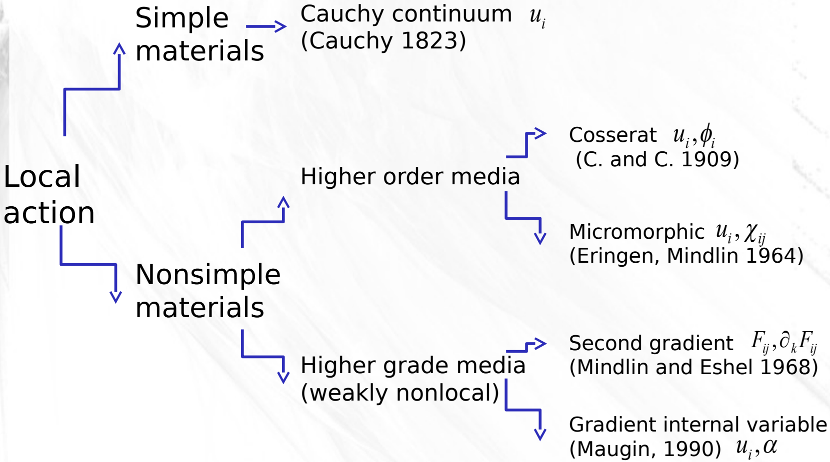
$$A_{ij} = \partial_{\psi_{ij}} S - \partial_k \left(\partial_{\partial_k \psi_{ij}} S \right), \quad B_{ij} = \partial_{\beta_{ij}} S - \partial_k \left(\partial_{\partial_k \beta_{ij}} S \right)$$

$$q_i = \lambda \partial_i \frac{1}{T}, \qquad \sigma_{ij} + \rho_0 T \partial_{\epsilon_{ij}} S = l_{11} \dot{\epsilon}_{ij} + l_{12} A_{ij} + l_{13} B_{ij},$$

$$\rho_0 \dot{\psi}_{ij} = l_{21} \dot{\epsilon}_{ij} + l_{22} A_{ij} + l_{23} B_{ij}, \quad \rho_0 \dot{\beta}_{ij} = l_{31} \dot{\epsilon}_{ij} + l_{32} A_{ij} + l_{33} B_{ij}$$

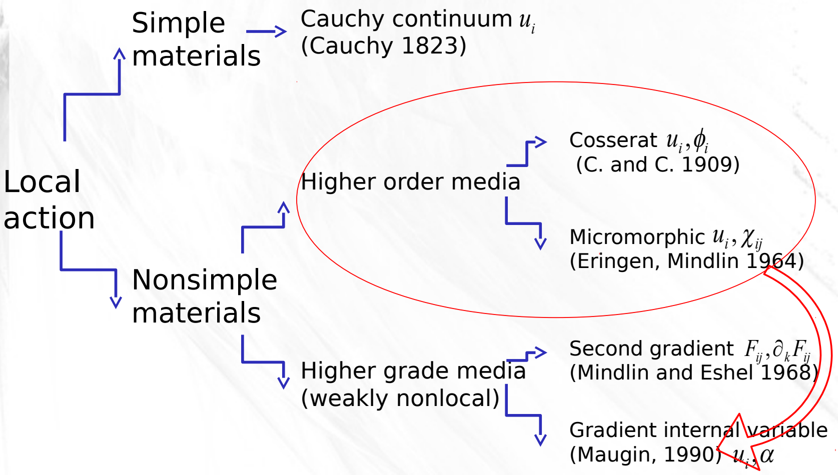
Casimir (gyroscopic) coupling, zero dissipation: $l_{23} = -l_{32} \neq 0$

Classification of continuum theories:



Encyclopedia of materials (2005)

Classification of continuum theories:



Encyclopedia of materials (2005)