Principes de construction des modèles mathématiques thermodynamiquement corrects des milieux continus hétérogènes

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What is a good mathematical model ?

- Physically reasonable
- Mathematically wellposed
- Thermodynamically consistent

About thermodynamics

Thermodynamics is a funny subject. The first time you go through it, you don't understand it at all. The second time you go through it, you think you understand it, excepting for one or two small point. The third time you go through it, you know you don't understand it, but by that time you are so used to the subject, it doesn't bother you any more...

La thermodynamique est amusante. La première fois que vous l'étudiez, vous ne la comprenez pas du tout. La seconde fois que vous l'étudiez, vous pensez l'avoir comprise, mis à part un ou deux points. La troisième fois que vous l'étudiez, vous savez pertinemment que vous ne la comprenez pas, mais vous vous y êtes tellement habitués que cela ne vous dérange plus...

Arnold Johannes Wilhelm SOMMERFELD (1868 — 1951)

What we learned from the thermodynamics (or thermostatics) ?

Paul Germain, Cours de Mécanique des Milieux Continus, Théorie générale, Masson et Cie, 1973 (Chapter concerning Constantin Carathéodory's axioms of thermodynamics).

A system is characterized by $n+1$ physical variables $\boldsymbol{\chi} = (\chi_0, \chi_1, \chi_2, ..., \chi_n) \in D \subset \mathcal{E},\ dim(\mathcal{E}) = n+1$. Let $E : D \to R$ be the equation of state called *internal energy*, $\delta W = \sum_{i=0}^{n} A_i d\chi_i$ and $\delta Q = \sum_{i=0}^{n} B_i d\chi_i$ be two 1 - differential forms, called *infinitesimal work done on the system* and *infinitesimal heat supplied to the system*, respectively.

The first law of thermodynamics

I. For a closed system (no exchange of the matter with surroundings) one has the Gibbs identity :

$$dE = \delta W + \delta Q. \tag{1}$$

The second law of thermodynamics (by Constantin Carathéodory, 1909)

II. In any neighborhood of arbitrary state χ there are states $\chi^{'}$ which can not be adiabatically accessible (i.e. without exchange of heat with surroundings) from χ.

Cela implique l'existence θ and η (C. Carathéodory, 1909, P. Germain, 1973) :

$$\delta Q = \theta d\eta. \tag{2}$$

and the inequality :

$$d\eta \geq 0 \tag{3}$$

for any adiabatically isolated system. The equality takes place only for reversible changes.

Equations of state for compressible fluids

$$\delta W = -p d\tau,\ \theta d\eta = d\varepsilon + p d\tau;\ \varepsilon = \varepsilon(\tau, \eta).$$

For a given $\varepsilon(\tau, \eta)$ it allows us to obtain the definition of the temperature θ and pressure p in the form

$$\theta = \frac{\partial \varepsilon}{\partial \eta}; p = -\frac{\partial \varepsilon}{\partial \tau}.$$

Equations of state for compressible fluids : examples

In practice, we can not obtain this function directly from experiments. We can only find intermediate equations of state : $p(\tau, \theta)$, $\varepsilon(\tau, \theta)$, and then derive $\varepsilon(\tau, \eta)$.

Polytropic gas.

$$p = \frac{R\theta}{\tau}, \ \varepsilon = c_v \theta, \ R = const, \ c_v = const.$$

Van der Waals gas.

$$p = \frac{R\theta}{\tau - b} - \frac{a}{\tau^2}, \ \varepsilon = -\frac{a}{\tau} + c_v \theta,$$

$$R = const, \ c_v = const; a = const, \ b = const.$$

Polytropic gas

The energy of the polytropic gas is convex : $\varepsilon_{\tau\tau} > 0, \varepsilon_{\tau\tau}\varepsilon_{\eta\eta} - (\varepsilon_{\eta\tau})^2 > 0$.
This is not the case of the Van der Waals equation of state.
For convex functions one can play with the Legendre transformation. I will consider only C^2 functions.

Legendre transformation

Let $e(\mathbf{u})$ be convex, i.e. its Hessian matrix is positive definite. The Legendre transform $e^*(\mathbf{v})$ of $e(\mathbf{u})$ is a function defined as

$$e^*(\mathbf{v}) = \mathbf{u} \cdot \mathbf{v} - e(\mathbf{u}),$$

where vector $\mathbf{u}$ is implicitly defined by the equation

$$\mathbf{v} = \boldsymbol{\nabla}_{\mathbf{u}} e(\mathbf{u}).$$

One also has :

$$\mathbf{u} = \boldsymbol{\nabla}_{\mathbf{v}} e^*(\mathbf{v}), \quad \mathbf{I} = e^{*\prime\prime}(\mathbf{v}) e^{\prime\prime}(\mathbf{u}).$$

The Legendre transform $e^*(\mathbf{v})$ is a convex function of $\mathbf{v}$. The Legendre transformation is involutive :

$$e^{**} = e.$$

Solid mechanics

In solid mechanics one usually works with the Helmholz free energy $\psi = \varepsilon - \theta\eta$. Thinking about applications related to the wave propagation in fluids and solids where the materials behave rather isentropically than isothermally, I will use everywhere the energy as a function of the entropy η and deformation gradient $\mathbf{F}$: $\varepsilon = \varepsilon(\mathbf{F}, \eta)$.
It cannot be a convex function of $\mathbf{F}$: $\varepsilon = \varepsilon(\eta, \mathbf{C})$, $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ is the right Cauchy-Green deformation tensor.

Rank-one convexity

The specific energy is *rank-one convex*, i.e. the function

$$\tilde{\varepsilon}(s) = \varepsilon(\mathbf{F} + s\mathbf{n} \otimes \mathbf{m})$$

is convex with respect to s for any $\mathbf{n}$ and $\mathbf{m}$ (Ball, Dafermos, Dacorogna, ...). The rank one convexity is equivalent the ellipticity condition (Legendre - Hadamard condition) in statics, or the hyperbolicity condition (in dynamics). We will see this later...
It is rather difficult (if not impossible) to use this definition in practice !

Solid mechanics : the case of isotropic solids

$$\varepsilon = \varepsilon(\eta, I_1, I_2, I_3),$$

or

$$\varepsilon = \varepsilon(\eta, J_1, J_2, J_3),\ J_n = \mathrm{tr}(\mathbf{C}^k) = \mathrm{tr}(\mathbf{B}^k),\ k = 1, 2, 3.$$

$\mathbf{C} = \mathbf{F}^T\mathbf{F}$ $\left(\mathbf{B} = \mathbf{F}\mathbf{F}^T\right)$ is the right (left) Cauchy-Green deformation tensor. One has

$$\frac{\partial J_k}{\partial \mathbf{C}} = k\mathbf{C}^{k-1}.$$

Example : Blatz-Ko equation of state

$$\varepsilon = \varepsilon(I_1, I_2, I_3) = \frac{\mu}{2}\left(\frac{I_2(\mathbf{C})}{I_3(\mathbf{C})} + 2\sqrt{I_3(\mathbf{C})} - 5\right).$$

It is not rank-one convex.

Dacorogna, 2001, Discret and Continuous Dynamical Systems- Series B, v.1, N2, 257-263 (Proposition 7).

Let k_i, $i = 1, 2, 3$, be singular values of $\mathbf{F}$, and $\varepsilon = \varepsilon(k_1, k_2, k_3)$. Then ε is rank-one convex, if the following conditions hold :

$$\varepsilon_{ii} \geq 0,$$

$$\frac{k_i \varepsilon_i - k_j \varepsilon_j}{k_i - k_j} \geq 0, \; k_i \neq k_j, \; 1 \leq i < j \leq 3,$$

$$\frac{\sqrt{\varepsilon_{ii}\varepsilon_{jj}}}{2} + \varepsilon_{ij} + \frac{\varepsilon_i - \varepsilon_j}{k_i - k_j} \geq 0, \; k_i \neq k_j, \; 1 \leq i < j \leq 3,$$

$$\frac{\sqrt{\varepsilon_{ii}\varepsilon_{jj}}}{2} - \varepsilon_{ij} + \frac{\varepsilon_i + \varepsilon_j}{k_i + k_j} \geq 0, \; k_i \neq k_j, \; 1 \leq i < j \leq 3.$$

Here $\varepsilon_i = \dfrac{\partial \varepsilon}{\partial k_i}$ etc.

Mathematically well-posed models

1. Existence
2. Uniqueness
3. Continuous dependence on the initial data

Hadamard's example

Cauchy Problem

$$
\begin{aligned}
u_t + v_x &= 0,\\
v_t - u_x &= 0,
\end{aligned}
$$
$$
u(0,x) = \frac{sin(nx)}{n^2}, \qquad v(0,x) = \frac{cos(nx)}{n^2}.
$$

Solution

$$
u(t,x) = \frac{sin(nx)}{n^2} e^{nt}, \qquad v(t,x) = \frac{cos(nx)}{n^2} e^{nt}.
$$

Algebraic friction doesn't help !

$$\begin{array}{l} u_t + v_x = -Ku, \\ v_t - u_x = -Kv \end{array}, \quad K > 0.$$

This does not help !

$$u' = e^{Kt} u, \qquad v' = e^{Kt} v.$$

Hyperbolic systems in a nutshell

- 1D hyperbolic systems of equations, characteristics, Riemann invariants, linearly degenerate fields, genuinely nonlinear fields, examples, fields which are not genuinely nonlinear.
- Rankine-Hugoniot relations, applications to the Euler equations of compressible fluids, admissibility of shock waves and the second law of thermodynamics
- Riemann problem, applications to the Euler equations

Hyperbolic equations : multiD case

Symmetric t-hyperbolic in the sense of Friedrichs systems (Kurt Otto Friedrichs, 1901-1982)

$$A\mathbf{U}_t+B\mathbf{U}_x+C\mathbf{U}_y+D\mathbf{U}_z=0,\ \mathbf{U}\in R^n,\ A=A^T>0,\ B=B^T,\ C=C^T,\ D=$$

The Cauchy problem

$$\mathbf{U}(0,\mathbf{x})=\mathbf{U}_0(\mathbf{x})$$

is well posed for small time.
1D hyperbolic models can always be written in symmetric form (a proof will be given).

Physically reasonable : Hamilton's principle

Definitions

- $E = T + W$ – total energy
- T – kinetic energy
- W – potential energy
- $L = T - W$ – Lagrangian
- $a = \int_{t_0}^{t_1} \int_{\mathcal{D}(t)} L dD dt$ - Hamilton's action

Hamilton's principle

The governing equations are stationary 'points' of Hamilton's action (under certain constraints to be defined).

Constraints

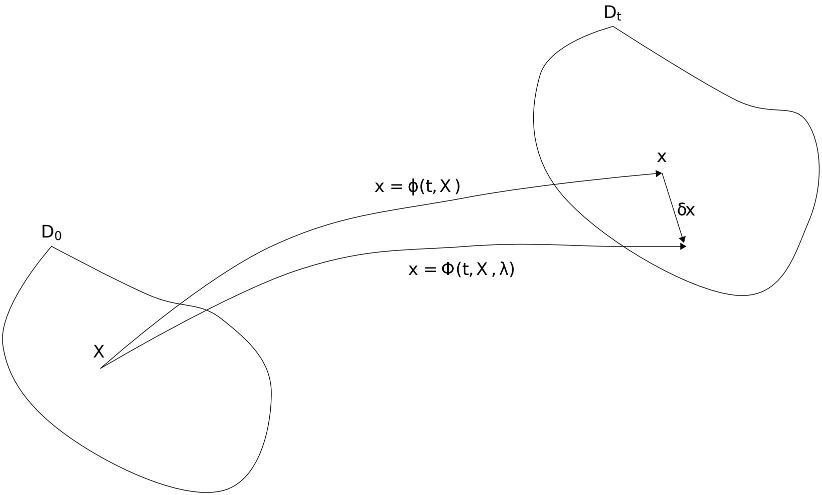
The constraints should be integrable in the reference configuration !

- Conservation of the mass
- Conservation of the entropy
- ...

Advantages

- Only one scalar function (Lagrangian) determines the governing equations
- Conservation laws are natural (Noether theorem)
- Invariance properties of governing equation are also determined by the Lagrangian
- One can naturally obtain the Rankine-Hugoniot relations

Motion and virtual motion



Motion and virtual motion

- $\mathbf{x} = \varphi(t, \mathbf{X}), \ \mathbf{x} = \left(x^1, x^2, x^3\right)^T, \ \mathbf{X} = \left(X^1, X^2, X^3\right)^T,$
- $\mathbf{x} = \mathbf{\Phi}(t, \mathbf{X}, \lambda),$
- $\delta\mathbf{x}(t, \mathbf{X}) = \frac{\partial}{\partial\lambda}\mathbf{\Phi}(t, \mathbf{X}, \lambda)|_{\lambda=0},$
- $\zeta(t, \mathbf{x}) = \delta\mathbf{x}\left(t, \varphi^{-1}(t, \mathbf{x})\right).$

Lagrangian and Eulerian variations

$$\tilde{f}(t, \mathbf{X}, \lambda), \;\; \hat{f}(t, \mathbf{x}, \lambda).$$

$$\tilde{\delta} f = \hat{\delta} f + \nabla f \cdot \delta \mathbf{x}.$$

Lagrangian variations

Berdichevskii, V. L. (2009), SG (2011)

- $\tilde{\delta}\rho = -\rho div(\zeta)$,
- $\tilde{\delta}\eta = 0,\ \tilde{\delta}\mathbf{F}^{-T} = -\left(\frac{\partial\zeta}{\partial\mathbf{x}}\right)^{T}\mathbf{F}^{-T}$,
- $\tilde{\delta}\mathbf{u} = \frac{\partial\delta\mathbf{x}}{\partial t}$.

Remark

$$\mathbf{F}^{-T} = \left(\mathbf{e}^1, \mathbf{e}^2, \mathbf{e}^3\right), \ \mathbf{e}^\beta = \nabla X^\beta.$$

We call $\mathbf{e}^\beta$ *curvilinear cobasis* (ot simply *cobasis*), which is dual to a natural curvilinear basis

$$\mathbf{e}_\beta = \frac{\partial \mathbf{x}}{\partial X^\beta}.$$

One has obviously

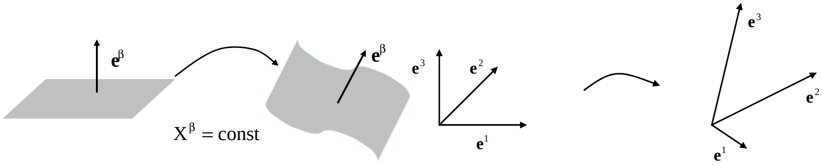
$$\mathrm{curl}\,\mathbf{e}^\beta = 0.$$

The Lagrangian variation of $\mathbf{e}^\beta$ is :

$$\tilde{\delta}\mathbf{e}^\beta = -\left(\frac{\partial \zeta}{\partial \mathbf{x}}\right)^T \mathbf{e}^\beta.$$

Finger tensor as a measure of deformation for isotropic solids

$$\mathbf{G} = \mathbf{B}^{-1} = \mathbf{F}^{-T}\mathbf{F}^{-1} = \sum_{i=1}^{3} \mathbf{e}^{\beta} \otimes \mathbf{e}^{\beta}.$$



Eulerian variations

- $\hat{\delta}\rho = -div(\rho\zeta)$,
- $\hat{\delta}\eta = -\nabla\eta \cdot \zeta, \quad \hat{\delta}\mathbf{e}^{\beta} = -\left(\frac{\partial\zeta}{\partial\mathbf{x}}\right)^{T}\mathbf{e}^{\beta} - \left(\frac{\partial\mathbf{e}^{\beta}}{\partial\mathbf{x}}\right)\zeta,$
- $\hat{\delta}\mathbf{u} = \frac{D\zeta}{Dt} - \frac{\partial\mathbf{u}}{\partial\mathbf{x}}\zeta.$

How to obtain the equations of motion ?

$$\delta a = \int_{t_0}^{t_1} \int_{\mathcal{D}(t)} \mathbf{M} \cdot \zeta dD \ dt = 0.$$

It implies

$$\mathbf{M} = \mathbf{0}.$$

Euler equations of compressible fluids

- $T = \int_{\mathcal{D}_t} \rho \frac{\|\mathbf{u}\|^2}{2} dD$
- $W = \int_{\mathcal{D}_t} \rho\varepsilon\left(\rho, \eta\right) dD.$

Constraints

$$\rho_t + div(\rho\mathbf{u}) = 0, \quad (\rho\eta)_t + div(\rho\eta\mathbf{u}) = 0.$$

Equations

$$\left(\rho\mathbf{u}\right)_t + div\left(\rho\mathbf{u} \otimes \mathbf{u} + p\mathbf{I}\right) = 0.$$

The convexity of the specific energy $\varepsilon(\tau, \eta)$, $\tau = 1/\rho$ implies the hyperbolicity.

Euler equations of compressible fluids : conservation laws

$$
\begin{gathered}
\rho_t + div(\rho \mathbf{u}) = 0, \\
(\rho \mathbf{u})_t + div\left(\rho \mathbf{u} \otimes \mathbf{u} + p\mathbf{I}\right) = 0, \\
\left(\rho\left(\frac{|\mathbf{u}|^2}{2} + \varepsilon\right)\right)_t + div\left(\rho \mathbf{u}\left(\frac{|\mathbf{u}|^2}{2} + \varepsilon\right) + p\mathbf{u}\right) = 0, \\
(\rho\eta)_t + div(\rho\eta\mathbf{u}) = 0.
\end{gathered}
$$

Theorem of Godunov-Friedrichs-Lax

Let a system of conservation laws

$$\mathbf{u}_t + \sum_{i=1}^{n} (\psi_i(\mathbf{u}))_{x_i} = 0$$

admits the additional conservation law

$$e_t + \sum_{i=1}^{n} (f_i(\mathbf{u}))_{x_i} = 0,$$

wher the function $e(\mathbf{u})$ is convex. Then the system can be written as a symmetric t-hyperbolic system in the sense of Friedrichs.

Proof The compatibility condition yields :

$$\frac{\partial e}{\partial \mathbf{u}}\frac{\partial \psi_i}{\partial \mathbf{u}} = \frac{\partial f_i}{\partial \mathbf{u}}.$$

Let

$$e^*(\mathbf{v}) = \mathbf{v}\cdot\mathbf{u} - e(\mathbf{u}),\ \mathbf{v} = \nabla_{\mathbf{u}} e, \quad f_i^*(\mathbf{v}) = \mathbf{v}\cdot\psi_i - f_i.$$

Then

$$(\nabla_{\mathbf{v}} e^*)_t + \sum_{i=1}^{n} (\nabla_{\mathbf{v}} f_i^*)_{x_i} = 0$$

Applications to the Euler equations of compressible fluids

$$E(\rho, \rho\mathbf{u}, \rho\eta) = \rho\left(\frac{|\mathbf{u}|^2}{2} + \varepsilon\right) = \left(\frac{(\rho|\mathbf{u}|)^2}{2\rho} + \rho\varepsilon\left(\frac{1}{\rho}, \frac{\rho\eta}{\rho}\right)\right).$$

$E(\rho, \rho\mathbf{u}, \rho\eta)$ is convex if and only if $|\mathbf{u}|^2/2 + \varepsilon(\tau, \eta)$ is convex with respect to $\mathbf{u}, \tau, \eta$.

Hyperelastic solids

- $T = \int_{\mathcal{D}_t} \rho \frac{\|\mathbf{u}\|^2}{2} dD$
- $W = \int_{\mathcal{D}_t} \rho\varepsilon\left(\mathbf{F}, \eta\right) dD, \ \mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}, \ \mathbf{F}^{-T} = \left(\mathbf{e}^1, \mathbf{e}^2, \mathbf{e}^3\right), \ \mathbf{e}^\beta = \nabla_{\mathbf{x}} X^\beta.$

Hyperelastic isotropic solids

$$\varepsilon\left(\mathbf{F}, \eta\right) = \varepsilon\left(J_1, J_2, J_3, \eta\right), \ J_k = \mathrm{tr}\left(\mathbf{G}^k\right), \ \mathbf{G} = \left(\mathbf{F}\mathbf{F}^T\right)^{-1}, \ k = 1, 2, 3.$$

Constraints

- $\rho_t + div(\rho\mathbf{u}) = 0,$
- $(\rho\eta)_t + div(\rho\eta\mathbf{u}) = 0,$
- $\mathbf{e}^\beta_t + \left(\frac{\partial\mathbf{e}^\beta}{\partial\mathbf{x}}\right)^T\mathbf{u} + \left(\frac{\partial\mathbf{u}}{\partial\mathbf{x}}\right)^T\mathbf{e}^\beta = 0,\ \ \mathrm{curl}\mathbf{e}^\beta = 0, \quad \beta = 1, 2, 3$

Equation for $\mathbf{e}^\beta$ comes from

$$\frac{\partial X^\beta}{\partial t} + \mathbf{u}\cdot\nabla X^\beta = 0.$$

Isotropic hyperelastic solids

$$(\rho \mathbf{u})_t + div\,(\rho \mathbf{u} \otimes \mathbf{u} - \boldsymbol{\sigma}) = 0.$$

Stress tensor :

$$\boldsymbol{\sigma} = -2\rho \frac{\partial \varepsilon}{\partial \mathbf{G}} \mathbf{G} = -2\rho \mathbf{G} \frac{\partial \varepsilon}{\partial \mathbf{G}}.$$

Separable form that matches perfectly with both solids and fluids :

$$\varepsilon = \varepsilon^h(\tau, \eta) + \varepsilon^e(\mathbf{g}),$$

$$\varepsilon^e(\mathbf{g}) = \varepsilon^e(j_1, j_2),\ j_k = \mathrm{tr}(\mathbf{g}^k), \quad \mathbf{g} = \frac{\mathbf{G}}{|\mathbf{G}|^{1/3}}, \quad \mathbf{G} = \sum_{\beta=1}^{3} \mathbf{e}^\beta \otimes \mathbf{e}^\beta,$$

$$\boldsymbol{\sigma} = -p\mathbb{I} + \mathbf{S}, \quad p = \rho^2 \frac{\partial \varepsilon^h}{\partial \rho}, \quad \mathbf{S} = -2\rho \frac{\partial \varepsilon^e}{\partial \mathbf{G}} \mathbf{G}.$$

Isotropic hyperelastic solids

Let $\varepsilon^e(j_1, j_2)$. Then

$$\mathbf{S} = -2\rho \frac{\partial e^e}{\partial \mathbf{G}} \mathbf{G} = -2\rho \left(\frac{\partial e^e}{\partial j_1} \left(\mathbf{g} - \frac{j_1}{3} \mathbf{I} \right) + 2 \frac{\partial e^e}{\partial j_2} \left(\mathbf{g}^2 - \frac{j_2}{3} \mathbf{I} \right) \right).$$

Criterion of hyperbolicity for a general stored specific energy

Theorem The equations are *hyperbolic*, if and only if the specific energy is rank - one convex (cf. C. Dafermos).

Polyconvexity et symmetrization

Let $\varepsilon(\mathbf{F}, \eta)$. Consider $\varepsilon = \mathcal{E}(|\mathbf{F}|, Cof\,\mathbf{F}, \mathbf{F}, \eta)$, $Cof\,\mathbf{F} = \dfrac{\mathbf{F}^{-T}}{|\mathbf{F}|}$.

Theorem (T. Qin, D. H. Wagner) Let $\mathcal{E}(|\mathbf{F}|, Cof\,\mathbf{F}, \mathbf{F}, \eta)$ be a convex function of its arguments (polyconvexity condition ; polyconvexity implies rank-one convexity). Then the equations for hyperelasticity can be rewritten as a symmetric-t hyperbolic system.

Remarks

- To find a polyconvex function from a given function is not an obvious exercise.
- In practice, we need only hyperbolicity, and not symmetric t -hyperbolic forms.
- This is a system of 23 scalar equations ! Difficult to solve ? Can we do better at least for isotropic hyperelastic solids ?

Back to the hyperelasticity

$$
\begin{gathered}
\rho_t + div(\rho \mathbf{u}) = 0, \\
(\rho \mathbf{u})_t + div\left(\rho \mathbf{u} \otimes \mathbf{u} - \boldsymbol{\sigma}\right) = 0, \\
(\rho \eta)_t + div(\rho \eta \mathbf{u}) = 0, \\
\mathbf{e}^{\beta}_t + \left(\frac{\partial \mathbf{e}^{\beta}}{\partial \mathbf{x}}\right)^T \mathbf{u} + \left(\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\right)^T \mathbf{e}^{\beta} = 0, \;\; \mathrm{curl}\mathbf{e}^{\beta} = 0, \quad \beta = 1, 2, 3.
\end{gathered}
$$

Separable form that matches perfectly with both solids and fluids :

$$
\varepsilon = \varepsilon^h(\tau, \eta) + \varepsilon^e(j_1, j_2),
$$

$$
j_k = \mathrm{tr}(\mathbf{g}^k), \quad \mathbf{g} = \frac{\mathbf{G}}{|\mathbf{G}|^{1/3}}, \quad \mathbf{G} = \sum_{\beta=1}^{3} \mathbf{e}^{\beta} \otimes \mathbf{e}^{\beta}.
$$

$$
\boldsymbol{\sigma} = -p\mathbf{I} + \mathbf{S}, \; \mathbf{S} = -2\rho \frac{\partial e^e}{\partial \mathbf{G}} \mathbf{G} = -2\rho \left(\frac{\partial e^e}{\partial j_1} \left(\mathbf{g} - \frac{j_1}{3} \mathbf{I} \right) + 2 \frac{\partial e^e}{\partial j_2} \left(\mathbf{g}^2 - \frac{j_2}{3} \mathbf{I} \right) \right).
$$

Nonconservative form

A non-conservative system is (ρ is considered as an independent variable) :

$$\frac{\partial \rho}{\partial t} + \bigtriangledown \rho \cdot \mathbf{u} + \rho div \mathbf{u} = 0,$$

$$\frac{\partial \mathbf{e}^\beta}{\partial t} + \frac{\partial \mathbf{e}^\beta}{\partial \mathbf{x}} \mathbf{u} + \left(\frac{\partial \mathbf{u}}{\partial \mathbf{x}} \right)^T \mathbf{e}^\beta = 0,$$

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{u}}{\partial \mathbf{x}} \mathbf{u} + \frac{\bigtriangledown p}{\rho} - \frac{div \mathbf{S}}{\rho} = 0,$$

$$\frac{\partial \eta}{\partial t} + \bigtriangledown \eta \cdot \mathbf{u} = 0$$

with

$$p = \rho^2 \frac{\partial e^h(\rho, \eta)}{\partial \rho}, \quad \mathbf{S} = -2\rho \left(\frac{\partial e^e}{\partial j_1} \left(\mathbf{g} - \frac{j_1}{3} \mathbf{I} \right) + 2 \frac{\partial e^e}{\partial j_2} \left(\mathbf{g}^2 - \frac{j_2}{3} \mathbf{I} \right) \right).$$

Rotational invariance

Theorem *The equations are invariant under rotations :*

$$t' = t, \quad \mathbf{x}' = O\mathbf{x}, \quad \mathbf{u}' = O\mathbf{u}, \quad \left(\mathbf{e}^{\beta}\right)' = O\mathbf{e}^{\beta},$$

$$\rho' = \rho, \quad \eta' = \eta.$$

where O is any element of $SO(3)$.

General definition of hyperbolicity

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{D}_x \frac{\partial \mathbf{U}}{\partial x} + \mathbf{D}_y \frac{\partial \mathbf{U}}{\partial y} + \mathbf{D}_z \frac{\partial \mathbf{U}}{\partial z} = 0,$$

where $\mathbf{D}_x, \mathbf{D}_y, \mathbf{D}_z$ are 14x14 matrices. Let us consider a smooth hypersurface $h\left(t, x, y, z\right) = 0$. We denote

$$\tau = \frac{\partial h}{\partial t}, \xi = \frac{\partial h}{\partial x}, \eta = \frac{\partial h}{\partial y}, \zeta = \frac{\partial h}{\partial z}.$$

The hypersurface is *characteristic* if

$$det\left(\tau \mathbf{I} + \xi \mathbf{D}_x + \eta \mathbf{D}_y + \zeta \mathbf{D}_z\right) = 0.$$

The system (46) is $t-$*hyperbolic*, if the eigenvalues τ are real and the matrix $\xi \mathbf{D}_x + \eta \mathbf{D}_y + \zeta \mathbf{D}_z$ is diagonalizable for any $\left(\xi, \eta, \zeta\right)^T$.

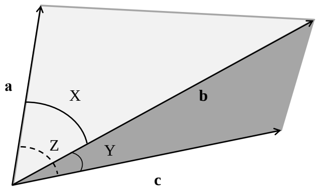
The hyperbolicity condition is thus reduced to 1D case due to the rotational invariance.

We present $\mathbf{F}^{-1}$ *in the form*

$$\mathbf{F}^{-1} = (\mathbf{a}, \mathbf{b}, \mathbf{c}),$$

i.e. $\mathbf{a}, \mathbf{b}, \mathbf{c}$ *are the columns of* $\mathbf{F}^{-1}$. Let us introduce the angles between vectors :

$$\frac{\mathbf{a} \cdot \mathbf{b}}{\|\mathbf{a}\| \, \|\mathbf{b}\|} = X, \;\; \frac{\mathbf{a} \cdot \mathbf{c}}{\|\mathbf{a}\| \, \|\mathbf{c}\|} = Y, \;\; \frac{\mathbf{b} \cdot \mathbf{c}}{\|\mathbf{b}\| \, \|\mathbf{c}\|} = Z.$$



Incompressibility condition

The condition $\det \mathbf{F} = 1$ can be written as

$$1 = \det\left(\mathbf{F}^{-1}\right) = \mathbf{a}\cdot(\mathbf{b}\wedge\mathbf{c})$$

$$= \left(\|\mathbf{b}\|^2\|\mathbf{c}\|^2 - (\mathbf{b}\cdot\mathbf{c})^2\right)\|\mathbf{a}\|^2$$

$$+\left((\mathbf{b}\cdot\mathbf{c})(\mathbf{a}\cdot\mathbf{c}) - (\mathbf{a}\cdot\mathbf{b})\|\mathbf{c}\|^2\right)(\mathbf{a}\cdot\mathbf{b})$$

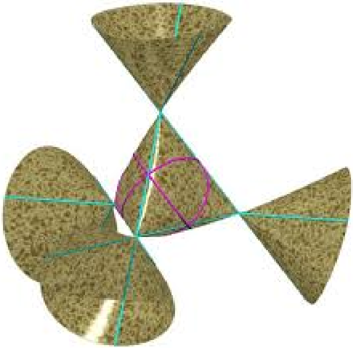
$$+\left((\mathbf{a}\cdot\mathbf{b})(\mathbf{b}\cdot\mathbf{c}) - (\mathbf{a}\cdot\mathbf{c})\|\mathbf{b}\|^2\right)(\mathbf{a}\cdot\mathbf{c}).$$

Or

$$X^2 + Y^2 + Z^2 - 2XYZ = 1 - \frac{1}{\|\mathbf{a}\|^2\|\mathbf{b}\|^2\|\mathbf{c}\|^2} < 1.$$

The inequality is a convex domain in R^3 bounded by the Cayley surface.

Cayley surface



Theorem (S. Ndanou, N. Favrie, SG, 2014, J. Elasticity) *Consider isotropic solids with the specific store energy in separable form*

$$e(\mathbf{G}, \eta) = e^h(\rho, \eta) + e^e(j_1, j_2).$$

The volume shear energy is :

$$E = \Delta e^e, \ \Delta = \det\left(\mathbf{F}^{-1}\right).$$

Let E'' *be the Hessian matrix of* E *with respect to* $\mathbf{a}$,

$$\mathbf{M} = \frac{\mathbf{F}^{-T} E'' \mathbf{F}^{-1}}{\Delta}, \ p = \rho^2 \frac{\partial e^h}{\partial \rho}.$$

Suppose that

- $c^2 = \frac{\partial p}{\partial \rho} > 0, \quad \frac{\partial p}{\partial \eta} > 0,$
- $\mathbf{M} \geq 0$ *for all angles (X,Y,Z) inside the domain having the Cayley surface as a boundary.*

Then the equations of hyperelasticity are hyperbolic.

Example

SG, Ndanou, Hank, 2016, J. Elasticity

$$e^e(j_1, j_2) = \frac{\mu}{4\rho_0}\left(\frac{1+a}{3}(j_2 - 3) + \frac{1-2a}{3}\left(j_1^2 - j_2 - 6\right)\right), \ -1 \le a \le 0.5.$$

$a = -1$ corresponds to the Neohookean materials, $e^e = \dfrac{\mu}{2\rho_0}(i_1 - 3)$,
$i_1 = \mathrm{tr}\left(\dfrac{\mathbf{B}}{|\mathbf{B}|^{1/3}}\right)$.
For small deformations the Hooke law is valid for any values of a.

Visco-plasticity

Plasticity as a relaxation phenomenon (Perzyna's model)

$$\frac{D\mathbf{e}^\beta}{Dt} + \left(\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\right)^T \mathbf{e}^\beta = \frac{\tilde{a}\mathbf{S}\mathbf{e}^\beta}{\tau_{rel}}, \;\; \beta = 1,2,3, \;\; \frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla,$$

$$\frac{D\mathbf{G}}{Dt} + \mathbf{G}\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \left(\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\right)^T \mathbf{G} = \frac{2\tilde{a}\mathbf{G}\mathbf{S}}{\tau_{rel}}, \;\; 2\tilde{a} = \frac{1}{(\mathbf{S}:\mathbf{S})^{1/2}},$$

$$\frac{1}{\tau_{rel}} = \begin{cases} \frac{1}{\tau_0}\left(\frac{\mathbf{S}:\mathbf{S}-\frac{2}{3}\sigma_Y^2}{\sigma_Y^2}\right)^n & \mathit{if} \quad \frac{\mathbf{S}:\mathbf{S}-\frac{2}{3}\sigma_Y^2}{\sigma_Y^2} > 0 \\ 0, & \mathit{if} \quad \frac{\mathbf{S}:\mathbf{S}-\frac{2}{3}\sigma_Y^2}{\sigma_Y^2} \leq 0 \end{cases}$$

Conservation of mass, entropy inequality and shear stresses decrease

- The equations are compatible with the mass conservation law
- The equations are compatible with the entropy inequality
- The intensity of shear stresses decays during the relaxation (Maxwell type model)

Conservation of mass

Let ρ_0 be a function conserving along trajectories :

$$\frac{D\rho_0}{Dt} = 0.$$

Then

$$\frac{D\rho}{Dt} = \frac{D\left(\rho_0 \left|\mathbf{G}\right|^{1/2}\right)}{Dt} = \rho_0 \frac{D\left|\mathbf{G}\right|^{1/2}}{Dt} = \frac{\rho_0}{2}\left|\mathbf{G}\right|^{-1/2} tr\left(\frac{\partial\left|\mathbf{G}\right|}{\partial\mathbf{G}}\frac{D\mathbf{G}}{Dt}\right)$$

$$= \frac{\rho_0}{2}\left|\mathbf{G}\right|^{-1/2} tr\left(\left|\mathbf{G}\right|\mathbf{G}^{-1}\left(-\mathbf{G}\frac{\partial\mathbf{v}}{\partial\mathbf{x}} - \left(\frac{\partial\mathbf{v}}{\partial\mathbf{x}}\right)^T\mathbf{G} + \frac{2\tilde{a}\mathbf{S}\mathbf{G}}{\tau_{rel}}\right)\right)$$

$$= \frac{\rho}{2} tr\left(-\frac{\partial\mathbf{v}}{\partial\mathbf{x}} - \mathbf{G}^{-1}\left(\frac{\partial\mathbf{v}}{\partial\mathbf{x}}\right)^T\mathbf{G} - \frac{2\tilde{a}\mathbf{S}}{\tau_{rel}}\right) = -\rho\,\mathrm{div}\mathbf{v}.$$

Entropy inequality

The energy equation is equivalent to

$$0 = \rho \frac{De}{Dt} - tr\left(\sigma \frac{\partial \mathbf{v}}{\partial \mathbf{x}}\right)$$

$$= \rho \frac{\partial e}{\partial \eta}\frac{D\eta}{Dt} + \rho tr\left(\frac{\partial e}{\partial \mathbf{G}}\left(-\mathbf{G}\frac{\partial \mathbf{v}}{\partial \mathbf{x}} - \left(\frac{\partial \mathbf{v}}{\partial \mathbf{x}}\right)^T \mathbf{G} + \frac{2\tilde{a}\mathbf{SG}}{\tau_{rel}}\right)\right) - tr\left(\boldsymbol{\sigma}\frac{\partial \mathbf{v}}{\partial \mathbf{x}}\right) =$$

$$= \rho \frac{\partial e}{\partial \eta}\frac{D\eta}{Dt} - \frac{\tilde{a}}{\tau_{rel}} tr\left(-2\rho \frac{\partial e}{\partial \mathbf{G}}\mathbf{GS}\right) = \rho\theta \frac{D\eta}{Dt} - \frac{\tilde{a}}{\tau_{rel}} tr\left(\boldsymbol{\sigma}\mathbf{S}\right)$$

Hence

$$\rho\theta \frac{D\eta}{Dt} = \frac{\tilde{a}}{\tau_{rel}} \mathbf{S} : \mathbf{S} \geq 0.$$

Singular value decomposition

$$\mathbf{F}^{-T} = \mathbf{UKV}^T, \qquad \mathbf{U}^T\mathbf{U} = \mathbb{I}, \qquad \mathbf{V}^T\mathbf{V} = \mathbb{I}, \qquad \mathbf{K} = \begin{pmatrix} k_1 & 0 & 0 \\ 0 & k_2 & 0 \\ 0 & 0 & k_3 \end{pmatrix}$$

The singular values k_α are related to the eigenvalues of $\mathbf{G}$ denoted by κ_α

$\kappa_\alpha = k_\alpha^2$

Relaxation equation

$$\frac{d\kappa_\alpha}{dt} = \frac{2\tilde{a}}{\tau_{rel}}\kappa_\alpha S_\alpha.$$

It admits the Lyapunov function $L = \mathbf{S} : \mathbf{S}$ in the case of a one parameter family of equations of state presented before.

Lyapunov function

In terms of singular values k_i of $\mathbf{F}^{-1}$ one has :

$$\frac{dk_\beta}{dt} = \tilde{a}\frac{S_\beta k_\beta}{\tau_{rel}}, \ \beta = 1, 2, 3.$$

One has the first integral :

$$k_1 k_2 k_3 = const.$$

Consider the materials with energy $e^e = \dfrac{\mu}{8\rho_0}(j_2 - 3)$.

$$S_\beta = -\frac{\mu}{2}\frac{\rho}{\rho_0}\left(\frac{k_\beta^4}{(k_1 k_2 k_3)^{\frac{4}{3}}} - \frac{1}{3}\sum_\alpha \frac{k_\alpha^4}{(k_1 k_2 k_3)^{\frac{4}{3}}}\right).$$

Hence

$$\frac{dL}{dt} = \frac{d}{dt}\sum_\beta S_\beta^2 = 2\sum_\beta S_\beta \frac{dS_\beta}{dt} = -\mu\frac{\rho}{\rho_0}\sum_\beta S_\beta \frac{4k_\beta^3}{(k_1 k_2 k_3)^{\frac{4}{3}}}\frac{dk_\beta}{dt} \le 0.$$

Lyapunov function

Remark The yield surface is attained in finite or infinite time depending on the exponent n in the definition of the relaxation time.
Remark In severe conditions the deviatoric part of the stress tensor can be neglected and we can take $Y = 0$. In this particular case formulas for the relaxation time can be found in Godunov and Romenskii (2002).

Solid-fluid interaction

Idea : to construct a multi-phase model from elementary “bricks” : hyperelastic solids and compressible fluids by Hamilton’s principle. The equation of state in separable form is thus very useful !