Chapter 6

Hyperelasticity with constraints

Motivation: From practical reasons, we need to be able to incorporate several types of constraints into our hyperelastic models. For instance many rubber-like materials are practically incompressible. Also some of the fiber-reinforced materials that we have met when discussing transversal anisotropy, can be almost inextensible in the direction of the fibers. This will lead to constrains of the form

- *Incompressibility*:
$$\det \mathbb{F} = 1 \, ,$$
- *Inextensibility* in the material direction ℓ:
$$\ell \cdot \mathbb{C}\ell = 1, .$$

Let us show, how such types of constraints can be incorporated into the theory of hyperelasticity. Interestingly, even though the world of hyperelasticity is a "reversible one" (no energy is lost or dissipated) a possibly most straightforward way is through a thermodynamic framework and entropy inequality. In particular, we will do in in the context of the so-called rational thermodynamics: we will first write down a particular form of second law of thermodynamics - so called Clausius-Duhem inequality - and then exploit it.

6.1 Clausius-Duhem inequality

Let us start by recalling the balances of mass, momentum, internal energy and entropy in Lagrange form, which we derived in the first exercise:

- *Balance of mass*
$$\rho(\mathbf{X},t)\det \mathbb{F}(\mathbf{X},t) = \rho_R(\mathbf{X}) \, , \tag{6.1.1}$$
where $\rho_R(\mathbf{X})$ is the reference density.
- *Balance of linear momentum*
$$\rho_R(\mathbf{X})\frac{\partial \mathbf{V}(\mathbf{X},t)}{\partial t} = \mathrm{Div}\mathbb{T}^{(1)}(\mathbf{X},t) + \rho_R(\mathbf{X})\mathbf{B}(\mathbf{X},t) \, , \tag{6.1.2}$$
where $\mathbb{T}^{(1)}$ is the first Piola-Kirchhoff stress tensor and $\mathbf{B}$ are the Lagrangian body forces mapped to the reference configuration by $\mathbf{B}(\mathbf{X},t) = \mathbf{b}(\boldsymbol{\chi}(\mathbf{X},t),t)$, where $\mathbf{b}$ is the standard Eulerian body force field.
- *Balance of angular momentum* (for a non-polar material)
$$\mathbb{T}^{(1)}(\mathbf{X},t)\mathbb{F}^T(\mathbf{X},t) = \mathbb{F}(\mathbf{X},t)(\mathbb{T}^{(1)})^T(\mathbf{X},t) \, , \tag{6.1.3}$$
- *Balance of internal energy*
$$\rho_R(\mathbf{X})\frac{\partial e_R(\mathbf{X},t)}{\partial t} = \dot{\mathbb{F}}(\mathbf{X},t) : \mathbb{T}^{(1)}(\mathbf{X},t) - \mathrm{Div}\mathbf{Q}(\mathbf{X},t) + \rho_R(\mathbf{X})R(\mathbf{X},t) \, , \tag{6.1.4}$$

where $e_R(\mathbf{X},t)$ is the Lagrangian internal energy density related with its Eulerian counterpart e via $e_R(\mathbf{X},t) = e(\boldsymbol{\chi}(\mathbf{X},t),t)$, $\mathbf{Q}(\mathbf{X},t)$ is the Lagrangian energy flux related with the Eulerian energy flux $\mathbf{q}$ via $\mathbf{Q}(\mathbf{X},t) = \det\mathbb{F}(\mathbf{X},t)\mathbb{F}^{-1}(\mathbf{X},t)\mathbf{q}(\boldsymbol{\chi}(\mathbf{X},t),t)$ and $R(\mathbf{X},t)$ are the energy sources related with their Eulerian counterpart r through $R(\mathbf{X},t) = r(\boldsymbol{\chi}(\mathbf{X},t),t)$.

- *Balance of entropy*

$$\rho_R(\mathbf{X})\frac{\partial\eta_R(\mathbf{X},t)}{\partial t} = -\mathrm{Div}\mathbf{J}_\eta(\mathbf{X},t) + \rho_R(\mathbf{X})R_\eta(\mathbf{X},t) + \xi_R(\mathbf{X},t)\ , \tag{6.1.5}$$

where $\mathbf{J}_\eta(\mathbf{X},t)$ is the Lagrangian entropy flux related with the Eulerian entropy flux $\mathbf{j}_\eta$ via $\mathbf{J}_\eta(\mathbf{X},t) = \det\mathbb{F}(\mathbf{X},t)\mathbb{F}^{-1}(\mathbf{X},t)\mathbf{j}_\eta(\boldsymbol{\chi}(\mathbf{X},t),t)$, R_η is Lagrangian entropy supply and $\xi_R(\mathbf{X},t)$ is the Lagrangian entropy production related to Eulerian entropy production by $\xi_R(\mathbf{X},t) = \det\mathbb{F}(\mathbf{X},t)\xi(\boldsymbol{\chi}(\mathbf{X},t))$.

The second law of thermodynamics in the Lagrangian form reads

$$\xi_R(\mathbf{X},t) \geq 0\ . \tag{6.1.6}$$

Exercise 14. Derive the Clausius-Duhem inequality by incorporating the second law of thermodynamics into the entropy balance, by employing an ansatz for the entropy flux and entropy supply in the form of energy flux and energy supply over absolute temperature and by making use of the internal energy balance.

Solution: As suggested, let us identify the entropy flux and entropy supply as follows

$$\mathbf{J}_\eta(\mathbf{X},t) = \frac{\mathbf{Q}(\mathbf{X},t)}{\vartheta_R(\mathbf{X},t)}\ , \qquad R_\eta(\mathbf{X},t) = \frac{R(\mathbf{X},t)}{\vartheta_R(\mathbf{X},t)} \tag{6.1.7}$$

where $\vartheta_R(\mathbf{X},t)$ is the thermodynamic temperature defined by $\vartheta_R(\mathbf{X},t) = \vartheta(\boldsymbol{\chi}(\mathbf{X},t),t)$. Introducing the Lagrangian Helmholtz specific free energy ψ_R by

$$\psi_R(\mathbf{X},t) \overset{\mathrm{def}}{=} e_R(\mathbf{X},t) - \vartheta_R(\mathbf{X},t)\eta_R(\mathbf{X},t)\ , \tag{6.1.8}$$

let us compute

$$\begin{aligned} \rho_R\dot{\psi}_R &= \rho_R(\dot{e}_R - \dot{\vartheta}_R\eta_R - \vartheta_R\dot{\eta}_R) \\ &= \dot{\mathbb{F}} : \mathbb{T}^{(1)} - \mathrm{Div}\mathbf{Q} + \rho_R R - \rho_R\eta_R\dot{\vartheta}_R - \vartheta_R\left(-\mathrm{Div}\left(\frac{\mathbf{Q}_\eta}{\vartheta_R}\right) + \frac{\rho_R R}{\vartheta_R} + \xi_R\right) \end{aligned} \tag{6.1.9}$$

Since

$$\begin{aligned} \mathrm{Div}\left(\frac{\mathbf{Q}}{\vartheta}\right) &= \frac{\mathrm{Div}\mathbf{Q}}{\vartheta} + \mathbf{Q}\cdot\mathrm{Grad}\left(\frac{1}{\vartheta}\right) \\ &= -\rho_r\dot{e_R} + \dot{\mathbb{F}} : \mathbb{T}^{(1)} + \rho_R R + \mathbf{Q}\cdot\mathrm{Grad}\left(\frac{1}{\vartheta}\right)\ . \end{aligned} \tag{6.1.10}$$

we obtain the following expression

$$\rho_R(\dot{\psi}_R + \eta_R\dot{\vartheta}_R) - \dot{\mathbb{F}} : \mathbb{T}^{(1)} - \vartheta_R\mathbf{Q}\cdot\mathrm{Grad}\left(\frac{1}{\vartheta_R}\right) = -\vartheta_R\xi_R\ . \tag{6.1.11}$$

making use of the second law of thermodynamics (6.1.6) allows to write it as an inequality

$$\boxed{\rho_R(\dot{\psi}_R + \eta_R\dot{\vartheta}_R) - \dot{\mathbb{F}} : \mathbb{T}^{(1)} - \vartheta_R\mathbf{Q}\cdot\mathrm{Grad}\left(\frac{1}{\vartheta_R}\right) \leq 0\ ,} \tag{6.1.12}$$

so-called **Clausius-Duhem inequality** (in the Lagrangian form).

6.2 Clausius-Duhem inequality for hyperelastic materials

Consider now an isothermal setting, i.e. take ϑ_R = const and let us rewrite the mechanical dissipation term a bit so that it involves the second Piola Kirchhoff stress:

$$\dot{\mathbb{F}} : \mathbb{T}^{(1)} = \dot{\mathbb{F}} : (\mathbb{F}\mathbb{T}^{(2)}) = \mathbb{F}^T\dot{\mathbb{F}} : \mathbb{T}^{(2)} = \mathrm{sym}(\mathbb{F}^T\dot{\mathbb{F}}) : \mathbb{T}^{(2)} = \frac{1}{2}(\mathbb{F}^T\dot{\mathbb{F}} + \dot{\mathbb{F}^T}\mathbb{F}) : \mathbb{T}^{(2)} = \frac{1}{2}\dot{\mathbb{C}} : \mathbb{T}^{(2)} \ , \tag{6.2.1}$$

where we used symmetry of the second Piola-Kirchhoff stress.

Finally, let us define Helmholtz free energy volumetric density W:

$$W(\mathbf{X}, t) = \rho_R(\mathbf{X})\psi_R(\mathbf{X}, t) \ , \tag{6.2.2}$$

which allows us to recast the Clausius-Duhem inequality (6.1.12) into the following form:

$$\dot{W} - \frac{1}{2}\mathbb{T}^{(2)} : \dot{\mathbb{C}} \leq 0 \ . \tag{6.2.3}$$

It is not a coincidence that we are using the same symbol W, which we have used for the free energy density in the models of hyperelasticity, as it is exactly the same thing. W is a volumetric density of the Helmholtz free energy (i.e. with units Joule per cubit meter), and is related with the standard Helmholtz potential ψ (with units Joule per kilogram) through (6.2.2).

Let us now consider an isotropic hyperelastic material. We know already that in such a case, ee can write $W = \hat{W}(\mathbb{C})$, where the dependence reduces to the dependence on scalar invariants of $\mathbb{C}$. Employing this in (6.2.3) yields:

$$\boxed{\left(\frac{\partial \hat{W}}{\partial \mathbb{C}} - \frac{\mathbb{T}^{(2)}}{2}\right) : \dot{\mathbb{C}} \leq 0 \ .} \tag{6.2.4}$$

6.3 Rational thermodynamics for hyperelastic materials with constraints

Speaking a bit vaguely, the main idea of a thermodynamic framework called *rational thermodynamics* is to (i) make some rather general constitutive ansatz for quantities that require constitutive closures (making use of principles such as material frame indifference, etc...) and (ii) to postulate the validity of the entropy inequality for arbitrary admissible process, defined as any process compatible with the basic balance laws - balances of mass, momentum and energy.

How does this work here in the realm of hyperelasticity? The thermodynamic ansatz would be for instance $W = \hat{W}(\mathbb{C})$ and $\mathbb{T}^{(2)} = \hat{\mathbb{T}}^{(2)}(\mathbb{C})$ and one would assert the validity of (6.2.4) for any values of $\mathbb{C}$ and $\dot{\mathbb{C}}$ (which are independent when considered as "point values" in space and time):

$$\boxed{\left(\frac{\partial \hat{W}(\mathbb{C})}{\partial \mathbb{C}} - \frac{\mathbb{T}^{(2)}(\mathbb{C})}{2}\right) : \dot{\mathbb{C}} \leq 0 \qquad \forall \mathbb{C}, \dot{\mathbb{C}}} \ . \tag{6.3.1}$$

Since the arguments in the parenthesis do not depend on $\dot{\mathbb{C}}$, it must be identically zero (otherwise taking suitable $\dot{\mathbb{C}}$ would violate the inequality). So we arrive at

$$\mathbb{T}^{(2)} = 2\frac{\partial W}{\partial \mathbb{C}} \ , \tag{6.3.2}$$

which is a general expression relating (for a hyperelastic isotropic material) the second Piola-Kirchhoff stress with the free energy - we have derived this expression before. This time, we derived it from a thermodynamic framework - making use of the second law of thermodynamics. In terms of results, nothing new so far, merely a consistence with what we have done previously (which is also good). But now we will see that the form of entropy inequality and the framework of rational thermodynamics as outlined is particularly suitable for incorporating constraints.

Let us consider a general scalar constraint of the form $f(\mathbb{C}) = 0$ and take the following modification of the Clausius-Duhem inequaltity, which reflects, that the admissible processes now have to respect the constraint (it is a subset of the original set of processes):

$$\boxed{\left(\frac{\partial \hat{W}(\mathbb{C})}{\partial \mathbb{C}} - \frac{\mathbb{T}^{(2)}(\mathbb{C})}{2}\right) : \dot{\mathbb{C}} \leq 0 \qquad \forall \mathbb{C}, \dot{\mathbb{C}} \text{ such that } f(\mathbb{C}) = 0} \tag{6.3.3}$$

The question is, what can we say about the form of $\mathbb{T}^{(2)}$ now? The answer is provided by the following linear-algebraic theorem:

Theorem 6.3.1. *Let $\mathbb{A}$ be a given matrix (with dimension $n \times m$), column vectors $\mathbf{b}$ (dimension $n \times 1$) and $\boldsymbol{\alpha}$ (dimension $m \times 1$), β a scalar. Consider the following equality (E) and inequality (I):*

$$\begin{aligned} \mathbb{A}\mathbf{x} + \mathbf{b} &= \mathbf{0} \qquad (E)\,, \\ \boldsymbol{\alpha} \cdot \mathbf{x} + \beta &\leq 0 \qquad (I)\,, \end{aligned}$$

for unknown column vector $\mathbf{x}$ (dimension $m \times 1$). Assume that (E) has a non-empty solution set S. Then the following statements are equivalent:

i) For all $\mathbf{x} \in S$, the inequality (I) holds.

ii) There exists a vector $\boldsymbol{\lambda} \neq \mathbf{0}$ (dimension $n \times 1$) such that:

$$\begin{aligned} \boldsymbol{\alpha}^T - \boldsymbol{\lambda}^T \mathbb{A} &= \mathbf{0} \\ \beta - \boldsymbol{\lambda} \cdot \mathbf{b} &\leq 0\,. \end{aligned}$$

Proof. I will add it at some point if you are interested. □

How do we apply the theorem? Taking time derivative of the constraint $f(\mathbb{C}) = 0$ yields $\frac{\partial f}{\partial \mathbb{C}} : \dot{\mathbb{C}} = 0$, which is equivalent to the original constraint provided that $f(\mathbb{C})$ is satisfied some initial time. Assuming that, we can view the constrained Clausius-Duhem inequality as composed of:

$$\text{inequality} \qquad \underbrace{\left(\frac{\partial W}{\partial \mathbb{C}} - \frac{\mathbb{T}^{(2)}}{2}\right)}_{\boldsymbol{\alpha}} : \underbrace{\dot{\mathbb{C}}}_{\mathbf{x}} \leq 0 \qquad \text{(I)} \tag{6.3.4}$$

$$\text{and equality} \qquad \underbrace{\frac{\partial f}{\partial \mathbb{C}}}_{\mathbb{A}} : \underbrace{\dot{\mathbb{C}}}_{\mathbf{x}} = 0 \qquad \text{(E)}\,, \tag{6.3.5}$$

i.e. exactly the structure considered by the theorem, provided that we set $\mathbf{b} = \mathbf{0}$ and $\beta = 0$. Now the theorem claims that the constrained Clausius-Duhem inequality (6.3.3) is equivalent to the following statement:

There exists a non-zero scalar λ such that

$$\boxed{\frac{\partial W}{\partial \mathbb{C}} - \frac{\mathbb{T}^{(2)}}{2} = \lambda \frac{\partial f}{\partial \mathbb{C}}}\,. \tag{6.3.6}$$

Note: Why is λ a scalar? What is the dimension of our $\mathbb{A}$? It is one equation for 6 unknown components of $\dot{\mathbb{C}}$, so the dimensions are n=1 and m=6, so λ is a 1×1 vector, i.e. scalar.

Exercise 15. (Homework) Consider the classical incompressibility in the form

$$\det \mathbb{F} = 1\,,$$

and express it as $f(\mathbb{C}) = 0$ for a suitable f. Apply the theory above to derive the form of $\mathbb{T}^{(2)}$, $\mathbb{T}^{(1)}$ and also Cauchy stress $\mathbb{T}$ for an incompressible isotropic hyperelastic material characterized by a free energy $W(\mathbb{C})$. HINT, For $\mathbb{T}$, you should arrive at:

$$\mathbb{T} = p\mathbb{I} + 2\mathbb{F}\frac{\partial W}{\partial C}\mathbb{F}^T\,, \tag{6.3.7}$$

i.e. extension of the original compressible formula by an isotropic tensor of the form: "constraint pressure" p (some scalar) times the identity tensor.

Exercise 16. (Homework) Consider now a transversally anisotropic hyperelastic material as in the fourth exercise (with isotropy axis given by vectors ℓ), and consider a constraint of the form

$$f(\mathbb{C}) = \ell \cdot \mathbb{C}\ell - 1 .$$

Verify that such a constraint indeed represents inextensibility in the ℓ direction and write down the forms of $\mathbb{T}^{(2)}$, $\mathbb{T}^{(1)}$ and $\mathbb{T}$ for such a general material.

6.4 Several examples of incompressible hyperelastic materials

Many real-world hyperelastic materials are considered as incompressible. In that case the expression for the free energy W is typically much simpler than for the compressible variant for the model, but when using the model, one has to employ (6.3.7) when writing down the corresponding Cauchy stress (an analogously with other stress measures). Let us give several examples of some incompressible hyperelastic material models:

- **The incompressible Mooney-Rivlin model** - the free energy function reads

$$W(\mathbb{B}) = c_1(I_1(\mathbb{B})-3) + c_2(I_2(\mathbb{B}) - 3) , \tag{6.4.1}$$

  where c_1 and c_2 are constant parameters.

- **The incompressible neo-Hookean model** - the free energy function reads

$$W(\mathbb{B}) = c_1(I_1(\mathbb{B})-3) , \tag{6.4.2}$$

  where c_1 is a constant parameter.

- **The incompressible Ogden model** - the free energy function reads

$$W(\lambda_1, \lambda_2, \lambda_3) = \sum_{k=1}^{N} \frac{\mu_k}{\alpha_k} \left(\lambda_1^{\alpha_k} + \lambda_2^{\alpha_k} + \lambda_3^{\alpha_k} - 3 \right) , \tag{6.4.3}$$

  where α_k are real constants and μ_k are (constant) shear moduli and it holds

$$\lambda_1 \lambda_2 \lambda_3 = 1 . \tag{6.4.4}$$

- **The incompressible Varga model** - the free energy function reads

$$W(\lambda_1, \lambda_2, \lambda_3) = c_1(\lambda_1 + \lambda_2 + \lambda_3 - 3) , \tag{6.4.5}$$

  where c_1 is a parameter and it holds

$$\lambda_1 \lambda_2 \lambda_3 = 1 . \tag{6.4.6}$$