DE LA RECHERCHE À L'INDUSTRIE

A Simple Elasticity Model at Large Deformations or where does come from the Wilkins model?

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Outline

Context and motivations

Context

- Wilkins model [Wilkins (MCP, 1964)] is widely used for elastic-plastic flows
- Recent cell-centered discretizations have been proposed [Maire et al. (JCP, 2012)] and [Sambasivan et al. (JCP, 2013)]
- Construction of cell-centered schemes relies on
  - Geometric conservation law
  - Total energy conservation
  - Entropy inequality
- Three main issues with the Wilkins model [Plohr (LAUR05 5471, 2005)]
  - Lack of thermodynamic consistency
  - Choice of an objective stress rate to ensure frame indifference
  - Non conservative form of the constitutive equation for stress tensor

Motivations

- Description of the theoretical weaknesses of the Wilkins model
- Presentation of an alternative hyperelasticity-based Lagrangian approach
- Connection with the Wilkins model by means of a linearization procedure

Wilkins model [Wilkins (MCP, 1964)]

Elastic flow written in updated Lagrangian form

$$\rho \frac{d}{dt}(\frac{1}{\rho}) - \nabla \cdot \boldsymbol{V} = 0, \qquad \text{volume conservation}$$

$$\rho \frac{d\boldsymbol{V}}{dt} + \nabla p - \nabla \cdot \mathrm{T}_0 = \mathbf{0}, \qquad \text{momentum conservation}$$

$$\rho \frac{dE}{dt} + \nabla \cdot (p\boldsymbol{V}) - \nabla \cdot (\mathrm{T}_0 \boldsymbol{V}) = 0, \qquad \text{total energy conservation}$$

$\mathrm{T} = \mathrm{T}_0 - p\mathrm{I}_d$ is the Cauchy stress tensor, which is symmetric.

Constitutive laws

- Equation of state: $p = p(\rho, e)$, where e is the specific internal energy
- Decomposition of the velocity gradient: $\nabla \boldsymbol{V} = \mathrm{D} + \mathrm{W}$, where $\mathrm{D} = \mathrm{D}^t$ is the strain rate and $\mathrm{W}^t = -\mathrm{W}$ is the rotation rate
- Frame invariant rate form of the Hooke's law for T_0 (deviatoric stress)

$$\frac{d}{dt}\mathrm{T}_0 + \mathrm{T}_0\mathrm{W} - \mathrm{W}\mathrm{T}_0 = 2\mu \mathrm{D}_0, \quad \textbf{Jaumann rate}.$$

Here, $\mathrm{D}_0 = \mathrm{D} - \frac{1}{3}\,\mathrm{tr}(\mathrm{D})\mathrm{I}_d$ is the deviatoric strain rate.

Frame-indifference [Gurtin (Cambridge, 2010)]

Principle of frame-indifference

Constitutive equations must be invariant under changes of frame

Change of frame

$$\boldsymbol{x} \mapsto \boldsymbol{x}^\star = \mathrm{Q}(t)\boldsymbol{x} + \boldsymbol{y}(t),$$

where $\boldsymbol{y}$ is a spatial point and Q a rotation, *i.e.*, $\mathrm{Q}\mathrm{Q}^t = \mathrm{I}_d$ and $\det \mathrm{Q} = 1$.

Frame-indifferent fields

- Scalars are invariant and vectors transform as $\boldsymbol{g}^\star = \mathrm{Q}\boldsymbol{g}$
- Second-order tensors transform as $\mathrm{G}^\star = \mathrm{Q}\mathrm{G}\mathrm{Q}^t$

Transformation rules for kinematic fields

- Velocity $\boldsymbol{V}^\star = \mathrm{Q}\boldsymbol{V} + \frac{d}{dt}\mathrm{Q}\boldsymbol{x} + \frac{d\boldsymbol{y}}{dt}$
- Velocity gradient $(\nabla \boldsymbol{V})^\star = \mathrm{Q}(\nabla \boldsymbol{V})\mathrm{Q}^t + \frac{d\mathrm{Q}}{dt}\mathrm{Q}^t$
- Rotation rate of the new frame $\Phi = \frac{d\mathrm{Q}}{dt}\mathrm{Q}^t$ with $\Phi^t = -\Phi$
- Strain rate tensor $\mathrm{D}^\star = \mathrm{Q}\mathrm{D}\mathrm{Q}^t$ **is frame-indifferent**
- Rotation rate tensor $\mathrm{W}^\star = \mathrm{Q}\mathrm{W}\mathrm{Q}^t + \Phi$ is not frame-indifferent

Frame-indifference [Gurtin (Cambridge, 2010)]

Fundamental requirement

Constitutive equations, when expressed in rate form require a frame-indifferent or objective rate

Frame-indifferent rate

- Let G be a frame-indifferent tensor $G^\star = QGQ^t$
- Its material derivative is not frame-indifferent
$$\frac{dG^\star}{dt} = Q\frac{dG}{dt}Q + \Phi G^\star - G^\star\Phi, \quad \text{where } \Phi = \frac{dQ}{dt}Q^t.$$
- Recalling that $\Phi = W^\star - QWQ^t$ leads to
$$\frac{dG^\star}{dt} + G^\star W - WG^\star = Q(\frac{dG}{dt} + GW - WG)Q^t$$
- **The Jaumann rate**, $\overset{\triangledown}{G} = \frac{dG}{dt} + GW - WG$, is **frame-indifferent**
- Other frame-indifferent rates may be derived by adding $f(D, G)$, for instance, the Oldroyd rate, $\overset{\diamond}{G} = \frac{dG}{dt} - (\nabla \boldsymbol{V})G - (\nabla \boldsymbol{V})^t G$, is also frame-indifferent

Thermodynamic consistency [Gavrilyuk, JCP 2008]

Internal energy balance

- Total energy writes $E = e + e_e + \frac{1}{2}\boldsymbol{V}^2$
- Elastic energy is given by $e_e = \frac{1}{4\mu\rho}(\mathrm{T}_0 : \mathrm{T}_0)$, where $\mathrm{G} : \mathrm{H} = \mathrm{tr}(\mathrm{G}^t\mathrm{H})$
- Subtracting kinetic energy equation to total energy equation leads to

$$\rho\frac{d}{dt}(e + e_e) + p\,\mathrm{tr}(\mathrm{D}) - \mathrm{T}_0 : \mathrm{D} = 0.$$

Entropy balance

- Substituting the constitutive law into the above equation yields

$$\rho\frac{d}{dt}e + p\rho\frac{d}{dt}(\frac{1}{\rho}) = \frac{(\mathrm{T}_0 : \mathrm{T}_0)}{4\mu^2\rho}\frac{d}{dt}(\mu\rho).$$

- Time rate of change of entropy writes

$$\rho\theta\frac{d\eta}{dt} = \frac{(\mathrm{T}_0 : \mathrm{T}_0)}{4\mu^2\rho}\frac{d}{dt}(\mu\rho).$$

- **Wilkins model does not preserve entropy for smooth elastic flows.**

Kinematics of deformations [Gurtin, 2010]

Motion of a continuum body $\mathcal{B}$

- Let Ω be the reference configuration of $\mathcal{B}$ and $\boldsymbol{X} \in \mathcal{B}$ a **material** position
- The motion $\Phi_t : \Omega \longrightarrow \mathbb{R}^3$ is the smooth time-dependent map of Ω

$$\boldsymbol{X} \mapsto \boldsymbol{x} = \Phi_t(\boldsymbol{X}), \quad \boldsymbol{x} \text{ is the } \textbf{spatial} \text{ position of } \boldsymbol{X} \text{ at time } t$$

- The deformation gradient is $\mathsf{F} = \nabla_X \Phi_t = \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}}$ and $J = \det \mathsf{F} > 0$
- $\omega(t) = \Phi_t(\Omega)$ is the deformed configuration at time t
- The velocity field is given by $\boldsymbol{V} = \frac{\partial \Phi_t}{\partial t}$

Geometric properties of the deformation gradient

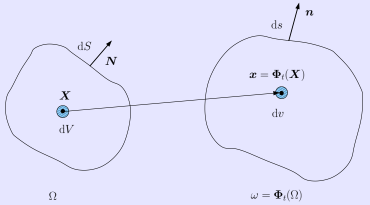
- The deformation of an infinitesimal fiber is characterized by $\mathrm{d}\boldsymbol{x} = \mathsf{F}\mathrm{d}\boldsymbol{X}$
- **The polar decomposition theorem** shows that $\mathsf{F} = \mathsf{R}\mathsf{U} = \mathsf{V}\mathsf{R}$, where R is a rotation and U, V are symmetric positive definite tensors
- Deformation measures which vanish when F is a rotation

$$\mid \mathrm{d}\boldsymbol{x} \mid^2 - \mid \mathrm{d}\boldsymbol{X} \mid^2 = (\mathsf{C} - \mathsf{I}_d)\mathrm{d}\boldsymbol{X} \cdot \mathrm{d}\boldsymbol{X}, \quad \mathsf{C} = \mathsf{F}^t\mathsf{F}, \text{ right Cauchy Green tensor}$$

$$\mid \mathrm{d}\boldsymbol{x} \mid^2 - \mid \mathrm{d}\boldsymbol{X} \mid^2 = (\mathsf{I}_d - \mathsf{B}^{-1})\mathrm{d}\boldsymbol{x} \cdot \mathrm{d}\boldsymbol{x}, \quad \mathsf{B} = \mathsf{F}\mathsf{F}^t, \text{ left Cauchy Green tensor}$$

From spatial to material representation

Material and spatial configurations



Transformation formulas

- For volume element

$$\mathrm{d}v = J\,\mathrm{d}V$$

- For surface element

$$\boldsymbol{n}\mathrm{d}s = J\mathsf{F}^{-t}\boldsymbol{N}\,\mathrm{d}S, \ \textbf{Nanson formula}$$

Divergence operator transformation

Employing divergence theorem and Nanson formula leads to

$$\nabla_x \cdot \mathsf{T} = J^{-1}\nabla_X \cdot (J\mathsf{T}\mathsf{F}^{-t})$$

Piola compatibility condition

The above formula for $\mathsf{T} = \mathsf{I}_d$ leads to the **Piola condition**

$$\nabla_X \cdot (J\mathsf{F}^{-t}) = 0$$

Geometrical interpretation: $\int_{\partial\omega(t)} \boldsymbol{n}\,\mathrm{d}s = \int_{\partial\Omega} J\mathsf{F}^{-t}\boldsymbol{N}\,\mathrm{d}S = \mathbf{0}$

Conservation laws for an isothermal solid

Spatial integral form

$$\frac{d}{dt}\int_{\omega(t)} \rho \,\mathrm{d}v = 0, \quad \text{mass conservation}$$

$$\frac{d}{dt}\int_{\omega(t)} \rho \boldsymbol{V} \,\mathrm{d}v - \int_{\partial\omega(t)} \mathsf{T}\boldsymbol{n} \,\mathrm{d}s = \boldsymbol{0}, \quad \text{momentum conservation}$$

$$\mathsf{T} = \mathsf{T}^t, \quad \text{angular momentum conservation.}$$

- Initial conditions: $\rho(\boldsymbol{x}, 0) = \rho^0(\boldsymbol{X})$ and $\boldsymbol{V}(\boldsymbol{x}, 0) = \boldsymbol{V}(\boldsymbol{X})^0$
- Boundary conditions: Let $\partial\omega = \partial\omega_k \cup \partial\omega_d$

$$\boldsymbol{V} = \boldsymbol{V}^\star \text{ for } \boldsymbol{x} \in \partial\omega_k, \quad \mathsf{T}\boldsymbol{n} = \boldsymbol{t}^\star \text{ for } \boldsymbol{x} \in \partial\omega_d$$

Free energy imbalance (thermodynamic-like inequality)

The specific free energy, ψ, satisfies

$$\frac{d}{dt}\int_{\omega(t)} \underbrace{\frac{1}{2}\rho \boldsymbol{V}^2 + \rho\psi \,\mathrm{d}v}_{\text{kinetic + free energy}} - \int_{\partial\omega(t)} \underbrace{\mathsf{T}\boldsymbol{n}\cdot\boldsymbol{V}}_{\text{external power}} \,\mathrm{d}s \le 0.$$

Spatial integral form

Balance of energy

Dot-multiplying the momentum equation by $\boldsymbol{V}$ and using the tensorial identity

$$\nabla \cdot (\mathsf{T}\boldsymbol{V}) = (\nabla \cdot \mathsf{T}^t) \cdot \boldsymbol{V} + \mathsf{T}^t : \nabla \boldsymbol{V}$$

leads to the balance equation

$$\frac{d}{dt} \int_{\omega(t)} \underbrace{\frac{1}{2}\rho \boldsymbol{V}^2 \,\mathrm{d}v}_{\text{kinetic energy}} + \int_{\omega(t)} \underbrace{\mathsf{T} : \nabla_x \boldsymbol{V}}_{\text{internal power}} \,\mathrm{d}v - \int_{\partial\omega(t)} \underbrace{\mathsf{T}\boldsymbol{n} \cdot \boldsymbol{V}}_{\text{external power}} \,\mathrm{d}s = 0.$$

Alertnative form of the free energy imbalance

Combining the free energy imbalance and the energy balance yields

$$\rho \frac{d}{dt}\psi - \mathsf{T} : \mathsf{D} \leq 0, \quad \text{where } \mathsf{D} = \frac{1}{2}[\nabla_x \boldsymbol{V} + (\nabla_x \boldsymbol{V})^t].$$

Constitutive law for the Cauchy stress shall be defined invoking

1. Material indifference principle
2. Thermodynamic consistency with the free energy imbalance

Material integral form

Conservation laws in material form

$$\frac{d}{dt}\int_\Omega \rho J \,\mathrm{d}V = 0, \quad \text{which under local form writes } \rho J = \rho^0$$

$$\frac{d}{dt}\int_\Omega \rho_0 \boldsymbol{V} \mathrm{d}V - \int_{\partial\Omega} J\mathsf{T}\mathsf{F}^{-t}\boldsymbol{N}\,\mathrm{d}S = \boldsymbol{0}, \quad \text{thanks to Nanson formula.}$$

First Piola Kirchhoff stress tensor

$$\mathsf{P} = J\mathsf{T}\mathsf{F}^{-t}$$

Note that P is not symmetric and we must enforce the angular momentum balance by imposing $\mathsf{P}\mathsf{F}^t = \mathsf{F}\mathsf{P}^t$.

Free energy imbalance

The material counterpart of the local free energy imbalance writes

$$\rho^0 \frac{\partial \psi}{\partial t} - \mathsf{P} : \nabla_X \boldsymbol{V} \leq 0.$$

We have also the integral form

$$\frac{d}{dt}\int_\Omega \rho^0 (\frac{1}{2}\boldsymbol{V}^2 + \psi)\,\mathrm{d}V - \int_{\partial\Omega} \mathsf{P}\boldsymbol{N} \cdot \boldsymbol{V} \mathrm{d}S \leq 0.$$

Material integral form

Evolution equation for F: Geometrical conservation law

The deformation gradient evolution is governed by

$$\frac{\partial \mathsf{F}}{\partial t} - \nabla_X \boldsymbol{V} = 0$$

This must be supplemented by the compatibility condition $\nabla_X \times \mathsf{F} = 0$ to ensure that F derives from a motion. This condition is an **involutive constraint which implies Piola condition.**

Power-conjugate pairings: Second Piola Kirchhoff stress tensor

Recalling that $\mathsf{T} : \mathsf{D}$ is the stress power per unit volume in the spatial configuration, it comes

$$\int_{\omega(t)} \mathsf{T} : \mathsf{D}\,\mathrm{d}v = \int_{\Omega} \mathsf{P} : \frac{\partial \mathsf{F}}{\partial t}\,\mathrm{d}V = \int_{\Omega} \mathsf{S} : \frac{1}{2}\frac{\partial \mathsf{C}}{\partial t}\,\mathrm{d}V, \text{ where } \mathsf{C} = \mathsf{F}^t\mathsf{F}.$$

Here, $\mathsf{S} = J\mathsf{F}^{-1}\mathsf{T}\mathsf{F}^{-t}$ is the **second Piola Kirchhoff stress tensor**, which is symmetric.

The proof relies on the fact that $\nabla_x \boldsymbol{V} = \frac{\partial \mathsf{F}}{\partial t}\mathsf{F}^{-1}$ and $\frac{\partial \mathsf{C}}{\partial t} = \frac{\partial \mathsf{F}^t}{\partial t}\mathsf{F} + \mathsf{F}^t\frac{\partial \mathsf{F}}{\partial t}$.

Material form

Summary of the model written under material form

- Geometric conservation law

$$\frac{\partial \mathsf{F}}{\partial t} - \nabla_X \boldsymbol{V} = 0, \quad \text{with } \nabla_X \times \mathsf{F} = 0.$$

- Balance laws

$$\rho J = \rho^0, \quad \rho^0 \frac{\partial}{\partial t} \boldsymbol{V} - \nabla_X \cdot \mathsf{P} = \mathbf{0}, \quad \mathsf{P}\mathsf{F}^t = \mathsf{F}\mathsf{P}^t.$$

- Free energy imbalance (dissipation inequality)

$$\rho^0 \frac{\partial \psi}{\partial t} - \mathsf{P} : \frac{\partial \mathsf{F}}{\partial t} \leq 0, \quad \rho^0 \frac{\partial \psi}{\partial t} - \frac{1}{2} \mathsf{S} : \frac{\partial \mathsf{C}}{\partial t} \leq 0.$$

Here, $\mathsf{C} = \mathsf{F}^t\mathsf{F}$ is the right Cauchy Green tensor, $\mathsf{P} = J\mathsf{T}\mathsf{F}^{-t}$ is the 1st P-K tensor and $\mathsf{S} = J\mathsf{F}\mathsf{T}\mathsf{F}^{-t}$ is the 2nd P-K tensor.

Constitutive law

Its remains to express the free energy and the stress in terms of a relevant deformation measure, invoking the frame-indifference and the thermodynamic consistency.

Constitutive theory

Elastic body

Analogy with classical mechanics where the force and the free energy within an elastic spring depend only on the change in length of the spring. In continuum mechanics, local length changes are characterized by the deformation gradient F. Thus, we define an elastic body through the constitutive equations

$$\psi = \psi(\mathsf{F}) \quad \text{and} \quad \mathsf{P} = \mathsf{P}(\mathsf{F})$$

Frame-indifference requirement

- Change of frame: $\boldsymbol{x} \mapsto \boldsymbol{x}^\star = \mathsf{Q}(t)\boldsymbol{x} + \boldsymbol{y}(t)$, where $\mathsf{Q}\mathsf{Q}^t = \mathsf{I}_d$ and $\det \mathsf{Q} = \mathsf{I}_d$
- Deformation gradient transforms according to $\mathsf{F}^\star = \mathsf{Q}\mathsf{F}$
- Free energy must satisfy $\psi(\mathsf{F}) = \psi(\mathsf{Q}\mathsf{F})$ for all rotations Q
- Using the polar decomposition $\mathsf{F} = \mathsf{R}\mathsf{U}$ and choose $\mathsf{Q} = \mathsf{R}$ yields

$$\psi(\mathsf{F}) = \psi(\mathsf{U}) = \psi(\sqrt{\mathsf{C}}) = \widetilde{\psi}(\mathsf{C})$$

- Stresses are characterized by $\mathsf{S} = \widetilde{\mathsf{S}}(\mathsf{C})$, $\mathsf{P} = \mathsf{F}\widetilde{\mathsf{S}}(\mathsf{C})$ and $\mathsf{T} = J^{-1}\mathsf{F}\widetilde{\mathsf{S}}(\mathsf{C})\mathsf{F}^t$
- Observe that $\mathsf{C} = \mathsf{C}^\star$ is an invariant measure of deformation

Constitutive theory

Thermodynamic restriction

- Substituting $\psi = \widetilde{\psi}(\mathsf{C})$ into the free energy imbalance, $\rho^0 \frac{\partial \psi}{\partial t} - \frac{1}{2}\mathsf{S} : \frac{\partial \mathsf{C}}{\partial t} \leq 0$, and knowing that $\frac{\partial \psi}{\partial t} = \frac{\partial \widetilde{\psi}}{\partial \mathsf{C}} : \frac{\partial \mathsf{C}}{\partial t}$ leads to

$$\mathsf{S} = 2\rho^0 \frac{\partial \widetilde{\psi}}{\partial \mathsf{C}}, \quad i.e., \quad \mathsf{S}_{ij} = 2\rho^0 \frac{\partial \widetilde{\psi}}{\partial \mathsf{C}_{ij}}$$

Materials consistent with this result are termed hyperelastic.

- 1st P-K and Cauchy stresses are given by

$$\mathsf{P} = 2\rho^0 \mathsf{F} \frac{\partial \widetilde{\psi}}{\partial \mathsf{C}}, \quad \mathsf{T} = 2\rho^0 J^{-1} \mathsf{F} \frac{\partial \widetilde{\psi}}{\partial \mathsf{C}} \mathsf{F}^t = 2\rho \mathsf{F} \frac{\partial \widetilde{\psi}}{\partial \mathsf{C}} \mathsf{F}^t.$$

Consequences on the dissipation

- For smooth constitutive processes the dissipation vanishes
- For non-smooth constitutive processes such as shock waves we have

$$\rho^0 \frac{\partial \psi}{\partial t} - \mathsf{P} : \frac{\partial \mathsf{F}}{\partial t} \leq 0,$$

since shock waves dissipate energy.

Constitutive theory

Isotropic material

An isotropic body is a body whose properties are the same in all directions. This means that the response function for the free energy is invariant for all rotation

$$\widetilde{\psi}(\mathrm{C}) = \widetilde{\psi}(\mathrm{Q}^t\mathrm{C}\mathrm{Q}), \quad \text{for all Q such that } \mathrm{Q}\mathrm{Q}^t = \mathrm{I}_d \text{ and } \det \mathrm{Q} = 1.$$

Using the polar decomposition $\mathrm{F} = \mathrm{R}\mathrm{U} = \mathrm{V}\mathrm{R}$ leads to $\mathrm{R}\mathrm{C}\mathrm{R}^t = \mathrm{B}$, where $\mathrm{B} = \mathrm{F}\mathrm{F}^t$ is the left Cauchy Green tensor. Thus, setting $\mathrm{Q} = \mathrm{R}^t$ in the above equation yields

$$\widetilde{\psi}(\mathrm{C}) = \widetilde{\psi}(\mathrm{B}).$$

Alternative form of the constitutive law using B

Substituting $\psi = \widetilde{\psi}(\mathrm{B})$ into the free energy imbalance, $\rho^0 \frac{\partial \psi}{\partial t} - \mathrm{P} : \frac{\partial \mathrm{F}}{\partial t} \leq 0$ leads to the following expression for the 1st P-K and Cauchy stress tensors

$$\mathrm{P} = 2\rho^0 \frac{\partial \widetilde{\psi}(\mathrm{B})}{\partial \mathrm{B}} \mathrm{F}, \quad \mathrm{T} = 2\rho \frac{\partial \widetilde{\psi}(\mathrm{B})}{\partial \mathrm{B}} \mathrm{B}.$$

Observe that T **depends uniquely on** B.

Constitutive theory

Free energy expressed in terms of invariants

The **representation theorem** [Gurtin (Cambridge, 2010)] asserts that an isotropic scalar function of a symmetric tensor B may be expressed as a function of its principal invariants

$$\psi = \hat{\psi}[I_1(\mathrm{B}), I_2(\mathrm{B}), I_3(\mathrm{B})], \text{ where } I_1 = \operatorname{tr}\mathrm{B},\; I_2 = \frac{1}{2}[\operatorname{tr}^2(\mathrm{B}) - \operatorname{tr}(\mathrm{B}^2)],\; I_3 = \det\mathrm{B}.$$

Expression of the Cauchy stress tensor in terms of invariants

The chain rule yields $\mathrm{T} = 2\rho(\sum_{i=1}^{3} \frac{\partial\hat{\psi}}{\partial I_i}\frac{\partial I_i}{\partial \mathrm{B}})\mathrm{B}$ knowing that

$$\frac{\partial I_1}{\partial \mathrm{B}} = \mathrm{I}_d,\;\; \frac{\partial I_2}{\partial \mathrm{B}} = I_1 \mathrm{I}_d - \mathrm{B} \;\text{ and }\; \frac{\partial I_3}{\partial \mathrm{B}} = I_3 \mathrm{B}^{-1}.$$

Finally, the Cauchy stress tensor writes

$$\mathrm{T} = 2\rho\left[I_3\frac{\partial\hat{\psi}}{\partial I_3}\mathrm{I}_d + \left(\frac{\partial\hat{\psi}}{\partial I_1} + I_1\frac{\partial\hat{\psi}}{\partial I_2}\right)\mathrm{B} - \frac{\partial\hat{\psi}}{\partial I_2}\mathrm{B}^2\right].$$

Isotropic elastic model in material form

Summary of the set of governing equations

- Geometric conservation law for the deformation gradient

$$\frac{\partial \mathrm{F}}{\partial t} - \nabla_X \boldsymbol{V} = 0, \quad \text{with the involutive constraint } \nabla_X \times \mathrm{F} = 0.$$

- Balance laws for mass and momentum

$$\rho J = \rho^0, \quad \rho^0 \frac{\partial}{\partial t} \boldsymbol{V} - \nabla_X \cdot \mathrm{P} = \mathbf{0}.$$

- Constitutive law for the free energy and the 1^{st} P-K stress tensor

$$\psi = \widetilde{\psi}(\mathrm{B}), \quad \mathrm{P} = 2\rho^0 \frac{\partial \widetilde{\psi}(\mathrm{B})}{\partial \mathrm{B}} \mathrm{F}, \quad \text{where } \mathrm{B} = \mathrm{F}\mathrm{F}^t.$$

- Thermodynamic-like dissipation inequality

$$\rho^0 \frac{\partial \widetilde{\psi}}{\partial t} - \mathrm{P} : \frac{\partial \mathrm{F}}{\partial t} \leq 0.$$

- Cell-centered discretization of a similar model in [Kluth, (JCP 2010)]

Isotropic elastic model in spatial form

Summary of the set of governing equations

- Balance laws for mass and momentum

$$(\text{since } \det \mathrm{B} = J^2),\ \rho\sqrt{\det \mathrm{B}} = \rho^0, \quad \rho \frac{d}{dt}\boldsymbol{V} - \nabla_x \cdot \mathrm{T} = \mathbf{0}.$$

- Constitutive law for the free energy and the Cauchy stress tensor

$$\psi = \widetilde{\psi}(\mathrm{B}), \quad \mathrm{T} = 2\rho \frac{\partial \widetilde{\psi}(\mathrm{B})}{\partial \mathrm{B}}\mathrm{B}, \quad \text{where } \mathrm{B} = \mathrm{F}\mathrm{F}^t.$$

- Thermodynamic-like dissipation inequality

$$\rho \frac{d\widetilde{\psi}}{dt} - \mathrm{T} : \mathrm{D} \leq 0, \quad \text{where } \mathrm{D} = \frac{1}{2}[\nabla_x \boldsymbol{V} + (\nabla_x \boldsymbol{V})^t].$$

Time rate of change of the left Cauchy Green tensor

Knowing that $\mathrm{B} = \mathrm{F}F^t$ and $\frac{\partial \mathrm{F}}{\partial t} = (\nabla_x \boldsymbol{V})\mathrm{F}$ leads to

$$\frac{d\mathrm{B}}{dt} - (\nabla_x \boldsymbol{V})\mathrm{B} - \mathrm{B}(\nabla_x \boldsymbol{V})^t = 0.$$

This is the Oldroyd rate (Lie derivative) of the left Cauchy Green tensor, which is frame-indifferent.

Links with the Wilkins model

Decomposition of the Cauchy stress tensor

- Isochoric and volumetric factors of the deformation gradient

$$\bar{\mathrm{F}} = J^{-\frac{1}{3}}\mathrm{F}\,\text{(isochoric since } \det \bar{\mathrm{F}} = 1), \quad \mathrm{F}^v = J^{\frac{1}{3}}\mathrm{I}d\,\text{(volumetric)}.$$

- Isochoric and volumetric factors of the left Cauchy Green tensor

$$\bar{\mathrm{B}} = J^{-\frac{2}{3}}\mathrm{B}\,\text{(isochoric since } \det \bar{\mathrm{B}} = 1), \quad \mathrm{B}^v = J^{\frac{2}{3}}\mathrm{I}d\,\text{(volumetric)}.$$

- Additive decomposition of the free energy

$$\psi = \bar{\psi}[I_1(\bar{\mathrm{B}}), I_2(\bar{\mathrm{B}})] + \psi^v(J),$$

where $I_1(\bar{\mathrm{B}}) = \operatorname{tr}\bar{\mathrm{B}}$ and $I_2(\bar{\mathrm{B}}) = \frac{1}{2}[\operatorname{tr}^2(\bar{\mathrm{B}}) - \operatorname{tr}\bar{\mathrm{B}}^2]$.

- Recalling that $\mathrm{T} = 2\rho\frac{\partial\psi(\mathrm{B})}{\partial\mathrm{B}}\mathrm{B}$, we finally obtain $\mathrm{T} = \mathrm{T}_0 - p\mathrm{I}_d$

$$p = -\rho^0\frac{d\psi^v}{dJ}, \quad \textbf{spherical component}$$

$$\mathrm{T}_0 = 2\rho\left\{\frac{\partial\bar{\psi}}{\partial I_1}\bar{\mathrm{B}}_0 + \frac{\partial\bar{\psi}}{\partial I_2}\left[\operatorname{tr}(\bar{\mathrm{B}})\bar{\mathrm{B}}_0 - (\bar{\mathrm{B}}^2)_0\right]\right\}, \quad \textbf{deviatoric component}.$$

Links with the Wilkins model

The Neo-Hookean model [Rivlin, 1948]

- Free energy is defined by

$$\psi = \frac{\mu}{2\rho^0}(\operatorname{tr}\bar{\mathrm{B}} - 3) + \frac{\kappa}{4\rho^0}\left[(J-1)^2 + \log^2 J\right], \quad \text{where } \bar{\mathrm{B}} = J^{-\frac{2}{3}}\mathrm{B},$$

  where μ is the shear modulus and κ the bulk modulus.

- Deviatoric Cauchy stress tensor writes

$$\mathrm{T}_0 = \mu J^{-1}\bar{\mathrm{B}}_0, \quad \text{where } \bar{\mathrm{B}}_0 = \bar{\mathrm{B}} - \frac{1}{3}\operatorname{tr}(\bar{\mathrm{B}})\mathrm{I}_d.$$

- Pressure is given by

$$p = -\frac{1}{2}\kappa(J - 1 + \frac{1}{J}\log J).$$

Links with the Wilkins model

Governing equations for the Neo-Hookean model

- Balance laws for mass and momentum

$$\rho\sqrt{\det \mathrm{B}} = \rho^0, \quad \rho\frac{d}{dt}\boldsymbol{V} + \nabla_x p - \nabla_x \cdot \mathrm{T}_0 = \mathbf{0}.$$

- Constitutive law for the pressure and the deviatoric stress

$$\mathrm{T}_0 = \mu J^{-1}\bar{\mathrm{B}}_0, \quad p = -\frac{1}{2}\kappa(J - 1 + \frac{1}{J}\log J).$$

- Thermodynamic-like dissipation inequality

$$\rho\frac{d\psi}{dt} - \mathrm{T} : \mathrm{D} \leq 0, \quad \text{where } \mathrm{D} = \frac{1}{2}[\nabla_x \boldsymbol{V} + (\nabla_x \boldsymbol{V})^t].$$

Evolution of the deviatoric left Cauchy Green tensor

Since $\bar{\mathrm{B}} = J^{-\frac{2}{3}}\mathrm{B}$, the evolution equation of B is equivalent to

$$\frac{d\bar{\mathrm{B}}}{dt} - (\nabla_x \boldsymbol{V})\bar{\mathrm{B}} - \bar{\mathrm{B}}(\nabla_x \boldsymbol{V})^t - \frac{2}{3}\mathrm{tr}(\mathrm{D})\bar{\mathrm{B}} = 0, \text{ and } \frac{dJ}{dt} - J\,\mathrm{tr}\,\mathrm{D} = 0.$$

Here, contrary to the Wilkins model, the proper variable for time integration of the constitutive law is the left Cauchy Green tensor.

Links with the Wilkins model

The small elastic strain case

Let us investigate the small strain limit assuming that the motion is such that F admits the following decomposition

$$\mathsf{F} = \alpha(\mathsf{I}_d + \mathsf{E})\mathsf{R}.$$

Here, $\alpha > 0$ characterizes the dilatational component of the motion, R is a rotation and E is symmetric and such that $\mid \mathsf{E} \mid \ll 1$, where $\mid \mathsf{E} \mid = \sqrt{\mathrm{tr}(\mathsf{E}^t\mathsf{E})}$. Employing this assumption leads to the following approximations

$$\mathsf{B} \approx \alpha^2(\mathsf{I}_d + 2\mathsf{E}),\ J \approx \alpha^3(1 + \mathrm{tr}\,\mathsf{E}),\ \bar{\mathsf{B}} \approx \mathsf{I}_d + 2\mathsf{E} \text{ and } \bar{\mathsf{B}}_0 \approx 2\mathsf{E}_0.$$

Limit of the left Cauchy Green tensor evolution equation

Employing the above approximations, the time rate of change of the deviatoric left Cauchy Green tensor turns into

$$\frac{d\mathsf{E}_0}{dt} - \mathsf{W}\mathsf{E}_0 + \mathsf{E}_0\mathsf{W} = \mathsf{D}_0 + \mathsf{D}_0\mathsf{E}_0 + \mathsf{E}_0\mathsf{D}_0.$$

We recover the **Jaumann derivative** of the elastic strain plus an extra term in the right-hand side.

Links with the Wilkins model

Order of magnitude of the extra term

- Recalling that $\mathsf{F} = \alpha(\mathsf{I}_d + \mathsf{E})\mathsf{R}$ with $\mid \mathsf{E} \mid \ll 1$ leads to
$$\nabla_x \boldsymbol{V} = \frac{d\mathsf{F}}{dt}\mathsf{F}^{-1} \approx \frac{d\alpha}{dt}\alpha^{-1} + \frac{d\mathsf{E}}{dt} + \Phi + \mathsf{E}\Phi - \Phi\mathsf{E}, \text{ where } \Phi = \frac{d\mathsf{R}}{dt}\mathsf{R}^t.$$
- The strain rate and the rotation rate small strain limits are given by
$$\mathsf{D} \approx \frac{d\alpha}{dt}\alpha^{-1}\mathsf{I}_d + \frac{d\mathsf{E}}{dt} + \mathsf{E}\Phi - \Phi\mathsf{E}, \text{ and } \mathsf{W} \approx \Phi.$$
- Therefore, the deviatoric strain rate and the extra term write
$$\mathsf{D}_0 \approx \frac{d\mathsf{E}_0}{dt} + \mathsf{E}_0\Phi - \Phi\mathsf{E}_0,$$
$$\mathsf{D}_0\mathsf{E}_0 + \mathsf{E}_0\mathsf{D}_0 \approx 2\mathsf{E}_0\frac{d\mathsf{E}_0}{dt} + \mathsf{E}_0^2\Phi - \Phi\mathsf{E}_0^2.$$

Limit of the left Cauchy Green tensor evolution equation

Provided that $\mid \mathsf{E} \mid \ll 1$ and $\mid \frac{d\mathsf{E}_0}{dt} \mid \ll 1$ the left Cauchy Green tensor evolution equation collapses to its **Jaumann derivative**.

Links with the Wilkins model

Neo-Hookean model in the small strain limit

- Balance laws for mass, Jacobian and momentum

$$\rho J = \rho^0, \quad \frac{dJ}{dt} - J \operatorname{tr} \mathrm{D} = 0, \quad \rho \frac{d}{dt}\boldsymbol{V} + \nabla_x p - \nabla_x \cdot \mathrm{T}_0 = \mathbf{0}.$$

- Constitutive law for the pressure and the deviatoric stress

$$J\mathrm{T}_0 = 2\mu \mathrm{E}_0, \quad p = -\frac{1}{2}\kappa(J - 1 + \frac{1}{J}\log J).$$

- Thermodynamic-like dissipation inequality

$$\rho\frac{d\psi}{dt} - \mathrm{T} : \mathrm{D} \leq 0, \quad \text{where } \mathrm{D} = \frac{1}{2}[\nabla_x \boldsymbol{V} + (\nabla_x \boldsymbol{V})^t].$$

Evolution equation for the small strain

Provided that $\mid \mathrm{E} \mid \ll 1$ and $\mid \frac{d\mathrm{E}_0}{dt} \mid \ll 1$

$$\frac{d\mathrm{E}_0}{dt} - \mathrm{W}\mathrm{E}_0 + \mathrm{E}_0\mathrm{W} = \mathrm{D}_0.$$

Here, evolution is written in terms of the elastic strain.

Conclusion and perspectives

A simple elasticity model at large deformations

- The model can be expressed in both material (Lagrangian) and spatial (Lagrangian updated) representation
- It relies on hyperelastic constitutive law
- The constitutive law satisfies the principle of material frame-indifference and is thermodynamically consistent
- The links with the Wilkins hypoelastic approach have been investigated under the small strain approximation

Perspectives

- Extension to thermoelasticity
- Extension to plasticity based on an additive decomposition of the strain rate [Volokh (EJM, 2013)]
- Lagrangian cell-centered discretization of the Lagrangian updated version of this model
- Comparison with the Wilkins model on relevant test cases