# On Classical and a Gradient Model of Finite Viscoplasticity

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# Outline

- **Phenomenological models with plastic flow co-axial with elastic stretch**
  - **General Theory**
  - **Finite Element Numerics**

- **Crystal Plasticity (with ‘Simple’ Gradient Hardening)**
  - **General Theory**
  - **Finite Element Numerics**
  - **Results**
    - **Polycrystal size effects**
    - **Cleavage of ductile materials**
    - **Orientation dependence of Fracture**

# Finite Phenomenological Viscoplasticity

- **Constitutive Description**
  - Elasticity – Isotropic Hyperelasticity
  - Rate Dependent
  - Strain Hardening
- **Finite Element Implementation**
  - Multiplicative Decomposition of Deformation Gradient
  - Plastic flow coaxial with elastic stretch
  - Rate-independent case is a trivial (one line) modification
  - Recovers fully-nonlinear hyperelastic response in the absence of inelasticity
  - Nonlinear Viscoelasticity is a straightforward modification

# Constitutive Model

| | |
|---|---|
| Multiplicative Decomposition | $\boldsymbol{F} = \boldsymbol{F}^{e}\boldsymbol{F}^{p}$ |
| Free Energy/vol | $\psi = \psi\left(\boldsymbol{C}^{e}\right)$ |
| Cauchy Stress | $\boldsymbol{T} = \boldsymbol{F}^{e}\dfrac{\partial\psi}{\partial\boldsymbol{C}^{e}}\boldsymbol{F}^{eT}$ |
| Flow-rule (*No plastic spin*) | $\boldsymbol{F}^{e}\dot{\boldsymbol{F}}^{p}\boldsymbol{F}^{p-1}\boldsymbol{F}^{e-1} = \dot{\gamma}\dfrac{\boldsymbol{T}^{dev}}{\left\Vert\boldsymbol{T}^{dev}\right\Vert}$ |
| Rate-Dependence | $\dot{\gamma} = p\left(\gamma,\sigma^{s}\right) \quad ; \quad \sigma^{s} = \left\Vert\boldsymbol{T}^{dev}\right\Vert / \sqrt{2}$ |

# Material Update

Kinematics

$$\text{for any } \boldsymbol{F}_{(\,)} \qquad \boldsymbol{C}_{(\,)} = \sum_A \left(\lambda^A_{(\,)}\right)^2 \boldsymbol{N}^A_{(\,)} \otimes \boldsymbol{N}^A_{(\,)} \quad ; \ \boldsymbol{n}^A_{(\,)} = \boldsymbol{F}_{(\,)} \boldsymbol{N}^A_{(\,)} / \lambda^A_{(\,)}$$

Isotropy

$$\boldsymbol{T} = \sum_A \sigma^A \boldsymbol{n}^A_e \otimes \boldsymbol{n}^A_e$$

Flow Rule

$$\boldsymbol{F}^e \dot{\boldsymbol{F}}^p \boldsymbol{F}^{p-1} \boldsymbol{F}^{e-1} = \frac{\dot{\gamma}}{\sqrt{2}\sigma^s} \sum_A S^A \boldsymbol{n}^A_e \otimes \boldsymbol{n}^A_e$$

$$\Rightarrow \dot{\boldsymbol{F}}^p = \frac{\dot{\gamma}}{\sqrt{2}\sigma^s} \left( \sum_A S^A \boldsymbol{N}^A_e \otimes \boldsymbol{N}^A_e \right) \boldsymbol{F}^p \quad ; \quad S^A := A^{th} \text{ e-value of } \boldsymbol{T}^{dev}$$

Discrete Update Formula

Weber & Anand, 1990

$$\boldsymbol{F}^p = \exp\left( \frac{\Delta\gamma}{\sqrt{2}\sigma^s} \sum_A S^A \boldsymbol{N}^A_e \otimes \boldsymbol{N}^A_e \right) \boldsymbol{F}^p_n \quad ; \quad \Delta\gamma = \dot{\gamma}\Delta t$$

$$\text{Note:} \quad \boldsymbol{F}^p_0 = \boldsymbol{I} \quad \Rightarrow \quad \det\left(\boldsymbol{F}^p\right) = 1$$

$$\text{since} \quad \det\left[\exp(\cdot)\right] = \exp\left(tr(\cdot)\right)$$

# Material Update

Elastic predictor

$$\boldsymbol{F}^e = \boldsymbol{F}\boldsymbol{F}^{p-1} = \boldsymbol{F}'\exp\left(\frac{-\Delta\gamma}{\sqrt{2}\sigma^s}\sum_A S^A \boldsymbol{N}_e^A \otimes \boldsymbol{N}_e^A\right) \quad ; \quad \boldsymbol{F}' = \boldsymbol{F}\boldsymbol{F}_n^{p-1}$$

$$\boldsymbol{R}^e\boldsymbol{U}^e \exp\left(\frac{\Delta\gamma}{\sqrt{2}\sigma^s}\sum_A S^A \boldsymbol{N}_e^A \otimes \boldsymbol{N}_e^A\right) = \boldsymbol{R}'\boldsymbol{U}'$$

Coaxiality and Uniqueness of Polar Decomposition

$$\boldsymbol{R}^e = \boldsymbol{R}' \quad ; \quad \boldsymbol{U}^e \exp\left(\frac{\Delta\gamma}{\sqrt{2}\sigma^s}\sum_A S^A \boldsymbol{N}_e^A \otimes \boldsymbol{N}_e^A\right) = \boldsymbol{U}'$$

$$\left.\begin{aligned} \lambda'^A &= \lambda_e^A \exp\left(S^A \frac{\Delta\gamma}{\sqrt{2}\sigma^s}\right) \\ \boldsymbol{N}'^A &= \boldsymbol{N}_e^A \end{aligned}\right\} \quad A = 1,2,3$$

# Update Equations

$$\varepsilon_e^A = \varepsilon'^A - \Delta\gamma \frac{S^A(\varepsilon_e)}{\sqrt{2}\sigma^s(S)} \qquad \varepsilon = \ln(\lambda)$$

$$\Delta\gamma = p(\gamma_n + \Delta\gamma, \sigma^s)\Delta t$$

$$\boldsymbol{F}^p = \exp\left(\frac{\Delta\gamma}{\sqrt{2}\sigma^s}\sum_A S^A \boldsymbol{N}'^A \otimes \boldsymbol{N}'^A\right)\boldsymbol{F}_n^p$$

$$\boldsymbol{U}^e = \sum_A \lambda_e^A \boldsymbol{N}'^A \otimes \boldsymbol{N}'^A$$

# Linearization of Virtual Work

$$R = \int_V \boldsymbol{T} : \delta \boldsymbol{L}\, dv = \int_{V_0} \boldsymbol{\tau} : \delta \boldsymbol{L}\, dv_0 \quad ; \quad \delta \boldsymbol{L} := \frac{\partial \delta \boldsymbol{x}}{\partial \boldsymbol{x}}$$

$$dR = \int_{V_0} d\boldsymbol{\tau} : \delta \boldsymbol{L}\, dv_0 + \int_V \boldsymbol{T} : d\delta \boldsymbol{L}\, dv$$

$$d\boldsymbol{\tau} = \sum_A d\tau^A \boldsymbol{n}_e^A \otimes \boldsymbol{n}_e^A + \sum_A \tau^A d\left(\boldsymbol{n}_e^A \otimes \boldsymbol{n}_e^A\right)$$

$$= \sum_A d\tau^A \boldsymbol{n}'^A \otimes \boldsymbol{n}'^A + \boldsymbol{F}' \left\{ \sum_A d\left( \frac{\boldsymbol{N}'^A \otimes \boldsymbol{N}'^A}{\mu'^A} \right) \right\} \boldsymbol{F}'^T + d\boldsymbol{L}\boldsymbol{\tau} + \boldsymbol{\tau}\, d\boldsymbol{L} \quad ; \quad \mu'^A = \left(\lambda'^A\right)^2$$

# Linearization: Geometric Stiffness (3 distinct e-values of Predictor Stretch)

Serrin, Cayley-Hamilton, Characteristic Equation:

(Simo, 1991)

$$\boldsymbol{F}'\left\{\sum_A d\left(\frac{\boldsymbol{N}'^A\otimes\boldsymbol{N}'^A}{\mu'^A}\right)\right\}\boldsymbol{F}'^T=\sum_A\frac{2\tau^A}{D'^A}\begin{bmatrix}\boldsymbol{II}_{B'}-\boldsymbol{B}'\otimes\boldsymbol{B}'+\dfrac{I_3'}{\mu_A'}\left(\boldsymbol{I}\otimes\boldsymbol{I}-\boldsymbol{II}\right)\\+\mu_A'\left(\boldsymbol{B}'\otimes\boldsymbol{m}'^A+\boldsymbol{m}'^A\otimes\boldsymbol{B}'\right)\\+\left(I_1'\mu_A'-4\mu_A'^2+I_3'\mu_A'^{-1}\right)\boldsymbol{m}'^A\otimes\boldsymbol{m}'^A\\-\dfrac{I'}{\mu_A'}\left(\boldsymbol{I}\otimes\boldsymbol{m}'^A+\boldsymbol{m}'^A\otimes\boldsymbol{I}\right)\end{bmatrix}:d\boldsymbol{D}$$

$$\boldsymbol{m}'^A:=\boldsymbol{n}'^A\otimes\boldsymbol{n}'^A$$

$$D'^A:=\left[\mu'^A-\mu'^{A+1}\right]\left[\mu'^A-\mu'^{A+2}\right]$$

symmetric

# Linearization: Material Stiffness
# (3 disinct e-values of Predictor Stretch)

$$\sum_{A} \delta \boldsymbol{D} : \boldsymbol{n}'^{A} \otimes \boldsymbol{n}'^{A} d\tau^{A} = \delta \boldsymbol{D} : \left[ \sum_{A} \sum_{B} \left( \boldsymbol{n}'^{A} \otimes \boldsymbol{n}'^{A} \right) H^{A}_{B} \left( \boldsymbol{n}'^{B} \otimes \boldsymbol{n}'^{B} \right) \right] : d\boldsymbol{D}$$

$$H := \left[ A^{B}_{A} + \frac{\Delta\gamma}{\sqrt{2}\tau^{s}} \left( \delta^{B}_{A} - \frac{1}{3} i^{A} i^{B} - \frac{1}{2} \left\{ 1 + \frac{\kappa}{\Delta\gamma J \tau^{s}} \right\} \tau^{d\,A} \tau^{d\,B} \right) + \frac{\kappa \sigma_{s} \tau^{d\,B}}{\sqrt{2}\tau^{s}} \sum_{C} A^{C}_{A} \right]^{-1}$$

Asymmetry due to Cauchy stress in flow rule

$$\kappa := \frac{\Delta t \partial_{\sigma^{s}} p}{\left( 1 - \Delta t \partial_{\gamma} p \right)} \qquad recall \quad \dot{\gamma} = p\left( \gamma, \sigma^{s} \right)$$

$$A := \left[ \frac{\partial \tau^{A}}{\partial \varepsilon^{B}} \right]^{-1}$$

← Nonlinear elasticity (symmetric)

$$i := (1,1,1) \quad ; \quad \tau^{s} = \left\| \tau^{dev} \right\| / \sqrt{2} \quad ; \quad \tau^{d\,A} = A^{th} \text{ e-value of } \tau^{dev}$$

If $\boldsymbol{F}^{p}$ in flow-rule (e.g. viscoelasticity) then additional asymmetry

# Linearization:
# Coalescence of e-values of Predictor Stretch

- **Geometric Stiffness is ‘highly’ singular in case of 1 or 2 repeated eigenvalues of the Predictor Stretch tensor**

- **These are not exceptional deformation states (e.g. the undeformed state)**

- **Perturbation of distinct e-value results (as suggested in Simo, 1990) does not work**

- **Need separate limit expressions**

# Linearization:
# Three repeated e-values of Predictor Stretch

- **Finite incremental response is completely elastic**
  - **i.e.** $\boldsymbol{F}^e = \boldsymbol{F}'$

- **'Approximation' (perhaps exact!)**

$$d\boldsymbol{\tau} = \left\{ B_{diag} - B_{off-diag} \right\} d\boldsymbol{D} + B_{off-diag}\, tr\left( d\boldsymbol{D} \right) \boldsymbol{I} \;\; ; \;\; B = \left[ \frac{\partial \tau^A}{\partial \varepsilon_e^B} \right]$$

Carlson & Hoger, 1986

# Linearization: 2 distinct e-values of Predictor Stretch

- Material Stiffness from expression for 3 distinct evalues case

- Use results from Hill (1978) for Lagrangian spin to derive singularity-free "limit" of geometric stiffness
  - Quadratic convergence up to $10^{-9}$ (nondimensional) for residual
  - Residual can be taken down to zero up to round-off
  - Expression involves non-unique e-vectors and principal dyads