1 REDBACK mechanics

1.1 Introduction

This document aims at describing the underlying structure of the mechanics implementation of REDBACK, which is built on top of MOOSE's TensorMechanics module. The current implementation of the FiniteStrainHyperElasticViscoPlastic material is using a finite strain formulation, which makes it helpful to document some definitions, link between variables in the code and mathematical variables, as well as some of the derivations used. See the related wiki page. As that page mentions, the two main references used are:

(Belytschko et al., 2014) for the Hyperelastic Viscoplastic J2 model;

(Ling et al., 2005) for the integration algorithm.

1.2 Symbols

Tab. 1.1 lists some of the main symbols used in this document. Equations from (Belytschko et al., 2014) are referred to as (B x.y.z)

Table 1.1: List of main symbols

Symbol	Name	Variable	Comment
σ	Cauchy stress	??	
σ'	Deviatoric stress	??	
σ_e	Effective stress	??	
C	right Cauchy–Green deformation tensor	??	$C = F^T . F = U.U$
\bar{C}^e	elastic right Cauchy–Green deformation tensor	_ce	$\bar{C}^e = F_e^T . F_e (B 5.7.3)$
	in intermediate configuration		
D	Rate of deformation tensor	??	$D = \frac{1}{2}(L + L^{T}) = F^{-T}.\dot{E}.F^{-1}$
E	Green-Lagrange strain	??	$E = \frac{1}{2}(F^T . F - I)$
\bar{E}^e	Elastic Green-Lagrange strain	_ee	$\bar{E}^e = \frac{1}{2}(\bar{C}^e - I)$
F	Deformation gradient	_deformation gradient	$F = \tilde{F^e}F^p$
F^e, F^p	elastic, plastic part of F	_fe, _fp	
J	Jacobian determinant	??	J = det(F)
L	Velocity gradient	??	$L = D + W = \dot{F}.F^{-1}$
S	2 nd Piola–Kirchhoff stress	pk2	$S = JF^{-1}\sigma F^{-T}$
S'	Deviatoric Piola–Kirchhoff stress	pk2_dev	$S' = JF^{-1}\sigma'F^{-T}$
T	Temperature	??	
W	Spin tensor	??	$W = \frac{1}{2}(L - L^T)$
p_f	Pore pressure	??	-

1.3 Piola-Kirchhoff stress

We use the convention that stresses are positive in tension. Using the finite strain formulation, the stress is expressed using the 2nd Piola–Kirchhoff stress tensor S, which is related to the Cauchy stress tensor σ by the relationship

$$S = JF^{-1}\sigma F^{-T} \tag{1.1}$$

where F is the deformation gradient and J = det(F) the Jacobian determinant. The deformation gradient can itself be decomposed in elastic (F^e) and plastic (F^p) components (Belytschko et al., 2014)

$$F = F^e F^p \tag{1.2}$$

1.3.1 Deviatoric stress

The deviatoric stress σ' is defined as

$$\sigma = \sigma' + pI \tag{1.3}$$

where the pressure p is defined as $p = \frac{Tr(\sigma)}{3}$ and I represents the identity.

Note that Belytschko defines the pressure as $p = -\frac{Tr(\sigma)}{3}$ (B 3.4.4), opposite of hydrostatic, so the deviatoric is $\sigma^{dev} = \sigma + pI$ (B 4.5.26)

The corresponding formulation for the 2nd Piola–Kirchhoff stress is

$$S' = JF^{-1}\sigma'F^{-T} \tag{1.4}$$

$$p = \frac{Tr(\sigma)}{3} = \frac{Tr\left(\frac{1}{J}FSF^{T}\right)}{3}$$

$$= \frac{1}{3J}Tr\left(F^{T}FS\right) \text{ since the trace is invariant under cyclic permutations}$$

$$= \frac{1}{3J}S:C \tag{1.5}$$

from the definition of the right Cauchy–Green deformation tensor $C = F^T F$. From Eq. (1.3) we get

$$S = S' + pJ F^{-1}F^{-T}$$

= S' + pJ C^{-1} (1.6)

Belytschko et al. (2014) uses the terms deviatoric and hydrostatic (opposite of his pressure). The hydrostatic component S^{hyd} can then be written (B 5.4.17a) as

$$S^{hyd} = pJ C^{-1} = (\frac{1}{3J} S : C)J C^{-1}$$
$$= \frac{1}{3}(S : C) C^{-1}$$
(1.7)

Note that HEVPFlowRatePowerLawJ2::computePK2Deviatoric uses the formula (B 5.7.39) from (Belytschko et al., 2014), in which the values are considered in the intermediate configuration

$$\bar{S}^{dev} = \bar{S} - \frac{1}{3}(\bar{S} : \bar{C}^e)\bar{C}^{e-1}$$
 (1.8)

1.3.2 von Mises effective stress

Using the relationship $A: B = Tr(AB^T)$, we note that

$$S': C = Tr(S'C^T) = Tr(S'C)$$

$$= Tr(JF^{-1}\sigma'F^{-T}F^TF)$$

$$= JTr(FF^{-1}\sigma') \quad \text{(trace invariance by permutation)}$$

$$= JTr(\sigma')$$

$$= 0 \tag{1.9}$$

The effective stress σ_e can be expressed as

$$\sigma_{e} = \sqrt{\frac{3}{2}} \sigma' : \sigma'$$

$$= \sqrt{\frac{3}{2}} Tr(\sigma'\sigma') \quad (\sigma' \text{ symmetric})$$

$$= \sqrt{\frac{3}{2}} Tr\left(\frac{1}{J}FS'F^{T}\frac{1}{J}FS'F^{T}\right)$$

$$= \frac{1}{J}\sqrt{\frac{3}{2}} Tr(FS'CS'F^{T})$$

$$= \frac{1}{J}\sqrt{\frac{3}{2}} Tr(S'CS'C) \quad (\text{trace invariance by permutation})$$

$$= \frac{1}{J}\sqrt{\frac{3}{2}} (S'C) : (S'C)^{T} \qquad (1.10)$$

Belytschko et al. (2014) is defining the von Mises effective stress $\bar{\sigma}$ (in the intermediate configuration) as (B 5.7.41)

$$\bar{\sigma}^2 = \frac{3}{2} \left(\bar{S}^{dev}.\bar{C}^e \right) : \left(\bar{S}^{dev}.\bar{C}^e \right)^T \tag{1.11}$$

Why is the 1/J different? Is Eq.1.4 correct?

as expressed in HEVPFlowRatePowerLawJ2::computeEqvStress.

1.3.3 Flow law – power law

Belytschko et al. (2014) defines the plastic flow rule, which determines \dot{F}^p , in the intermediate configuration (B 5.7.15).

$$\bar{L}^p = \dot{\lambda}\bar{r}(\bar{S}, \bar{q}) \tag{1.12}$$

where \bar{L}^p is the plastic velocity gradient (see B 5.7.9), \bar{r} is the plastic flow direction, $\dot{\lambda}$ is the plastic rate parameter and \bar{q} is a set of internal variables.

The UserObject HEVPFlowRatePowerLawJ2::computeValue implements a power law of the form

$$\dot{\epsilon_{eq}} = \dot{\epsilon_0} \left(\frac{\sigma_e}{\sigma_s} \right)^m \tag{1.13}$$

where σ_s is the strength, itself a UserObject (to handle dependency on ϵ_{eq}^p for example). The function HEVPFlowRatePowerLawJ2::computeDerivative computes the derivatives of ϵ_{eq} with respect to other scalar parameters. In practice, it deals only with the

strength σ_s

$$\frac{\partial \dot{\epsilon_{eq}}}{\partial \sigma_s} = -\frac{\dot{\epsilon_0}}{\sigma_s} m \left(\frac{\sigma_e}{\sigma_s}\right)^m \tag{1.14}$$

The function HEVPFlowRatePowerLawJ2::computeTensorDerivative computes the derivatives of ϵ_{eq} with respect to tensor parameters. In practice, it deals only with the 2nd Piola–Kirchhoff stress.

which
stress exactly?...

$$\frac{\partial \dot{\epsilon_{eq}}}{\partial \bar{S}_{ij}} = \frac{\partial \dot{\epsilon_{eq}}}{\partial \sigma_e} \frac{\partial \bar{S}_{kl}^{dev}}{\partial \bar{S}_{ij}}^T \frac{\partial \sigma_e}{\partial \bar{S}_{kl}^{dev}}??? \tag{1.15}$$

TODO: derive that term...

1.3.4 Flow direction – J2 plasticity

For a J2 yield criterion, the (associated) flow potential is

$$f(\sigma) = \sigma_e - Y \tag{1.16}$$

The flow direction $\vec{n} = \frac{\partial f}{\partial \sigma}$ is computed as follows, (switching to indices notation for the derivation)

$$\vec{n}_{ij} = \frac{\partial \left(\sqrt{\frac{3}{2}}\sigma'_{kl}\sigma'_{kl} - Y\right)}{\partial \sigma_{ij}}$$

$$= \frac{3}{2\sigma_e}\sigma'_{kl}\frac{\partial \sigma'_{kl}}{\partial \sigma_{ij}}$$

$$= \frac{3}{2\sigma_e}\sigma'_{kl}\left(\delta_{ik}\delta_{jl} - \frac{1}{3}\delta_{kl}\delta_{ij}\right)$$

$$= \frac{3}{2\sigma_e}\left(\sigma'_{ij} - \frac{1}{3}\sigma'_{kk}\delta_{ij}\right)$$

$$= \frac{3\sigma'_{ij}}{2\sigma_e} \quad \text{(since } \sigma'_{kk} = 0\text{)}$$

$$(1.17)$$

Using Eq. (1.4) we obtain

$$\vec{n} = \frac{3}{2 J \sigma_e} F S' F^T \tag{1.18}$$

Belytschko et al. (2014) defines the flow direction (B 5.7.40) as

$$\vec{n} = sym(\bar{r}) = \frac{3}{2\bar{\sigma}_e} \bar{C}^e.\bar{S}^{dev}.\bar{C}^e$$
(1.19)

as expressed in HEVPFlowRatePowerLawJ2::computeDirection.

$$\begin{split} \vec{n}_{ij} &= \frac{\partial \left(\sqrt{\frac{3}{2}} \left(\bar{S}^{dev}.\bar{C}^e \right)_{kl} \left(\bar{S}^{dev}.\bar{C}^e \right)_{lk} - Y \right)}{\partial \bar{S}_{ij}} \\ &= \frac{\partial \left(\sqrt{\frac{3}{2}} \left(\bar{S}^{dev}.\bar{C}^e \right)_{kl} \left(\bar{S}^{dev}.\bar{C}^e \right)_{lk} \right)}{\partial \bar{S}^{dev}} \frac{\partial \bar{S}^{dev}_{ij}}{\partial \bar{S}_{ij}} \\ &= \frac{\partial \left(\sqrt{\frac{3}{2}} \left(\bar{S}^{dev}.\bar{C}^e \right)_{kl} \left(\bar{S}^{dev}.\bar{C}^e \right)_{lk} \right)}{\partial \bar{S}^{dev}} \quad \text{(since } \frac{\partial \bar{S}^{dev}_{ij}}{\partial \bar{S}_{ij}} = 1 \text{)} \\ &= \frac{3}{4\bar{\sigma}_e} \frac{\partial \left[\left(\bar{S}^{dev}.\bar{C}^e \right)_{kl} \left(\bar{S}^{dev}.\bar{C}^e \right)_{lk} \right]}{\partial \bar{S}^{dev}} \\ &= \frac{3}{4\bar{\sigma}_e} \left[\frac{\partial \left(\bar{S}^{dev}.\bar{C}^e \right)_{kl} \left(\bar{S}^{dev}.\bar{C}^e \right)_{lk} + \left(\bar{S}^{dev}.\bar{C}^e \right)_{kl} \frac{\partial \left(\bar{S}^{dev}.\bar{C}^e \right)_{lk} }{\partial \bar{S}^{dev}} \right] \\ &= \frac{3}{4\bar{\sigma}_e} \left[\frac{\partial \left(\bar{S}^{dev}.\bar{C}^e \right)_{kl} \left(\bar{S}^{dev}.\bar{C}^e \right)_{lk} + \left(\bar{S}^{dev}.\bar{C}^e \right)_{kl} \frac{\partial \left(\bar{S}^{dev}.\bar{C}^e \right)_{lk} }{\partial \bar{S}^{dev}} \right] \\ &= \frac{3}{4\bar{\sigma}_e} \left[\bar{C}^e_{jl} \left(\bar{S}^{dev}.\bar{C}^e \right)_{li} + \left(\bar{S}^{dev}.\bar{C}^e \right)_{ki} \bar{C}^e_{jk} \right] \\ &= \frac{3}{4\bar{\sigma}_e} \left[2 \left(\bar{C}^e.\bar{S}^{dev}.\bar{C}^e \right)_{ji} \right] \\ &= \frac{3}{4\bar{\sigma}_e} \left[\bar{C}^e_{il}.\bar{S}^{dev}.\bar{C}^e \right)_{ij} \quad \text{(by symmetry)} \end{aligned}$$

Bibliography

- T. Belytschko, W.K. Liu, B. Moran, K. Elkhodary, Nonlinear Finite Elements for Continua and Structures. No Longer used (Wiley, ???, 2014). ISBN 9781118632703. https://books.google.com.au/books?id=BQpfAQAAQBAJ
- D. Gaston, C. Newman, G. Hansen, D. Lebrun-Grandi, Moose: A parallel computational framework for coupled systems of nonlinear equations. Nuclear Engineering and Design **239**(10), 1768–1778 (2009). doi:10.1016/j.nucengdes.2009.05.021
- X. Ling, M.F. Horstemeyer, G.P. Potirniche, On the numerical implementation of 3d rate-dependent single crystal plasticity formulations. International Journal for Numerical Methods in Engineering 63(4), 548–568 (2005). doi:10.1002/nme.1289