Stabilized Mixed Finite Element Formulation

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Definitions

F: Deformation gradient
I: second-order unit tensor
$\boldsymbol{u}$: Displacement
J: determinant of the deformation gradient
C: Right Cauchy-Green Strain Tensor
$\mathcal{W}(\mathbf{F})$: strain energy function
P: first Piola-Kirchhoff stress tensor
S: second PK stress tensor

α: cracks are represented by a scalar phase-field variable
p: Lagrange multiplier, hydrostatic pressure field
κ: bulk modulus

$$\kappa = \frac{E}{3(1-2\nu)} \tag{0.1}$$

μ: shear modulus

$$\mu = \frac{E}{2(1+\nu)} \tag{0.2}$$

λ: Lamé modulus

$$\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)} \tag{0.3}$$

For Plane Stress

$$\kappa = \frac{3-\nu}{1+\nu}, \quad \lambda = \frac{E\nu}{(1-\nu)^2} \tag{0.4}$$

$\mathcal{E}_\ell$: potential energy functional
$a(\alpha)$ is the decreasing stiffness modulation function
$w(\alpha)$ is an increasing function representing the specific energy dissipation per unit of volume
c_w is a normalization constant

1 Hyperelastic Phase-Field Fracture Models

Deformation Gradient

$$\mathbf{F} = \mathbf{I} + \nabla \otimes \boldsymbol{u} \tag{1.1}$$

where $J = \det \mathbf{F}$ and $\mathbf{C} = \mathbf{F}^T\mathbf{F}$.

The strain energy function $\mathcal{W}(\mathbf{F})$ is defined per unit reference volume such that the first PK and second PK

$$\mathbf{P} = \frac{\partial \mathcal{W}(\mathbf{F})}{\partial \mathbf{F}} \tag{1.2a}$$

$$\mathbf{S} = 2\frac{\partial \mathcal{W}(\mathbf{F})}{\partial \mathbf{C}} \tag{1.2b}$$

where $\mathbf{P} = \mathbf{F}\mathbf{S}$.

Non-modified strain energy function is the compressible Neo-Hookean:

$$\mathcal{W}(\mathbf{F}) = \frac{\mu}{2}(I_1 - 3 - 2\ln J) \tag{1.3}$$

For incompressible hyperelastic materials, the strain energy function is defined using the Lagrangian formulation

$$\widetilde{\mathcal{W}}(\mathbf{F}) = \mathcal{W}(\mathbf{F}) + p\,(J-1)\,, \tag{1.4}$$

If we consider the perturbed lagrangian formulation

$$\widetilde{\mathcal{W}}(\mathbf{F}) = \mathcal{W}(\mathbf{F}) + p\,(J-1) - \frac{p^2}{2\kappa}, \tag{1.5}$$

Decreasing stiffness modulation function is $a(\alpha)$ and $w(\alpha)$ is an increasing function representing the specific energy dissipation per unit of volume

$$a(\alpha) = (1-\alpha)^2 \quad w(\alpha) = \alpha \tag{1.6}$$

In the code, we have the following definition

$$b(\alpha) = (1-\alpha)^3 = \sqrt{a^3(\alpha)}$$

The normalization constant is defined as:

$$c_w = \int_0^1 \sqrt{w(\alpha)}d\alpha \tag{1.7}$$

1.1 Derivation from 2020 Li and Bouklas Paper

Here, unlike Eq. 21 from Bin2020, we drop λ_b which is not a consideration in this formulation

$$\mathcal{E}_\ell(\boldsymbol{u}, \alpha) = \int_\Omega a(\alpha)\mathcal{W}(\mathbf{F}, \alpha)d\Omega + \frac{G_c}{c_w}\int_\Omega \left(\frac{w(\alpha)}{\ell} + \ell\|\nabla\alpha\|^2\right)d\Omega \tag{1.8}$$

We want to enforce the following relationship for pressure with a Lagrange multiplier

$$p = -\sqrt{a^3(\alpha)}\kappa\,(J-1) \tag{1.9}$$

Giving us Eq. 25 in the 2020 Li and Bouklas paper where κ is the bulk modulus

$$\mathcal{E}_\ell\left(\boldsymbol{u}, p, \Lambda, \alpha\right) = \mathcal{E}_\ell(\boldsymbol{u}, \alpha) + \int_\Omega \frac{p^2}{2\kappa}d\Omega + \int_\Omega \Lambda(p + \sqrt{a^3(\alpha)}\kappa(J-1))d\Omega \tag{1.10}$$

Identify the stationary point of the energy functional with respect to pressure (not Λ)

$$\frac{\partial \mathcal{E}_\ell}{\partial p} = \int_\Omega \frac{p}{\kappa} d\Omega + \int_\Omega \Lambda d\Omega$$
$$0 = \frac{p}{\kappa} + \Lambda \rightarrow \Lambda = -p/\kappa$$

Substituting this relationship into the energy functional yields:

$$\begin{aligned}
\mathcal{E}_\ell\left(\boldsymbol{u}, p, \alpha\right) &= \mathcal{E}_\ell(\boldsymbol{u}, \alpha) + \int_\Omega \frac{p^2}{2\kappa} d\Omega + \int_\Omega -\frac{p}{\kappa}(p + \sqrt{a^3(\alpha)}\kappa(J-1))d\Omega \\
&= \mathcal{E}_\ell(\boldsymbol{u}, \alpha) + \int_\Omega \frac{p^2}{2\kappa} d\Omega - \int_\Omega \frac{p^2}{\kappa} d\Omega - \int_\Omega \frac{p}{\kappa}\sqrt{a^3(\alpha)}\kappa(J-1))d\Omega \qquad (1.11) \\
\mathcal{E}_\ell\left(\boldsymbol{u}, p, \alpha\right) &= \mathcal{E}_\ell(\boldsymbol{u}, \alpha) - \int_\Omega \frac{p^2}{2\kappa} d\Omega - \int_\Omega \sqrt{a^3(\alpha)}p(J-1))d\Omega
\end{aligned}$$

Substitute in $\mathcal{E}_\ell(\boldsymbol{u}, \alpha)$ and substitute Eq. 1.3

$$\mathcal{E}_\ell\left(\boldsymbol{u}, p, \alpha\right) = \int_\Omega a(\alpha)\mathcal{W}(\mathbf{F}) d\Omega + \frac{G_c}{c_w}\int_\Omega \left(\frac{w(\alpha)}{\ell} + \ell\|\nabla\alpha\|^2\right) d\Omega - \int_\Omega \frac{p^2}{2\kappa} d\Omega - \int_\Omega \sqrt{a^3(\alpha)}p(J-1)d\Omega$$

The prior equation includes the full weak form, unless we want to consider linear interpolation of all fields. In that case, we can introduce the stabilization term

$$-\frac{\varpi h^2}{2\mu}\sqrt{a^3(\alpha)}\sum_{e=1}^{n_{el}}\int_{\Omega^e} J\mathbf{C}^{-1} : \left(\nabla p \cdot \nabla q\right) dV = 0$$

1.2 Summary

Therefore the modified strain energy functional

$$\widetilde{W}(\mathbf{F}, \alpha) = a(\alpha)\mathcal{W}(\mathbf{F}) + a^3(\alpha)\kappa(J-1)^2 - \frac{p^2}{2\kappa}$$
$$\widetilde{W}(\mathbf{F}, \alpha) = a(\alpha)\mathcal{W}(\mathbf{F}) - \sqrt{a^3(\alpha)}p(J-1) - \frac{p^2}{2\kappa}$$

Following the code, we have a small number for numerical purposes

$$\widetilde{W}(\mathbf{F}, \alpha) = \left(a(\alpha) + k_\ell\right)\frac{\mu}{2}(I_c - 3 - 2\ln J) - b(\alpha)p(J-1) - \frac{p^2}{2\kappa}$$

The first Piola-Kirchhoff stress tensor is given:

$$\begin{aligned}
\mathbf{P} &= \frac{\partial \widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{\partial \mathbf{F}} \\
&= \frac{\partial}{\partial \mathbf{F}}\left[a(\alpha)\mathcal{W}(\mathbf{F}) + a^3(\alpha)\frac{1}{2}\kappa\left(J-1\right)^2\right] \\
&= a(\alpha)\frac{\partial \mathcal{W}(\mathbf{F})}{\partial \mathbf{F}} + a^3(\alpha)\frac{1}{2}\kappa\frac{\partial (J-1)^2}{\partial \mathbf{F}} \qquad (1.12) \\
&= a(\alpha)\frac{\partial \mathcal{W}(\mathbf{F})}{\partial \mathbf{F}} + a^3(\alpha)\kappa\left(J-1\right)\frac{\partial J}{\partial \mathbf{F}} \quad \text{where } \frac{\partial J}{\partial \mathbf{F}} = J\mathbf{F}^{-T} \\
&= a(\alpha)\frac{\partial \mathcal{W}(\mathbf{F})}{\partial \mathbf{F}} + a^3(\alpha)\kappa(J-1)J\mathbf{F}^{-T} \quad \text{substituting in pressure equation} \\
\mathbf{P} &= a(\alpha)\mu(\mathbf{F} - \mathbf{F}^{-T}) - b(\alpha)pJ\mathbf{F}^{-T}
\end{aligned}$$

1.3 Changes for 2D Plane-Stress Models

Recalling the 1st PK stress in Eq. 1.12.

$$\mathbf{P} = a(\alpha)\mu(\mathbf{F} - \mathbf{F}^{-T}) - b(\alpha)pJ\mathbf{F}^{-T}$$

In a plane-stress case, the $\mathbf{P_{33}}$ component is zero:

$$P_{33} = a(\alpha)\mu(F_{33} - F_{33}^{-1}) - b(\alpha)pJF_{33}^{-1} = 0$$

This can be multiplied by its associated test function to obtain the weak form

$$\int_\Omega \left(a(\alpha)\mu(F_{33} - F_{33}^{-1}) - b(\alpha)pJF_{33}^{-1} \right) v_{F_{33}} dV = 0$$

In the FEniCS code, we expand the solution space to include displacement, pressure, and a component of the deformation gradient $\mathbf{F_{33}}$. Therefore, we include a change to the invariants of the deformation tensors:

```
J = det(F)*F33
Ic = tr(C) + F33**2
```

Together with the weak form from above:

```
F_u = derivative(elastic_potential, w_p, v_q) \
      + (a(alpha)*mu*(F33 - 1/F33) - b(alpha)*p*J/F33)*v_F33*dx
```

1.3.1 Changes for 2D Discrete Crack Model

If we are considering a discrete fracture method

$$\mathcal{E}_\ell\left(\boldsymbol{u}, p, \alpha\right) = \int_\Omega a(\alpha)\mathcal{W}(\mathbf{F})d\Omega + \frac{G_c}{c_w}\int_\Omega \left(\frac{w(\alpha)}{\ell} + \ell\|\nabla\alpha\|^2\right)d\Omega - \int_\Omega \frac{p^2}{2\kappa}d\Omega - \int_\Omega \sqrt{a^3(\alpha)}p(J-1)d\Omega$$
$$\mathcal{E}_\ell\left(\boldsymbol{u}, p, \alpha\right) = \int_\Omega \mathcal{W}(\mathbf{F})d\Omega - \int_\Omega \frac{p^2}{2\kappa}d\Omega - \int_\Omega p(J-1)d\Omega$$

where we have assumed for the energy functional

$$\widetilde{\mathcal{W}}(\mathbf{F}, \alpha) = \frac{\mu}{2}(I_c - 3 - 2\ln J) - p(J-1) - \frac{p^2}{2\lambda}$$

Therefore, we can calculate the 1st Piola Kirchoff Stress as:

$$\begin{aligned} \mathbf{P} &= \frac{\mu}{2}(2\mathbf{F} - \frac{2}{J}J\mathbf{F}^{-T}) - pJ\mathbf{F}^{-T} \\ &= \mu(\mathbf{F} - \mathbf{F}^{-T}) - pJ\mathbf{F}^{-T} \end{aligned}$$

Taking the third component to be zero

$$\begin{aligned} P_{33} &= \mu(F_{33} - F_{33}^{-1}) - pJF_{33}^{-1} = 0 \\ &= F_{33} - F_{33}^{-1} - \frac{pJ}{\mu}F_{33}^{-1} = 0 \\ P_{33} &= F_{33}^2 - 1 - \frac{pJ}{\mu} = 0 \end{aligned}$$

with the stabilization term and plane stress in the weak form

$$
\begin{aligned}
-\frac{\varpi h^2}{2\mu}\int_\Omega J\mathbf{C}^{-1} : \big(\nabla p \cdot \nabla q\big)\, dV = 0 \\
\int_\Omega \left(\mathbf{F}_{33}^2 - 1 - \frac{pJ}{\mu}\right) v_{F_{33}} dV = 0
\end{aligned}
$$

1.3.2 Changes for 2D displacement formulation

Removing pressure terms

$$
\begin{aligned}
\mathcal{E}_\ell\left(\boldsymbol{u}, p, \alpha\right) &= \int_\Omega a(\alpha)\mathcal{W}(\mathbf{F})d\Omega + \frac{G_c}{c_w}\int_\Omega \left(\frac{w(\alpha)}{\ell} + \ell\|\nabla\alpha\|^2\right) d\Omega - \int_\Omega \frac{p^2}{2\kappa} d\Omega - \int_\Omega \sqrt{a^3(\alpha)}p(J-1)d\Omega \\
\mathcal{E}_\ell\left(\boldsymbol{u}, p, \alpha\right) &= \int_\Omega a(\alpha)\mathcal{W}(\mathbf{F})d\Omega + \frac{G_c}{c_w}\int_\Omega \left(\frac{w(\alpha)}{\ell} + \ell\|\nabla\alpha\|^2\right) d\Omega
\end{aligned}
$$

with plane stress in the weak form (no need for stabilization terms)

$$
\int_\Omega \big(a(\alpha)\mu(F_{33} - F_{33}^{-1})\big) v_{F_{33}} dV = 0
$$

We have assumed the modified energy functional

$$
\widetilde{W}(\mathbf{F}, \alpha) = a(\alpha)\frac{\mu}{2}(I_c - 3 - 2\ln J) \tag{1.13}
$$

Therefore, we can calculate the 1st Piola Kirchoff Stress as:

$$
\begin{aligned}
\mathbf{P} &= a(\alpha)\frac{\mu}{2}(2\mathbf{F} - \frac{2}{J}J\mathbf{F}^{-T}) \\
&= a(\alpha)\mu(\mathbf{F} - \mathbf{F}^{-T})
\end{aligned}
$$

Taking the third component to be zero

$$
P_{33} = a(\alpha)\mu(F_{33} - F_{33}^{-1}) = 0
$$

2 Obtaining the Critical Stretch

Assuming a Neo-Hookean energy where μ is the shear modulus

$$
\begin{aligned}
W(I_1, I_2) &= \beta_1(I_1 - 3) + \beta_2(I_2 - 3) \quad \text{where } \beta_1 = \frac{\mu}{2},\ \beta_2 = 0 \\
W(I_1, I_2) &= \frac{\mu}{2}(I_1 - 3) \quad \text{where } I_1 = I_2 = \lambda_A^2 + \lambda_A^{-2} + 1 \\
W(I_1, I_2) &= \frac{\mu}{2}\left(\lambda_A^2 + \frac{1}{\lambda_A^2} - 2\right) \\
W(I_1, I_2) &= \frac{\mu}{2}\left(\lambda_A - \frac{1}{\lambda_A}\right)^2
\end{aligned}
$$

The J-integral for a pure shear strip geometry can be calculated as:

$$
\begin{aligned}
J &= 2h_0 W(I_1, I_2) \\
J &= h_0 \mu \left(\lambda_A - \frac{1}{\lambda_A} \right)^2
\end{aligned}
$$

where for the stretch:

$$
\lambda_A = 1 + \frac{\Delta}{h_0}
$$

where the total height of the strip is $2h_0$ and Δ is the loading

Theoretically the criticial fracture energy is equivalent to the energy release rate

$$
G_c = J
$$

In order to obtain the critical stretch of a particular specimen in Krishnan 2008, we can equate our dissipated energy or critical fracture energy density

$$
\int_\Gamma G_c \, d\mathbf{S} = \frac{G_c}{c_w} \int_\Omega \left(\frac{w(\alpha)}{\ell} + \ell \|\nabla \alpha\|^2 \right) d\Omega
$$

3 Strain energy decomposition

The Heaviside function is defined as

$$
H(x) = \frac{x + |x|}{2x} = \begin{cases} 1, & x \geq 0, \\ 0, & x < 0 \end{cases}
$$

The Macaulay bracket is defined

$$
M(x) = \frac{x + |x|}{2} = \begin{cases} x, & x \geq 0, \\ 0, & x < 0 \end{cases}
$$

3.1 Following Ye 2020 and Tang 2019

In the Ye 2020 paper, the internal energy is expressed as:

$$
W_{int}(\mathbf{F}, \alpha, \nabla \alpha) = [a(\alpha) + k_\ell] W_{act} + W_{pas} + G_c \left(\frac{\alpha^2}{2\ell} + \frac{\ell}{2} |\nabla \alpha|^2 \right)
$$

Now in section 3.2.3 of Ye 2020, is stated the decomposition for a Mooney Rivlin constitutive law:

$$
\begin{aligned}
W_{MR}(I_1, I_2) &= C_1(I_1 - 3) + C_2(I_2 - 3) \\
W_{MR}(\lambda_1, \lambda_1, \lambda_3) &= C_1(\lambda_1^2 + \lambda_2^2 + \lambda_3^2 - 3) + C_2(\lambda_1^{-2} + \lambda_2^{-2} + \lambda_3^{-2} - 3) \\
&= C_1 \sum_{i=1}^{3} (\lambda_i^2 - 1) + C_2 \sum_{i=1}^{3} (\lambda_i^{-2} - 1)
\end{aligned}
$$

Which can be decomposed to active and passive internal energy terms. First we can rewrite:

$$
\begin{aligned}
W_{MR}(\lambda_1, \lambda_1, \lambda_3) = C_1 \sum_{i=1}^{3} H(\lambda_i - 1)(\lambda_i^2 - 1) + C_2 \sum_{i=1}^{3} H(\lambda_i - 1)(\lambda_i^{-2} - 1) \\
+ C_1 \sum_{i=1}^{3} H(1 - \lambda_i)(\lambda_i^2 - 1) + C_2 \sum_{i=1}^{3} H(1 - \lambda_i)(\lambda_i^{-2} - 1)
\end{aligned}
$$

The active and passive terms can be stated as follows where the active part represents the crack-driven energy.

$$
\begin{aligned}
W_{act} &= C_1 \sum_{i=1}^{3} H(\lambda_i - 1)(\lambda_i^2 - 1) + C_2 \sum_{i=1}^{3} H(\lambda_i - 1)(\lambda_i^{-2} - 1) \\
W_{pas} &= C_1 \sum_{i=1}^{3} H(1 - \lambda_i)(\lambda_i^2 - 1) + C_2 \sum_{i=1}^{3} H(1 - \lambda_i)(\lambda_i^{-2} - 1)
\end{aligned}
$$

One way to better understand these is to consider some cases 1) triaxial tension $\lambda_i > 1$ 2) other stress states where $\lambda_i < 1$:

$$
\begin{aligned}
&\text{For } \lambda_i > 1: \\
&\qquad W_{act} = C_1 \sum_{i=1}^{3} (\lambda_i^2 - 1) + C_2 \sum_{i=1}^{3} (\lambda_i^{-2} - 1) \\
&\qquad W_{pas} = 0 \\
&\text{For } \lambda_i < 1: \\
&\qquad W_{act} = 0 \\
&\qquad W_{pas} = C_1 \sum_{i=1}^{3} (\lambda_i^2 - 1) + C_2 \sum_{i=1}^{3} (\lambda_i^{-2} - 1)
\end{aligned}
$$

For this second case, we end up with a negative energy component (first term of the passive energy).

We can also note the definitions within Tang 2019 for Model M_I. In this model, we consider the free energy density of a neo-Hookean constitutive law:

$$
W(\mathbf{F}) = \frac{\mu}{2}(I_1 - 3 - 2\ln J) + \frac{\kappa}{2}(\ln J)^2
$$

which can also be rephrased in terms of stretches

$$
\begin{aligned}
W(\lambda_1, \lambda_2, \lambda_3) &= W_1 + W_2 \\
&= \frac{\mu}{2} \sum_{i=1}^{3} (\lambda_i^2 - 1 - 2\ln \lambda_i) + \frac{\kappa}{2}(\ln J)^2
\end{aligned}
$$

where we note that W_1 is a linear function of $\ln \lambda_i$ and W_2 is a nonlinear function of $\ln J$
The free energy is stated as

$$
G_{rub} = [(1 - K)\alpha^2 + K]W^+ + W^-
$$

Note that K is not κ. No definition is provided in the paper. This is another way of coupling the damage to the free energy density, and I believe we can rewrite our own version where:

$$G_{rub} = [a(\alpha) + k_\ell]W^+ + W^-$$

Now we turn to the definition of W^+ and W^- which refers to the energy with tensile stretching

$$W^+ = W(\lambda_i^+, J^+) = \frac{\mu}{2}\sum_{i=1}^{3}((\lambda_i^+)^2 - 1 - 2\ln\lambda_i^+) + \frac{\kappa}{2}(\ln J^+)^2$$

and the energy with compression respectively.

$$W^- = W(\lambda_i^-, J^-) = \frac{\mu}{2}\sum_{i=1}^{3}((\lambda_i^-)^2 - 1 - 2\ln\lambda_i^-) + \frac{\kappa}{2}(\ln J^-)^2$$

The definitions for these superscript + and - terms gives us

$$\lambda_i^+ = \begin{cases}\lambda_i, & \lambda_i > 1,\\ 1, & \lambda_i \le 1\end{cases} \qquad J^+ = \begin{cases}J, & J > 1,\\ 1, & J \le 1\end{cases}$$
$$\lambda_i^- = \begin{cases}\lambda_i, & \lambda_i < 1,\\ 1, & \lambda_i \ge 1\end{cases} \qquad J^- = \begin{cases}J, & J < 1,\\ 1, & J \ge 1\end{cases}$$

This isn't the definition for the heaviside function, but it could be a shifted Macaulay bracket

$$M_s(x) = \frac{x - 1 + |x-1|}{2} + 1 = \begin{cases}x, & x > 1,\\ 1, & x \le 1\end{cases}$$

Now we can consider some examples.

$$\begin{aligned}
&\text{For } J > 1:\\
&\qquad W^+ = \frac{\mu}{2}\sum_{i=1}^{3}((\lambda_i^+)^2 - 1 - 2\ln\lambda_i^+) + \frac{\kappa}{2}(\ln J)^2\\
&\qquad W^- = \frac{\mu}{2}\sum_{i=1}^{3}((\lambda_i^-)^2 - 1 - 2\ln\lambda_i^-)\\
&\text{For } J < 1:\\
&\qquad W^+ = \frac{\mu}{2}\sum_{i=1}^{3}((\lambda_i^+)^2 - 1 - 2\ln\lambda_i^+)\\
&\qquad W^- = \frac{\mu}{2}\sum_{i=1}^{3}((\lambda_i^-)^2 - 1 - 2\ln\lambda_i^-) + \frac{\kappa}{2}(\ln J)^2
\end{aligned}$$

If we consider the same stress states as in Ye2020, 1) triaxial tension $\lambda_i > 1$ 2) all other stress states $\lambda_i < 1$:

$$
\begin{aligned}
&\text{For } J > 1,\ \lambda_i > 1: \\
&\qquad W^+ = \frac{\mu}{2}\sum_{i=1}^{3}(\lambda_i^2 - 1 - 2\ln\lambda_i) + \frac{\kappa}{2}(\ln J)^2 \\
&\qquad W^- = 0 \\
&\text{For } J < 1,\ \lambda_i > 1: \\
&\qquad W^+ = \frac{\mu}{2}\sum_{i=1}^{3}(\lambda_i^2 - 1 - 2\ln\lambda_i) \\
&\qquad W^- = \frac{\kappa}{2}(\ln J)^2
\end{aligned}
$$

Now for all other stress states:

$$
\begin{aligned}
&\text{For } J > 1,\ \lambda_i < 1: \\
&\qquad W^+ = \frac{\kappa}{2}(\ln J)^2 \\
&\qquad W^- = \frac{\mu}{2}\sum_{i=1}^{3}(\lambda_i^2 - 1 - 2\ln\lambda_i) \\
&\text{For } J < 1,\ \lambda_i < 1: \\
&\qquad W^+ = 0 \\
&\qquad W^- = \frac{\mu}{2}\sum_{i=1}^{3}(\lambda_i^2 - 1 - 2\ln\lambda_i) + \frac{\kappa}{2}(\ln J)^2
\end{aligned}
$$

This should be roughly equivalent to the considerations in the Ye2020 paper.

3.2 Our strain energy decomposition

Following the section above, we can consider our modified strain energy

$$
\begin{aligned}
\widetilde{W}(\mathbf{F},\alpha) &= a(\alpha)\frac{\mu}{2}(I_c - 3 - 2\ln J) - b(\alpha)p(J-1) - \frac{p^2}{2\kappa} \quad \text{where } p = -b(\alpha)\kappa(J-1) \\
\widetilde{W}(\mathbf{F},\alpha) &= a(\alpha)\frac{\mu}{2}(I_c - 3 - 2\ln J) + \frac{\kappa}{2}a(\alpha)^3(J-1)^2
\end{aligned}
$$

We can also rewrite the first term with regards to stretches

$$
\widetilde{W}(\mathbf{F},\alpha) = a(\alpha)\frac{\mu}{2}\sum_{i=1}^{3}(\lambda_i^2 - 1 - 2\ln\lambda_i) + \frac{\kappa}{2}a(\alpha)^3(J-1)^2
$$

Following Tang 2019 we rewrite the strain energy as

$$
\widetilde{W}(\mathbf{F},\alpha) = \widetilde{W}_{\text{act}}(\mathbf{F},\alpha) + \widetilde{W}_{\text{pas}}(\mathbf{F},\alpha) \tag{3.1}
$$

where the active and passive parts of the strain energy can be written as:

$$\widetilde{W}_{act}(\mathbf{F},\alpha) = a(\alpha)\frac{\mu}{2}\sum_{i=1}^{3}((\lambda_i^+)^2 - 1 - 2\ln\lambda_i^+) + \frac{\kappa}{2}a(\alpha)^3(J^+ - 1)^2$$

$$\widetilde{W}_{pas}(\mathbf{F},\alpha) = a(\alpha)\frac{\mu}{2}\sum_{i=1}^{3}((\lambda_i^-)^2 - 1 - 2\ln\lambda_i^-) + \frac{\kappa}{2}a(\alpha)^3(J^- - 1)^2$$

where the definitions of the superscript + and - terms remain the same as in Tang2020:

$$\begin{aligned}
&\text{For } J > 1: \\
&\qquad \widetilde{W}_{act}(\mathbf{F},\alpha) = a(\alpha)\frac{\mu}{2}\sum_{i=1}^{3}((\lambda_i^+)^2 - 1 - 2\ln\lambda_i^+) + \frac{\kappa}{2}a(\alpha)^3(J - 1)^2 \\
&\qquad \widetilde{W}_{pas}(\mathbf{F},\alpha) = a(\alpha)\frac{\mu}{2}\sum_{i=1}^{3}((\lambda_i^-)^2 - 1 - 2\ln\lambda_i^-) \\
&\text{For } J \leq 1: \\
&\qquad \widetilde{W}_{act}(\mathbf{F},\alpha) = a(\alpha)\frac{\mu}{2}\sum_{i=1}^{3}((\lambda_i^+)^2 - 1 - 2\ln\lambda_i^+) \\
&\qquad \widetilde{W}_{pas}(\mathbf{F},\alpha) = a(\alpha)\frac{\mu}{2}\sum_{i=1}^{3}((\lambda_i^-)^2 - 1 - 2\ln\lambda_i^-) + \frac{\kappa}{2}a(\alpha)^3(J - 1)^2
\end{aligned} \tag{3.2}$$

Now considering the same two cases of, triaxial tension and

$$\begin{aligned}
&\text{For } J > 1,\ \lambda_i > 1: \\
&\qquad \widetilde{W}_{act}(\mathbf{F},\alpha) = a(\alpha)\frac{\mu}{2}\sum_{i=1}^{3}(\lambda_i^2 - 1 - 2\ln\lambda_i) + \frac{\kappa}{2}a(\alpha)^3(J - 1)^2 \\
&\qquad \widetilde{W}_{pas}(\mathbf{F},\alpha) = 0 \\
&\text{For } J \leq 1,\ \lambda_i > 1: \\
&\qquad \widetilde{W}_{act}(\mathbf{F},\alpha) = a(\alpha)\frac{\mu}{2}\sum_{i=1}^{3}(\lambda_i^2 - 1 - 2\ln\lambda_i) \\
&\qquad \widetilde{W}_{pas}(\mathbf{F},\alpha) = \frac{\kappa}{2}a(\alpha)^3(J - 1)^2
\end{aligned}$$

all other cases:

$$\begin{aligned}
&\text{For } J > 1,\ \lambda_i < 1: \\
&\qquad \widetilde{W}_{act}(\mathbf{F},\alpha) = \frac{\kappa}{2}a(\alpha)^3(J - 1)^2 \\
&\qquad \widetilde{W}_{pas}(\mathbf{F},\alpha) = a(\alpha)\frac{\mu}{2}\sum_{i=1}^{3}(\lambda_i^2 - 1 - 2\ln\lambda_i) \\
&\text{For } J \leq 1,\ \lambda_i < 1: \\
&\qquad \widetilde{W}_{act}(\mathbf{F},\alpha) = 0 \\
&\qquad \widetilde{W}_{pas}(\mathbf{F},\alpha) = a(\alpha)\frac{\mu}{2}\sum_{i=1}^{3}(\lambda_i^2 - 1 - 2\ln\lambda_i) + \frac{\kappa}{2}a(\alpha)^3(J - 1)^2
\end{aligned}$$

These can be concisely summarized with the following expressions, where the active part of the strain energy is

$$\widetilde{W}_{\text{act}}\left(\mathbf{F},\alpha\right) = a(\alpha)\frac{\mu}{2}\sum_{i=1}^{3} H(\lambda_i - 1)\left(\lambda_i^2 - 1 - 2\ln\lambda_i\right) + a^3(\alpha)H(J-1)\frac{1}{2}\kappa\left(J-1\right)^2, \tag{3.3}$$

and the passive part of the strain energy is

$$\widetilde{W}_{\text{pas}}\left(\mathbf{F},\alpha\right) = a(\alpha)\frac{\mu}{2}\sum_{i=1}^{3} H(1-\lambda_i)\left(\lambda_i^2 - 1 - 2\ln\lambda_i\right) + a^3(\alpha)H(1-J)\frac{1}{2}\kappa\left(J-1\right)^2, \tag{3.4}$$

3.2.1 Compute the principal stretches λ_i

The eigenvalues of Cauchy-Green strain tensor $\mathbf{C}$ are λ_i^2, $i = 1, 2, 3$. With following definitions

$$d = \frac{Tr\mathbf{C}}{3}, \quad e = \sqrt{\frac{Tr(\mathbf{C} - d\mathbf{I})^2}{6}}, \quad f = \frac{1}{e}\left(\mathbf{C} - d\mathbf{I}\right), \quad g = \frac{\det f}{2}, \tag{3.5}$$

and assuming the eigenvalues satisfying $\lambda_3^2 \leq \lambda_2 \leq \lambda_1$, we could obtain (**?**)

$$\lambda_1^2 = d + 2e\cos\left(\frac{\arccos g}{3}\right), \quad \lambda_3^2 = d + 2e\cos\left(\frac{\arccos g}{3} + \frac{2\pi}{3}\right), \quad \lambda_2^2 = 3d - \lambda_1^2 - \lambda_3^3. \tag{3.6}$$

3.3 Hybrid Formulation

The principal stretches can be computed as shown above, but for spherical stretch ($\mathbf{C} = constant\mathbf{I}$) leading to NaN error. This means that for 3D strain decomposition using the explicit eigenvalue formulation, the computation of the first variation and second variation are nontrivial. FEniCS auto-differential function cannot detect these special cases.

The workaround is to consider the Hybrid model in Ambati 2015: A review on phase-field models of brittle fracture and a new fast hybrid formulation.

$$\sigma(\mathbf{u},\alpha) = (1-\alpha)^2\frac{\partial W(\epsilon)}{\partial\epsilon}$$
$$-l^2\nabla^2\alpha + \alpha = \frac{2l}{G_c}(1-\alpha)\mathcal{H}^+$$

Again, we consider our modified strain energy

$$\widetilde{W}(\mathbf{F},\alpha) = a(\alpha)\frac{\mu}{2}(I_c - 3 - 2\ln J) + \frac{\kappa}{2}a(\alpha)^3(J-1)^2$$

Then the active and

$$\widetilde{W}_{\text{act}}\left(\mathbf{F},\alpha\right) = a(\alpha)\frac{\mu}{2}\sum_{i=1}^{3} H(\lambda_i - 1)\left(\lambda_i^2 - 1 - 2\ln\lambda_i\right) + a^3(\alpha)H(J-1)\frac{1}{2}\kappa\left(J-1\right)^2, \tag{3.7}$$

the passive part of the strain energy is

$$\widetilde{W}_{\text{pas}}\left(\mathbf{F},\alpha\right) = \frac{\mu}{2}\sum_{i=1}^{3} H(1-\lambda_i)\left(\lambda_i^2 - 1 - 2\ln\lambda_i\right) + H(1-J)\frac{1}{2}\kappa\left(J-1\right)^2, \tag{3.8}$$

4 Following Borden: Derivations of Analytical Phase Field

Note the full potential energy functional, which can also be called the lagrangian

$$\mathcal{E}_\ell(\boldsymbol{u}, p, \alpha) = \int_\Omega a(\alpha)\mathcal{W}(\mathbf{F})d\Omega - \int_\Omega \sqrt{a^3(\alpha)}p(J-1)d\Omega - \int_\Omega \frac{p^2}{2\kappa}d\Omega + \frac{G_c}{c_w}\int_\Omega \left(\frac{w(\alpha)}{\ell} + \ell\|\nabla\alpha\|^2\right)d\Omega$$

We can use the Euler-Lagrange equations to arrive at the equations of motion by taking the derivative with respect to displacement, pressure, and the scalar damage field. Starting with displacement:

$$\frac{\partial \mathcal{E}_\ell}{\partial \boldsymbol{u}} = \int_\Omega a(\alpha)\frac{\partial \mathcal{W}(\mathbf{F})}{\partial \mathbf{u}}d\Omega$$

$$\frac{\partial \mathcal{E}_\ell}{\partial p} = -\int_\Omega \frac{p}{\kappa}d\Omega - \int_\Omega \sqrt{a^3(\alpha)}(J-1)d\Omega$$

$$\frac{\partial \mathcal{E}_\ell}{\partial \alpha} = -\int_\Omega 2(1-\alpha)\,\mathcal{W}(\mathbf{F})\,d\Omega + \int_\Omega 3p(1-\alpha)^2(J-1)d\Omega + \frac{G_c}{c_w}\int_\Omega \left[\frac{1}{\ell} + 2\ell\nabla^2\alpha\right]d\Omega$$

Therefore we have three equations:
First is mechanical eq,

$$\begin{aligned} \frac{\partial \mathcal{W}(\mathbf{F})}{\partial u_i} &= 0 \\ \frac{\partial}{\partial x_j}\left(\frac{\partial \mathcal{W}}{\partial \epsilon_{ij}}\right) &= 0 \\ \frac{\partial \sigma_{ij}}{\partial x_j} &= 0 \end{aligned}$$

Second is an equation for pressure,

$$\begin{aligned} -\frac{p}{\kappa} - \sqrt{a^3(\alpha)}(J-1) &= 0 \\ -\frac{p}{\kappa} - (1-\alpha)^3(J-1) &= 0 \\ -\kappa(J-1)(1-\alpha)^3 &= p \end{aligned}$$

Lastly,

$$-2(1-\alpha)\,\mathcal{W}(\mathbf{F}) + 3p(1-\alpha)^2(J-1) + \frac{G_c}{c_w}\left[\frac{1}{\ell} + 2\ell\nabla^2\alpha\right] = 0$$

Substitute second equation into third

$$-2(1-\alpha)\,\mathcal{W}(\mathbf{F}) - 3\kappa(1-\alpha)^5(J-1)^2 + \frac{G_c}{c_w}\left[\frac{1}{\ell} + 2\ell\nabla^2\alpha\right] = 0$$

4.1 Homogeneous Solution

We can study the homogeneous solution by ignoring spatial derivatives of α. If we don't substitute p:

$$-2(1-\alpha_h)\,\mathcal{W}(\mathbf{F}) + 3p(1-\alpha_h)2(J-1) + \frac{G_c}{c_w\ell} = 0$$

or if we substitute pressure

$$-2(1-\alpha_h)\,\mathcal{W}(\mathbf{F}) - 3\kappa(1-\alpha_h)^5(J-1)^2 + \frac{G_c}{c_w\ell} = 0$$

4.2 Non-Homogeneous Solution

Now for the Non-homogenous solution, we have the following

$$-2(1-\alpha)\,\mathcal{W}(\mathbf{F}) + 3p(1-\alpha)^2(J-1) + \frac{G_c}{c_w}\left[\frac{1}{\ell} + 2\ell\nabla^2\alpha\right] = 0$$

Multiply by $d\alpha/dx$

$$\begin{aligned}
\frac{d\alpha}{dx}\left[-2(1-\alpha)\,\mathcal{W}(\mathbf{F}) + 3p(1-\alpha)^2(J-1) + \frac{G_c}{c_w}\left(\frac{1}{\ell} + 2\ell\nabla^2\alpha\right)\right] &= 0\\
\frac{d}{dx}\int\left[-2(1-\alpha)\,\mathcal{W}(\mathbf{F}) + 3p(1-\alpha)^2(J-1) + \frac{G_c}{c_w}\left(\frac{1}{\ell} + 2\ell\nabla^2\alpha\right)\right]d\alpha &= 0\\
\frac{d}{dx}\left[(1-\alpha)^2\,\mathcal{W}(\mathbf{F}) - p(1-\alpha)^3(J-1) + \frac{G_c}{c_w}\left(\frac{\alpha}{\ell} + 2\ell\nabla^2\alpha\right)\right] &= 0
\end{aligned}$$

now integrate from x to infinity

$$\begin{aligned}
\left[(1-\alpha)^2\,\mathcal{W}(\mathbf{F}) - p(1-\alpha)^3(J-1) + \frac{G_c}{c_w}\left(\frac{\alpha}{\ell} + 2\ell\nabla^2\alpha\right)\right]\Bigg|_0^\infty &= 0\\
(1-\alpha)^2\,\mathcal{W}(\mathbf{F}) - p(1-\alpha)^3(J-1) + \frac{G_c}{c_w}\left(\frac{\alpha}{\ell} + 2\ell\nabla^2\alpha\right)&\\
-\left[(1-\alpha_h)^2\,\mathcal{W}(\mathbf{F}) - p(1-\alpha_h)^3(J-1) + \alpha_h\frac{G_c}{c_w\ell}\right] &= 0
\end{aligned}$$

with some rearrangement we can call the bracketed section

$$a_{hom} = (1-\alpha_h)^2\,\mathcal{W}(\mathbf{F}) - p(1-\alpha_h)^3(J-1) + \alpha_h\frac{G_c}{c_w\ell} \tag{4.1}$$

which can yield an expression that can solve for the phase field profile

$$\begin{aligned}
-(1-\alpha)^2\,\mathcal{W}(\mathbf{F}) + p(1-\alpha)^3(J-1) - \frac{G_c}{c_w}\frac{\alpha}{\ell} + \left[a_{hom}\right] &= 2\ell\nabla^2\alpha\frac{G_c}{c_w}\\
\frac{c_w}{2\ell G_c}\left[-(1-\alpha)^2\,\mathcal{W}(\mathbf{F}) + p(1-\alpha)^3(J-1)\right] - \frac{\alpha}{2\ell^2} + \frac{c_w}{2\ell G_c}\left[a_{hom}\right] &= \frac{d^2\alpha}{dx^2}
\end{aligned}$$

This expression needs to be non-dimensionalized accurately in order to be plotted

$$ \tag{4.2} $$