

Stabilized Mixed Finite Element Formulation

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Definitions

F: Deformation gradient

I: second-order unit tensor

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

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

μ : shear modulus

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

λ : Lamé modulus

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

For Plane Stress

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

\mathcal{E}_ℓ : 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

$$\mathbf{F} = \mathbf{I} + \nabla \otimes \mathbf{u} \quad (1.1)$$

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

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

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

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

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

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

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

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

If we consider the perturbed lagrangian formulation

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

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

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

In the code, we have the following definition

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

The normalization constant is defined as:

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

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

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

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

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

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

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

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

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

Substituting this relationship into the energy functional yields:

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

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

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

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

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

1.2 Summary

Therefore the modified strain energy functional

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

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

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

The first Piola-Kirchhoff stress tensor is given:

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

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:

$$J = \det(\mathbf{F}) * F_{33}$$

$$I_c = \text{tr}(\mathbf{C}) + F_{33} * 2$$

Together with the weak form from above:

$$\begin{aligned} F_u = & \text{derivative}(\text{elastic_potential}, w_p, v_q) \setminus \\ & + (a(\alpha) * \mu * (F_{33} - 1/F_{33}) - b(\alpha) * p * J/F_{33}) * v_F_{33} * dx \end{aligned}$$

1.3.1 Changes for 2D Discrete Crack Model

If we are considering a discrete fracture method

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

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 Kirchhoff 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

$$-\frac{\varpi h^2}{2\mu} \int_{\Omega} J \mathbf{C}^{-1} : (\nabla p \cdot \nabla q) dV = 0$$

$$\int_{\Omega} \left(\mathbf{F}_{33}^2 - 1 - \frac{pJ}{\mu} \right) v_{F_{33}} dV = 0$$

1.3.2 Changes for 2D displacement formulation

Removing pressure terms

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

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

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

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

We have assumed the modified energy functional

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

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

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

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

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

$$W(I_1, I_2) = \beta_1 (I_1 - 3) + \beta_2 (I_2 - 3) \quad \text{where } \beta_1 = \frac{\mu}{2}, \beta_2 = 0$$

$$W(I_1, I_2) = \frac{\mu}{2} (I_1 - 3) \quad \text{where } I_1 = I_2 = \lambda_A^2 + \lambda_A^{-2} + 1$$

$$W(I_1, I_2) = \frac{\mu}{2} \left(\lambda_A^2 + \frac{1}{\lambda_A^2} - 2 \right)$$

$$W(I_1, I_2) = \frac{\mu}{2} \left(\lambda_A - \frac{1}{\lambda_A} \right)^2$$

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

$$\begin{aligned} J &= 2h_0W(I_1, I_2) \\ J &= h_0\mu\left(\lambda_A - \frac{1}{\lambda_A}\right)^2 \end{aligned} \quad (2.1)$$

where for the stretch:

$$\lambda_A = 1 + \frac{\Delta}{h_0} \quad (2.2)$$

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

Theoretically, the critical condition for crack initiation is where the fracture energy is equivalent to the energy release rate

$$G_c = J$$

Determining whether the length of the strip is long enough:

1. Choose height of strip, h_0 , shear modulus, μ , and critical fracture energy G_c
2. Use Matlab to calculate the critical stretch λ_c

$$G_c = h_0\mu\left(\lambda_c - \frac{1}{\lambda_c}\right)^2$$

3. Calculate the critical displacement Δ_c using eq. 2.2

$$\Delta_c = h_0(\lambda_c - 1)$$

4. Run two simulations using 2D-planestress-TH-BL.py

- (a) Assign a displacement slightly below the predicted Δ_c
- (b) Change P3 point to either $2hsize$ before or after the crack center to calculate an energy max and energy min
- (c) Calculate J numerical

$$J_n = -\frac{E_{max} - E_{min}}{4hsize}$$

- (d) Calculate percentage error with J analytical from Eq (2.1)

$$\%Error = \left(\frac{J_a - J_n}{J_a}\right)100\%$$

Note that there is an effective critical energy release rate

$$G_c^e = G_c\left(1 + \frac{3hsize}{8\ell}\right) \quad (2.3)$$

where $hsize$ is the element size and ℓ is the width of the phase-field

Once a length is determined, we can then run both a phase field and discrete trial and determine where the crack initiates

1. The strip has a length of 6 and a total width of 1.0 where $h_0 = 0.5$
2. $hsize = 0.002$, $\ell = 0.01$
3. Used an exponential function to ramp the displacement in order to obtain a close agreement

3 Strain energy decomposition

The Heaviside function is defined as

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

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:

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

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 $\lambda_i < 1$:

For $\lambda_i > 1$:

$$W_{act} = C_1 \sum_{i=1}^3 (\lambda_i^2 - 1) + C_2 \sum_{i=1}^3 (\lambda_i^{-2} - 1)$$

$$W_{pas} = 0$$

For $\lambda_i < 1$:

$$W_{act} = 0$$

$$W_{pas} = C_1 \sum_{i=1}^3 (\lambda_i^2 - 1) + C_2 \sum_{i=1}^3 (\lambda_i^{-2} - 1)$$

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

$$\lambda_i^+ = \begin{cases} \lambda_i, & \lambda_i > 1, \\ 1, & \lambda_i \leq 1 \end{cases} \quad J^+ = \begin{cases} J, & J > 1, \\ 1, & J \leq 1 \end{cases}$$

$$\lambda_i^- = \begin{cases} \lambda_i, & \lambda_i < 1, \\ 1, & \lambda_i \geq 1 \end{cases} \quad J^- = \begin{cases} J, & J < 1, \\ 1, & J \geq 1 \end{cases}$$

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

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

Now we can consider some examples.

For $J > 1$:

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

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

For $J < 1$:

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

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

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

For $J > 1, \lambda_i > 1$:

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

$$W^- = 0$$

For $J < 1, \lambda_i > 1$:

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

$$W^- = \frac{\kappa}{2} (\ln J)^2$$

Now for all other stress states:

For $J > 1$, $\lambda_i < 1$:

$$W^+ = \frac{\kappa}{2}(\ln J)^2$$

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

For $J < 1$, $\lambda_i < 1$:

$$W^+ = 0$$

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

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

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

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

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

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

For $J > 1$:

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

For $J \leq 1$:

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

Now considering the same two cases of, triaxial tension and

For $J > 1, \lambda_i > 1$:

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

For $J \leq 1, \lambda_i > 1$:

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

all other cases:

For $J > 1, \lambda_i < 1$:

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

For $J \leq 1, \lambda_i < 1$:

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

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

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

and the passive part of the strain energy is

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

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

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

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

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

3.3 Hybrid Formulation

The principal stretches can be computed as shown above, but for spherical stretch ($\mathbf{C} = \text{constant} \mathbf{I}$) 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.

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

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

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

the passive part of the strain energy is

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

4 Gateaux Derivative

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

The Gateaux derivative with respect to (\mathbf{u}, α) in direction (\mathbf{v}, β) under the irreversibility condition $\dot{\alpha} \geq 0$.

$$d\mathcal{E}_\ell(\mathbf{u}, \alpha; \mathbf{v}, \beta) \geq 0. \quad (4.1)$$

Calculation of the Gateaux derivative

$$\begin{aligned} d\mathcal{E}_\ell(\mathbf{u}, \mathbf{v})(\alpha, \beta) &= \frac{d}{d\delta} \mathcal{E}_\ell(\mathbf{u} + \delta \mathbf{v}, \alpha + \delta \beta) \Big|_{\delta=0} \\ &= \frac{d}{d\delta} \mathcal{E}_\ell(\mathbf{u} + \delta \mathbf{v}, \alpha) \Big|_{\delta=0} + \frac{d}{d\delta} \mathcal{E}_\ell(\mathbf{u}, \alpha + \delta \beta) \Big|_{\delta=0} \end{aligned}$$

Starting with the first term:

$$\begin{aligned} \frac{d}{d\delta} \mathcal{E}_\ell(\mathbf{u} + \delta \mathbf{v}, \alpha) \Big|_{\delta=0} &= \frac{d}{d\delta} \left[\int_{\Omega} \widetilde{\mathcal{W}}(\mathbf{I} + \nabla(\mathbf{u} + \delta \mathbf{v}), \alpha) d\Omega - \int_{\partial_N \Omega} \tilde{\mathbf{g}}_0 \cdot (\mathbf{u} + \delta \mathbf{v}) dA \right] \Big|_{\delta=0} \\ &= \left[\int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{I} + \nabla(\mathbf{u} + \delta \mathbf{v}), \alpha)}{d\delta} d\Omega - \int_{\partial_N \Omega} \tilde{\mathbf{g}}_0 \cdot \frac{d(\mathbf{u} + \delta \mathbf{v})}{d\delta} dA \right] \Big|_{\delta=0} \quad \text{chain rule} \\ &= \left[\int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{I} + \nabla(\mathbf{u} + \delta \mathbf{v}), \alpha)}{d(\mathbf{I} + \nabla(\mathbf{u} + \delta \mathbf{v}))} \frac{d(\mathbf{I} + \nabla(\mathbf{u} + \delta \mathbf{v}))}{d\delta} d\Omega - \int_{\partial_N \Omega} \tilde{\mathbf{g}}_0 \cdot \frac{d(\mathbf{u} + \delta \mathbf{v})}{d\delta} dA \right] \Big|_{\delta=0} \\ &= \left[\int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{I} + \nabla \mathbf{u} + \delta \nabla \mathbf{v}, \alpha)}{d(\mathbf{I} + \nabla \mathbf{u} + \delta \nabla \mathbf{v})} \frac{d(\mathbf{I} + \nabla \mathbf{u} + \delta \nabla \mathbf{v})}{d\delta} d\Omega - \int_{\partial_N \Omega} \tilde{\mathbf{g}}_0 \cdot \mathbf{v} dA \right] \Big|_{\delta=0} \\ &= \left[\int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{I} + \nabla \mathbf{u} + \delta \nabla \mathbf{v}, \alpha)}{d(\mathbf{I} + \nabla \mathbf{u} + \delta \nabla \mathbf{v})} \nabla \mathbf{v} d\Omega - \int_{\partial_N \Omega} \tilde{\mathbf{g}}_0 \cdot \mathbf{v} dA \right] \Big|_{\delta=0} \\ &= \int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{I} + \nabla \mathbf{u}, \alpha)}{d(\mathbf{I} + \nabla \mathbf{u})} \nabla \mathbf{v} d\Omega - \int_{\partial_N \Omega} \tilde{\mathbf{g}}_0 \cdot \mathbf{v} dA \\ \frac{d}{d\delta} \mathcal{E}_\ell(\mathbf{u} + \delta \mathbf{v}, \alpha) \Big|_{\delta=0} &= \int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{d\mathbf{F}} \nabla \mathbf{v} d\Omega - \int_{\partial_N \Omega} \tilde{\mathbf{g}}_0 \cdot \mathbf{v} dA \end{aligned}$$

Second term:

$$\begin{aligned}
& \frac{d}{d\delta} \mathcal{E}_\ell(\mathbf{u}, \alpha + \delta\beta) \Big|_{\delta=0} \\
&= \frac{d}{d\delta} \left[\int_{\Omega} \widetilde{\mathcal{W}}(\mathbf{F}, \alpha + \delta\beta) d\Omega + \frac{\mathcal{G}_c}{c_w} \int_{\Omega} \left(\frac{w(\alpha + \delta\beta)}{\ell} + \ell \|\nabla(\alpha + \delta\beta)\|^2 \right) dV \right] \Big|_{\delta=0} \\
&= \left[\int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha + \delta\beta)}{d\delta} d\Omega + \frac{\mathcal{G}_c}{c_w} \frac{d}{d\delta} \int_{\Omega} \left(\frac{w(\alpha + \delta\beta)}{\ell} + \ell \|\nabla(\alpha + \delta\beta)\|^2 \right) dV \right] \Big|_{\delta=0} \\
&= \left[\int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha + \delta\beta)}{d(\alpha + \delta\beta)} \frac{d(\alpha + \delta\beta)}{d\delta} d\Omega + \frac{\mathcal{G}_c}{c_w} \frac{1}{\ell} \int_{\Omega} \frac{dw(\alpha + \delta\beta)}{d\delta} dV + \frac{\mathcal{G}_c}{c_w} \ell \int_{\Omega} \frac{\|\nabla(\alpha + \delta\beta)\|^2}{d\delta} dV \right] \Big|_{\delta=0} \\
&= \left[\int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha + \delta\beta)}{d(\alpha + \delta\beta)} \beta d\Omega + \frac{\mathcal{G}_c}{c_w} \frac{1}{\ell} \int_{\Omega} \frac{dw(\alpha + \delta\beta)}{d(\alpha + \delta\beta)} \frac{d(\alpha + \delta\beta)}{d\delta} dV + \frac{\mathcal{G}_c}{c_w} \ell \int_{\Omega} 2\nabla(\alpha + \delta\beta) \frac{\nabla(\alpha + \delta\beta)}{d\delta} dV \right] \Big|_{\delta=0} \\
&= \int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{d\alpha} \beta d\Omega + \left[\frac{\mathcal{G}_c}{c_w} \frac{1}{\ell} \int_{\Omega} \frac{dw(\alpha + \delta\beta)}{d(\alpha + \delta\beta)} \beta dV + \frac{\mathcal{G}_c}{c_w} \ell \int_{\Omega} 2\nabla(\alpha + \delta\beta) \nabla\beta dV \right] \Big|_{\delta=0} \\
&= \int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{d\alpha} \beta d\Omega + \frac{\mathcal{G}_c}{c_w} \frac{1}{\ell} \int_{\Omega} \frac{dw(\alpha)}{d\alpha} \beta dV + 2\ell \frac{\mathcal{G}_c}{c_w} \int_{\Omega} \nabla\alpha \cdot \nabla\beta dV \\
&= \int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{d\alpha} \beta d\Omega + \frac{\mathcal{G}_c}{c_w \ell} \int_{\Omega} \left[\frac{dw(\alpha)}{d\alpha} \beta + 2\ell^2 (\nabla\alpha \cdot \nabla\beta) \right] dV
\end{aligned}$$

First, consider Eq. 1.9

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

Multiplying this by test function q and integrating over volume, we obtain an equation that can be combined with the equations from the Gateaux Derivative.

$$\int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{d\mathbf{F}} \nabla \mathbf{v} d\Omega - \int_{\partial_N \Omega} \tilde{\mathbf{g}}_0 \cdot \mathbf{v} dA = 0 \quad (4.2a)$$

$$\int_{\Omega} \left(-\sqrt{a^3(\alpha)} (J - 1) - \frac{p}{\kappa} \right) q dV = 0 \quad (4.2b)$$

$$\int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{d\alpha} \beta d\Omega + \frac{\mathcal{G}_c}{c_w \ell} \int_{\Omega} \left[\frac{dw(\alpha)}{d\alpha} \beta + 2\ell^2 (\nabla\alpha \cdot \nabla\beta) \right] dV \geq 0 \quad (4.2c)$$

The strong form

$$\text{Div } \mathbf{P} = 0 \quad \text{in } \Omega \quad (4.3a)$$

$$\mathbf{u} = \tilde{\mathbf{u}}_0 \quad \text{in } \partial_D \Omega \quad (4.3b)$$

$$[\mathbf{FS}] \mathbf{n} = \tilde{\mathbf{g}}_0 \quad \text{on } \partial_N \Omega, \quad (4.3c)$$

where from Eq. 1.12 we can substitute Eq. 1.9

$$\begin{aligned}
\mathbf{P} &= a(\alpha) \frac{\mathcal{W}(\mathbf{F})}{\partial \mathbf{F}} + a^3(\alpha) \kappa (J - 1) \frac{\partial J}{\partial \mathbf{F}} \quad \text{where } p = -\sqrt{a^3(\alpha)} \kappa (J - 1) \\
\mathbf{P} &= a(\alpha) \frac{\mathcal{W}(\mathbf{F})}{\partial \mathbf{F}} - p \sqrt{a^3(\alpha)} \frac{\partial J}{\partial \mathbf{F}}
\end{aligned}$$

and write the mechanical equilibrium equation in Eq. 3.11:

$$\text{Div} \left[a(\alpha) \frac{\mathcal{W}(\mathbf{F})}{\partial \mathbf{F}} - p \sqrt{a^3(\alpha)} \frac{\partial J}{\partial \mathbf{F}} \right] = 0 \quad (4.4)$$

Derivation of the KKT condition equations where $\nabla \beta \cdot \nabla \alpha = \nabla(\beta \nabla \alpha) - \beta \Delta \alpha$

$$\begin{aligned} \int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{d\alpha} \beta d\Omega + \frac{\mathcal{G}_c}{c_w \ell} \int_{\Omega} \left[\frac{dw(\alpha)}{d\alpha} \beta + 2\ell^2 (\nabla \alpha \cdot \nabla \beta) \right] dV &\geq 0 \\ \int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{d\alpha} \beta d\Omega + \frac{\mathcal{G}_c}{c_w \ell} \int_{\Omega} \frac{dw(\alpha)}{d\alpha} \beta dV + \frac{\mathcal{G}_c}{c_w \ell} \int_{\Omega} 2\ell^2 (\nabla \alpha \cdot \nabla \beta) dV &\geq 0 \\ \int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{d\alpha} \beta d\Omega + \frac{\mathcal{G}_c}{c_w \ell} \int_{\Omega} \frac{dw(\alpha)}{d\alpha} \beta dV + \frac{\mathcal{G}_c}{c_w \ell} \int_{\Omega} 2\ell^2 (\nabla(\beta \nabla \alpha)) dV - \frac{\mathcal{G}_c}{c_w \ell} \int_{\Omega} 2\ell^2 (\beta \Delta \alpha) dV &\geq 0 \\ \int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{d\alpha} \beta d\Omega + \frac{\mathcal{G}_c}{c_w \ell} \int_{\Omega} \frac{dw(\alpha)}{d\alpha} \beta dV - \frac{\mathcal{G}_c}{c_w \ell} \int_{\Omega} 2\ell^2 (\beta \Delta \alpha) dV &\geq 0 \\ \left[\int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{d\alpha} d\Omega + \frac{\mathcal{G}_c}{c_w \ell} \int_{\Omega} \left(\frac{dw(\alpha)}{d\alpha} - 2\ell^2 \Delta \alpha \right) dV \right] \beta &\geq 0 \\ \int_{\Omega} \frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{d\alpha} d\Omega + \frac{\mathcal{G}_c}{c_w \ell} \int_{\Omega} \left(\frac{dw(\alpha)}{d\alpha} - 2\ell^2 \Delta \alpha \right) dV &\geq 0 \end{aligned}$$

Grouping terms, we obtain

$$\frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{d\alpha} + \frac{\mathcal{G}_c}{c_w \ell} \left(\frac{dw(\alpha)}{d\alpha} - 2\ell^2 \Delta \alpha \right) \geq 0 \quad \text{in } \Omega \quad (4.5a)$$

$$\dot{\alpha} \geq 0 \quad \text{in } \Omega \quad (4.5b)$$

$$\dot{\alpha} \left[\frac{d\widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{d\alpha} + \frac{\mathcal{G}_c}{c_w \ell} \left(\frac{dw(\alpha)}{d\alpha} - 2\ell^2 \Delta \alpha \right) \right] \geq 0 \quad \text{in } \Omega \quad (4.5c)$$

$$(4.5d)$$

Lastly, we have the following, (Neumann?)

$$\frac{\partial \alpha}{\partial \mathbf{n}} \geq 0 \quad \text{and} \quad \dot{\alpha} \frac{\partial \alpha}{\partial \mathbf{n}} = 0 \quad \text{on } \partial \Omega \quad (4.6)$$

Multiply Eq. 3.12 with weighting function $\mathbf{v} + (\varpi h^2)/(2\mu)\mathbf{F}^{-T}\nabla q$

$$\begin{aligned}
& \int_{\Omega} \text{Div} \mathbf{P} \cdot \left[\mathbf{v} + \frac{\varpi h^2}{2\mu} \mathbf{F}^{-T} \nabla q \right] dV = 0 \\
& \int_{\Omega} \text{Div} \mathbf{P} \cdot \mathbf{v} dV + \int_{\Omega} \text{Div} \mathbf{P} \cdot \left[\frac{\varpi h^2}{2\mu} \mathbf{F}^{-T} \nabla q \right] dV = 0 \\
& \int_{\Omega} \text{Div} \mathbf{P} \cdot \mathbf{v} dV + \frac{\varpi h^2}{2\mu} \sum_{e=1}^{n_{el}} \int_{\Omega^e} \text{Div} \mathbf{P} \cdot (\mathbf{F}^{-T} \nabla q) dV = 0 \\
& \int_{\Omega} \text{Div} \mathbf{P} \cdot \mathbf{v} dV \\
& + \frac{\varpi h^2}{2\mu} \sum_{e=1}^{n_{el}} \int_{\Omega^e} \text{Div} \left[a(\alpha) \frac{\mathcal{W}(\mathbf{F})}{\partial \mathbf{F}} \right] \cdot (\mathbf{F}^{-T} \nabla q) dV - \frac{\varpi h^2}{2\mu} \sum_{e=1}^{n_{el}} \int_{\Omega^e} \text{Div} \left[p \sqrt{a^3(\alpha)} \frac{\partial J}{\partial \mathbf{F}} \right] \cdot (\mathbf{F}^{-T} \nabla q) dV = 0 \\
& \quad \text{""} + \text{""} - \frac{\varpi h^2}{2\mu} \sum_{e=1}^{n_{el}} \int_{\Omega^e} \nabla (p \sqrt{a^3(\alpha)}) J \mathbf{F}^{-T} \cdot (\mathbf{F}^{-T} \nabla q) dV = 0 \\
& \quad \text{""} + \text{""} - \frac{\varpi h^2}{2\mu} \sum_{e=1}^{n_{el}} \int_{\Omega^e} \nabla (p \sqrt{a^3(\alpha)}) J \mathbf{F}^{-1} \mathbf{F}^{-T} \cdot (\mathbf{F}^{-1} \mathbf{F}^{-T} \nabla q) dV = 0 \\
& \quad \text{""} + \text{""} - \frac{\varpi h^2}{2\mu} \sum_{e=1}^{n_{el}} \int_{\Omega^e} \nabla (p \sqrt{a^3(\alpha)}) J \cdot (\mathbf{C}^{-1} \nabla q) dV = 0 \\
& \quad \text{""} + \text{""} - \frac{\varpi h^2}{2\mu} \sum_{e=1}^{n_{el}} \int_{\Omega^e} J \mathbf{C}^{-1} : \left[\nabla (p \sqrt{a^3(\alpha)}) \cdot \nabla q \right] dV = 0
\end{aligned}$$

where $\mathbf{P} = a(\alpha) \frac{\mathcal{W}(\mathbf{F})}{\partial \mathbf{F}} - p \sqrt{a^3(\alpha)} \frac{\partial J}{\partial \mathbf{F}}$

We also want to deal with the first term where $(fg)' = f'g + fg'$

$$\int_{\Omega} \text{Div} \mathbf{P} \cdot \mathbf{v} dV = \int_{\Omega} (\mathbf{F} \cdot \mathbf{v})_{,X} dV - \int_{\Omega} \mathbf{P} \cdot \frac{\partial \mathbf{v}}{\partial X} dV$$

Leaving

$$\int_{\Omega} \text{Div} \mathbf{P} \cdot \mathbf{v} dV + \frac{\varpi h^2}{2\mu} \sum_{e=1}^{n_{el}} \int_{\Omega^e} \text{Div} \left[a(\alpha) \frac{\mathcal{W}(\mathbf{F})}{\partial \mathbf{F}} \right] \cdot (\mathbf{F}^{-T} \nabla q) dV - \frac{\varpi h^2}{2\mu} \sum_{e=1}^{n_{el}} \int_{\Omega^e} J \mathbf{C}^{-1} : \left[\nabla (p \sqrt{a^3(\alpha)}) \cdot \nabla q \right] dV \quad (4.7)$$

5 Following Borden: Derivations of Analytical Phase Field

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

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

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:

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

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

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

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

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

5.1 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

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

5.2 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

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

with some rearrangement we can call the bracketed section

$$a_{hom} = (1 - \alpha_h)^2 \mathcal{W}(\mathbf{F}) - p(1 - \alpha_h)^3(J - 1) + \alpha_h \frac{G_c}{c_w \ell} \quad (5.1)$$

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