

# stabilized mixed finite element formulation

Bin Li

*Sibley School of Mechanical and Aerospace Engineering, Cornell University, NY, USA*

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## Abstract

*Keywords:* Elastomer, Phase-field model, Incompressibility, Nucleation, Stabilization

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## 1. Introduction

Brink and Stein (1996) Klaas et al. (1999) Li and Bouklas (2020) Li et al. (2015) Li et al. (2018)  
Li and Maurini (2019) Adler et al. (2014)

## 2. Hyperelastic phase-field fracture models

The deformation gradient  $\mathbf{F} = \mathbf{I} + \nabla \otimes \mathbf{u}$  with  $\mathbf{I}$  being the second-order unit tensor and  $J = \det \mathbf{F}$  is the determinant of the deformation gradient. The right Cauchy-Green strain tensor  $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ . The homogeneous hyperelastic material postulates (Holzapfel, 2000) the existence of a strain energy function  $\mathcal{W}(\mathbf{F})$  defined per unit reference volume such that  $\mathbf{P} = \partial \mathcal{W}(\mathbf{F}) / \partial \mathbf{F}$ , where  $\mathbf{P}$  is the first Piola-Kirchhoff stress tensor. The second Piola-Kirchhoff stress tensor  $\mathbf{S} = 2 \partial \mathcal{W}(\mathbf{F}) / \partial \mathbf{C}$  with relationship  $\mathbf{P} = \mathbf{F} \mathbf{S}$ .

### 2.1. Phase-field fracture model

In the regularized approximation of brittle fracture, cracks are represented by a phase-field variable (scalar order parameter)  $\alpha$ , which is 0 away from the crack, 1 inside a cracked zone, and changes from 0 to 1 smoothly (Pham et al., 2011; Marigo et al., 2016; Li and Bouklas, 2020). For incompressible hyperelastic materials, the strain energy function is defined as (Holzapfel, 2000)

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

where the incompressibility constraint is enforced through a Lagrange multiplier  $p$  that can be identified as a hydrostatic pressure field. However, note that the damaged materials are no longer incompressible because of the microcrack growth or crack opening, accordingly the incompressibility constraint should be relaxed in the damaged regions in an appropriate way. To this end, we instead consider a damage dependent relaxation of the incompressibility constraint and the phase-field couples to the strain energy through the modified function (Li and Bouklas, 2020)

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

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\*Corresponding author

Email address: b1736@cornell.edu (Bin Li)

where  $a(\alpha) = (1 - \alpha)^2$  is a decreasing stiffness modulation function. However, we choose to damage the bulk modulus  $\kappa$  faster than the shear modulus  $\mu$  ensuring that the incompressibility constraint does not impose a barrier to the physical opening of crack. Effectively, it allows the damaged phase to bypass the incompressibility constraint. In the intact material the incompressibility is ensured by setting the bulk modulus  $\kappa \gg \mu$  sufficiently large. Thus, the first Piola-Kirchhoff stress tensor is written as

$$\mathbf{P} = \frac{\partial \widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{\partial \mathbf{F}} = a(\alpha) \frac{\mathcal{W}(\mathbf{F})}{\partial \mathbf{F}} + a^3(\alpha) \kappa (J - 1) \frac{\partial J}{\partial \mathbf{F}}, \quad (3)$$

where  $\partial J / \partial \mathbf{F} = J \mathbf{F}^{-T}$ . However, when applied to the finite element discretization, this formulation near the incompressible limit exhibits severe volumetric locking issue (Auricchio et al., 2013). To circumvent this numerical difficulties, we resort to the classical mixed formulation and introduce the pressure-like field

$$p = -\sqrt{a^3(\alpha)} \kappa (J - 1), \quad (4)$$

as an independent variable along with the displacement field.

The potential energy functional of a possibly fractured elastic body with isotropic surface energy, under traction force on the boundary  $\partial_N \Omega$ , is modeled by

$$\mathcal{E}_\ell(\mathbf{u}, \alpha) = \int_\Omega \widetilde{\mathcal{W}}(\mathbf{F}, \alpha) d\Omega + \frac{\mathcal{G}_c}{c_w} \int_\Omega \left( \frac{w(\alpha)}{\ell} + \ell \|\nabla \alpha\|^2 \right) dV - \int_{\partial_N \Omega} \tilde{\mathbf{g}}_0 \cdot \mathbf{u} dA, \quad (5)$$

where  $w(\alpha)$  is an increasing function representing the specific energy dissipation per unit of volume, the  $c_w = \int_0^1 \sqrt{w(\alpha)} d\alpha$  is normalization constant.

## 2.2. Plane-stress case

Consider an hyperelastic model

$$\mathcal{W}(\mathbf{F}) = \frac{\mu}{2} (\text{tr } \mathbf{C} - 3 - 2 \ln J), \quad (6)$$

and with additional pressure-like field  $p$ , thus

$$\widetilde{\mathcal{W}}(\mathbf{F}, \alpha) = a(\alpha) \frac{\mu}{2} (\text{tr } \mathbf{C} - 3 - 2 \ln J) - \sqrt{a^3(\alpha)} p (J - 1) - \frac{p^2}{2\kappa}. \quad (7)$$

The first Piola-Kirchhoff stress is

$$\mathbf{P} = 2\mathbf{F} \frac{\partial \widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{\partial \mathbf{C}} = a(\alpha) \mu (\mathbf{F} - \mathbf{F}^{-T}) - \sqrt{a^3(\alpha)} p J \mathbf{F}^{-T}. \quad (8)$$

Following the plane stress assumptions made in Knowles and Sternberg (1983), we have

$$F_{31} = F_{13} = F_{13} = F_{23} = 0, \quad (9)$$

thus

$$\mathbf{F} = \begin{bmatrix} F_{11} & F_{12} & 0 \\ F_{21} & F_{22} & 0 \\ 0 & 0 & F_{33} \end{bmatrix}, \quad (10)$$

and

$$F_{33}^{-T} = \frac{1}{J} \frac{J}{F_{33}} = \frac{1}{F_{33}}. \quad (11)$$

44 Set the component  $P_{33}$  of  $\mathbf{P}$  to be zero

$$\begin{aligned} P_{33} &= \mu \left( F_{33} - F_{33}^{-T} \right) - (1 - \alpha) p J F_{33}^{-T} \\ &= \mu \left( F_{33} - \frac{1}{F_{33}} \right) - (1 - \alpha) \frac{p J}{F_{33}} \\ &= 0, \end{aligned}$$

45 and then

### 46 3. Stabilized Finite Element Method

#### 47 3.1. Gateaux derivative

48 The Gateaux derivative with respect to  $(\mathbf{u}, \alpha)$  in direction  $(\mathbf{v}, \beta)$  (Pham et al., 2011)

$$d\mathcal{E}_\ell(\mathbf{u}, \alpha; \mathbf{v}, \beta) \geq 0. \quad (12)$$

49 under the irreversibility condition  $\dot{\alpha} \geq 0$ . Enforcing the Eq. (4) in a weak sense, we arrive at  
50 following mixed formulations

$$\begin{aligned} \int_{\Omega} \frac{\partial \widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{\partial \mathbf{F}} : \nabla \otimes \mathbf{v} \, dV - \int_{\partial_N \Omega} \tilde{\mathbf{g}}_0 \cdot \mathbf{v} \, dA &= 0, \\ \int_{\Omega} \left( -\sqrt{a^3(\alpha)} (J - 1) - \frac{1}{\kappa} p \right) q \, dV &= 0, \\ \int_{\Omega} \frac{\partial \widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{\partial \alpha} \beta \, d\Omega + \frac{\mathcal{G}_c}{c_w \ell} \int_{\Omega} \left( \frac{\partial w(\alpha)}{\partial \alpha} \beta + \ell^2 \nabla \alpha \cdot \nabla \beta \right) dV &\geq 0. \end{aligned} \quad (13)$$

51 Thus, the strong form for displacement field

$$\begin{aligned} \text{Div} \left[ a(\alpha) \frac{\partial \mathcal{W}(\mathbf{F})}{\partial \mathbf{F}} - \sqrt{a^3(\alpha)} p \frac{\partial J}{\partial \mathbf{F}} \right] &= 0 \quad \text{in } \Omega, \\ \mathbf{u} &= \tilde{\mathbf{u}}_0 \quad \text{in } \partial_D \Omega, \\ [\mathbf{F}\mathbf{S}] \mathbf{n} &= \tilde{\mathbf{g}}_0 \quad \text{on } \partial_N \Omega, \end{aligned} \quad (14)$$

52 where the Eq. (4) is substituted and  $\mathbf{n}$  is outward normal to the boundary. And the damage  
53 evolution problem is formulated in form of the Karush–Kuhn–Tucker conditions as (Pham et al.,  
54 2011)

$$\begin{aligned} \frac{\partial \mathcal{W}(\tilde{\mathbf{F}}, \alpha)}{\partial \alpha} + \frac{\mathcal{G}_c}{c_w \ell} \left( \frac{\partial w(\alpha)}{\partial \alpha} - \ell^2 \Delta \alpha \right) &\geq 0 \quad \text{in } \Omega, \\ \dot{\alpha} &\geq 0 \quad \text{in } \Omega, \\ \frac{\partial \alpha}{\partial \mathbf{n}} &\geq 0 \quad \text{and} \quad \dot{\alpha} \frac{\partial \alpha}{\partial \mathbf{n}} = 0, \quad \text{on } \partial \Omega, \\ \dot{\alpha} \left[ \frac{\partial \mathcal{W}(\tilde{\mathbf{F}}, \alpha)}{\partial \alpha} + \frac{\mathcal{G}_c}{c_w \ell} \left( \frac{\partial w(\alpha)}{\partial \alpha} - \ell^2 \Delta \alpha \right) \right] &\geq 0 \quad \text{in } \Omega. \end{aligned} \quad (15)$$

55 Following the derivation in Klaas et al. (1999), we multiply Eq. (14)<sub>1</sub> by the perturbed weighting  
 56 function  $\mathbf{v} + (\varpi h^2)/(2\mu)\mathbf{F}^{-T}\nabla q$ , where  $h$  is a characteristic mesh length, and the non dimensional,  
 57 non negative stability parameter  $\varpi$  depends only on the element type (Klaas et al., 1999). The  
 58 perturbation is applied element wise, integrating it over the reference domain we have

$$\int_{\Omega} \text{Div} [\mathbf{FS}] \cdot \mathbf{v} dV + \frac{\varpi h^2}{2\mu} \sum_{e=1}^{n_{el}} \int_{\Omega^e} \text{Div} [\mathbf{FS}] \cdot (\mathbf{F}^{-T}\nabla q) dV = 0. \quad (16)$$

59 Now we focus on the derivation of the stabilization term in Eq. (16), noting that Eqs. (3) and  
 60 (4), and employing the Piola identity  $\text{Div} (J\mathbf{F}^{-T}) = 0$  (Holzapfel, 2000), we have

$$\begin{aligned} & \text{Div} \left[ a(\alpha) \frac{\partial \mathcal{W}(\mathbf{F})}{\partial \mathbf{F}} \right] \cdot (\mathbf{F}^{-T}\nabla q) - \left[ J\mathbf{F}^{-T} \cdot \nabla \left( \sqrt{a^3(\alpha)} p \right) \right] \cdot (\mathbf{F}^{-T}\nabla q) \\ &= \text{Div} \left[ a(\alpha) \frac{\partial \mathcal{W}(\mathbf{F})}{\partial \mathbf{F}} \right] \cdot (\mathbf{F}^{-T}\nabla q) - \nabla \left( \sqrt{a^3(\alpha)} p \right) J\mathbf{F}^{-1}\mathbf{F}^{-T}\nabla q \\ &= \text{Div} \left[ a(\alpha) \frac{\partial \mathcal{W}(\mathbf{F})}{\partial \mathbf{F}} \right] \cdot (\mathbf{F}^{-T}\nabla q) - J\mathbf{C}^{-1} : \left[ \nabla \left( \sqrt{a^3(\alpha)} p \right) \otimes \nabla q \right]. \end{aligned} \quad (17)$$

61 Consequently, we obtain the stabilized mixed formulation corresponding to Eq. (13)

$$\begin{aligned} & \int_{\Omega} \frac{\partial \widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{\partial \mathbf{F}} : \nabla \otimes \mathbf{v} dV - \int_{\partial_N \Omega} \tilde{\mathbf{g}}_0 \cdot \mathbf{v} dA = 0, \\ & \int_{\Omega} \left( -\sqrt{a^3(\alpha)} (J-1) - \frac{1}{\kappa} p \right) q dV - \frac{\varpi h^2}{2\mu} \sum_{e=1}^{n_{el}} \int_{\Omega^e} J\mathbf{C}^{-1} : \left[ \nabla \left( \sqrt{a^3(\alpha)} p \right) \otimes \nabla q \right] dV \\ & \quad + \frac{\varpi h^2}{2\mu} \sum_{e=1}^{n_{el}} \int_{\Omega^e} \text{Div} \left[ a(\alpha) \frac{\partial \mathcal{W}(\mathbf{F})}{\partial \mathbf{F}} \right] \cdot (\mathbf{F}^{-T}\nabla q) dV = 0, \\ & \int_{\Omega} \frac{\partial \widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{\partial \alpha} \beta dV + \frac{\mathcal{G}_c}{c_w \ell} \int_{\Omega} \left( \frac{\partial w(\alpha)}{\partial \alpha} \beta + \ell^2 \nabla \alpha \cdot \nabla \beta \right) dV \geq 0. \end{aligned} \quad (18)$$

62 Since we are interested in the linear shape functions for the displacements. Thus the divergence  
 63 of the stresses will be vanished considering that assumption. Accordingly, the weak form Eq. (18)  
 64 reduces to

$$\begin{aligned} & \int_{\Omega} \frac{\partial \widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{\partial \mathbf{F}} : \nabla \otimes \mathbf{v} dV - \int_{\partial_N \Omega} \tilde{\mathbf{g}}_0 \cdot \mathbf{v} dA = 0, \\ & \int_{\Omega} \left( -\sqrt{a^3(\alpha)} (J-1) - \frac{1}{\kappa} p \right) q dV - \frac{\varpi h^2}{2\mu} \sum_{e=1}^{n_{el}} \int_{\Omega^e} J\mathbf{C}^{-1} : \left[ \nabla \left( \sqrt{a^3(\alpha)} p \right) \otimes \nabla q \right] dV = 0, \\ & \int_{\Omega} \frac{\partial \widetilde{\mathcal{W}}(\mathbf{F}, \alpha)}{\partial \alpha} \beta dV + \frac{\mathcal{G}_c}{c_w \ell} \int_{\Omega} \left( \frac{\partial w(\alpha)}{\partial \alpha} \beta + \ell^2 \nabla \alpha \cdot \nabla \beta \right) dV \geq 0. \end{aligned} \quad (19)$$

65 **Remark 1.** Regarding the FEniCS implementation, we confine ourselves to alternate minimiza-  
 66 tion algorithm (Bourdin, 2007) to minimize the energy functional Eq. (5), so that  $\nabla \sqrt{a^3(\alpha)} = 0$ .  
 67 Thus, Eq. (18)<sub>2</sub> simplifies as

$$\int_{\Omega} \left( -\sqrt{a^3(\alpha)} (J-1) - \frac{1}{\kappa} p \right) q dV - \frac{\varpi h^2}{2\mu} \sum_{e=1}^{n_{el}} \int_{\Omega^e} J\mathbf{C}^{-1} : \sqrt{a^3(\alpha)} (\nabla p \otimes \nabla q) dV = 0. \quad (20)$$

68

**Remark 2.** For the characteristic element length  $h$ , we set  $h$  equals to the cell diameter for given mesh, and the non dimensional, non negative stability parameter  $\varpi$  are given as.

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71 h = CellDiameter(mesh)
72 varpi_ = 1.0
73 varpi = project(varpi_*h**2/(2.0*mu), FunctionSpace(mesh, 'DG', 0))

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#### 4. Strain energy decomposition

Following Tang et al. (2019), we rewritten the strain energy as

$$\widetilde{W}(\mathbf{F}, \alpha) = \widetilde{W}_{\text{act}}(\mathbf{F}, \alpha) + \widetilde{W}_{\text{pas}}(\mathbf{F}, \alpha), \quad (21)$$

where the active part of the strain energy is

$$\widetilde{W}_{\text{act}}(\mathbf{F}, \alpha) = a(\alpha) \frac{\mu}{2} \sum_{i=1}^3 H(\lambda_i - 1) (\lambda_i^2 - 1 - 2 \ln \lambda_i) + a^3(\alpha) H(J - 1) \frac{1}{2} \kappa (J - 1)^2, \quad (22)$$

and the passive part of the strain energy is

$$\widetilde{W}_{\text{pas}}(\mathbf{F}, \alpha) = \frac{\mu}{2} \sum_{i=1}^3 H(1 - \lambda_i) (\lambda_i^2 - 1 - 2 \ln \lambda_i) + H(1 - J) \frac{1}{2} \kappa (J - 1)^2, \quad (23)$$

where  $\lambda_i$ ,  $i = 1, 2, 3$  are principal stretches,  $H(x) = \begin{cases} 1 & x \geq 0 \\ 0 & x < 0 \end{cases}$  is the Heaviside step function. This decomposition scheme meets the non-negativeness of strain energy constraint (Ye et al., 2020).

##### 4.1. Compute the principal stretches $\lambda_i$

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

$$d = \frac{\text{tr } \mathbf{C}}{3}, \quad e = \sqrt{\frac{\text{tr}((\mathbf{C} - d\mathbf{I})^2)}{6}}, \quad f = \frac{1}{e}(\mathbf{C} - d\mathbf{I}), \quad g = \frac{\det f}{2}, \quad (24)$$

and assuming the eigenvalues satisfying  $\lambda_3^2 \leq \lambda_2^2 \leq \lambda_1^2$ , we could obtain (Smith, 1961)

$$\lambda_1^2 = d + 2e \cos\left(\frac{\arccos g}{3}\right), \quad \lambda_3^2 = d + 2e \cos\left(\frac{\arccos g}{3} + \frac{2\pi}{3}\right), \quad \lambda_2^2 = 3d - \lambda_1^2 - \lambda_3^2. \quad (25)$$

**Remark 3.** For coding in FEniCS with UFL language is straightforward.

#### 5. Numerical examples

##### 5.1. Benchmark : Uniaxial tension of a hyperelastic bar

We consider a three-dimensional hyperelastic bar of length  $L = 1.0$ , height  $H = 0.1$  and thickness  $W = 0.02$  in a state of uniaxial stress  $\sigma_1 = \sigma$  and  $\sigma_2 = \sigma_3 = 0$  with the imposed displacement boundary conditions on the left end  $u_x = 0$  and on the right end  $u_x = tL$ . Let the stretch along the axis of the loading direction be  $\lambda_1 = \lambda$ . The incompressibility results in that

the stretches in the directions transverse to the axial loading direction are  $\lambda_2 = \lambda_3 = 1/\sqrt{\lambda}$ . The critical value of  $t_c$  is determined by

$$a'(0) \frac{\mu}{2} (\text{tr } \mathbf{C} - 3) + \frac{\mathcal{G}_c}{c_w} \frac{w'(0)}{\ell} = 0, \quad (26)$$

which can be reformulated as

$$\lambda^3 + p_0 \lambda + q_0 = 0, \quad p_0 = -\frac{3 c_w \mu \ell + \mathcal{G}_c}{c_w \mu \ell}, \quad q_0 = 2, \quad (27)$$

giving the critical loading

$$t_c = 2 \sqrt{-\frac{p_0}{3}} \cos \left( \frac{1}{3} \arccos \left( \frac{3q_0}{2p_0} \sqrt{\frac{-3}{p_0}} \right) \right) - 1. \quad (28)$$

## 5.2. Revisiting crack nucleation in elastomer

Regarding the nucleation issues in elastomer, see the Section 3.1 in the work of Kumar et al. (2018).

“ When deformed, because of their typical near incompressibility, elastomers are prone to feature regions where the hydrostatic part of the stress is very large while, at the same time, the strain energy is comparatively small (because the strain is small). This has been long known to be the case, for instance, near reinforcing fillers in filled elastomers; see, e.g., the analysis in Lefèvre et al. (2015). As outlined in the Introduction, it is precisely in those regions that the nucleation of internal fracture often occurs first. Physically, this can be understood at once from the recognition that the concentration of large hydrostatic stresses – in spite of the absence of strain – triggers the growth of the underlying microscopic defects, and thus, the nucleation of fracture at macroscopic length scales. ”

**Remark 4.** In the generic variational phase-field model, nucleation is due to the loss of stability, i.e. the strain energy reaches the critical value defined by

$$\mathcal{W}(\mathbf{F}) \propto -\frac{\mathcal{G}_c w'(0)}{c_w \ell a'(0)},$$

which is inconsistent with the experiments (Kumar and Lopez-Pamies, 2020). Consequently, they introduce a external driving force  $\mathcal{C}_e$  which is purely phenomenological, furthermore, contaminates the variational feature. The ideal one could be the one preserves the variational feature and also captures the experiments well (Possibly Chad Landis will bring his idea.).

**Remark 5.** TO DO: If not, herein, other possibility is checking this reference (Pourmodheji et al., 2019) to see if it relates to the issues.

- 5.3. (ida) *Imposing asymptotic displacements field (Long and Hui, 2015) and comparing the crack opening displacements*
- 5.4. (jason) *Some comparison with the XFEM prediction (Legrain et al., 2005; Rashetnia and Mohammadi, 2015)*
- 5.5. (ida) *Maybe or NOT one showcase simulation*
- 5.6. (ida) *or nucleation following the paper by kumar and oscar lopez pamies*

## 6. Concluding and remarks

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