# Thermo-mechanical phase-field model for porous-ductile fracture

J. Schulte \* <sup>1</sup>, M. Dittmann<sup>1</sup>, F. Aldakheel<sup>2</sup> and C. Hesch<sup>1</sup>

<sup>1</sup>Chair of Computational Mechanics, University of Siegen, Paul-Bonatz-Strasse 9-11, 57076 Siegen, Germany <sup>2</sup>Institute of Continuum Mechanics, Leibnitz University Hannover, Appelstr. 11, 30167 Hannover, Germany

#### Abstract.

Phase-field methods to regularize sharp interfaces represent a well established technique nowadays. In fracture mechanics, recent works have shown the capability of the method for brittle as well as ductile problems formulated within the fully non-linear regime [2, 3].

In this contribution, we propose a novel framework to simulate porous-ductile fracture in isotropic thermoelasto-plastic solids undergoing large deformations [1]. Therefore, a modified Gurson-Tvergaard-Needelman GTN-type plasticity model is combined with a phase-field fracture approach to account for a temperaturedependent growth of voids on micro-scale followed by crack initiation and propagation on macro-scale. The multi-physical formulation is completed by the incorporation of an energy transfer into thermal field such that on the other hand the temperature distribution depends on the evolution of the plastic strain and the crack phase-field.

Eventually, a number of numerical investigations show not only the possibilities of the approach for a multiphysical analysis of complex material behavior, but also the accordance with experimental results in terms of hardening, necking, crack initiation and propagation. Moreover, a further example based on the third Sandia Fracture Challenge is applied to demonstrate the capability of the model for the prediction of three-dimensional fracture pattern in complex geometries.

#### Introduction

The analysis of crack initiation and propagation in ductile materials plays an important role in predicting failure mechanisms for various engineering applications. The phase-field approach to fracture has been proven to be a very powerful technique to simulate crack phenomena in multi-physical environments [2, 3]. The goal of this work is to present a theoretical and a computationally efficient framework for ductile, porous materials undergoing thermomechanical loading conditions in order to study the influence of the growth of micro-voids, as well as the final rupture at the macro-scale [1].

#### 1 Governing equations

A theory for coupled thermomechanical response at fracture undergoing large deformations is outlined in this section. The underlying, three-dimensional (d = 3) system leads to a multi-field setting with seven fields

$$\{\boldsymbol{\varphi}, \boldsymbol{\mathfrak{s}}, \boldsymbol{\theta}, \boldsymbol{\alpha}, r^{\mathrm{p}}, \boldsymbol{F}^{\mathrm{p}}, f\},$$
(1)

which are the deformation map, the crack phase-field, the absolute temperature and the four plastic fields, which are the equivalent plastic strain, its dual hardening force, the plastic deformation gradient and the void volume fraction. Here, the void volume fraction is defined as

$$f = 1 - \frac{1 - f_0}{J^{\rm p}} \tag{2}$$

<sup>\*</sup>Corresponding author: jonathan.schulte@uni-siegen.de

and is assumed as a micro-mechanically motivated damage variable, related to the plastic deformation gradient through its determinant  $J^{p}$ .  $f_{0}$  is the initial void volume fraction.

The deformation gradient  $\mathbf{F} = \mathbf{F}^{e} \mathbf{F}^{p}$  and its determinant  $J = J^{e} J^{p}$  are decomposed multiplicatively into elastic and plastic parts. Moreover, the fracture insensitive isochoric and volumetric parts are given by

$$\tilde{\bar{F}}^{\mathrm{e}} = \sum_{a} \left[ (J^{\mathrm{e}})^{-1/d} \lambda_{a}^{\mathrm{e}} \right]^{g(\mathfrak{s})} \boldsymbol{n}_{a} \otimes \boldsymbol{N}_{a} \quad \text{and} \quad \tilde{J}^{\mathrm{e}} = \begin{cases} (J^{\mathrm{e}})^{g(\mathfrak{s})} & \text{if} \quad J^{\mathrm{e}} > 1\\ J^{\mathrm{e}} & \text{else} \end{cases},$$
(3)

postulating that fracture requires a local state of tensile/shear deformation.  $\lambda_a^e$  are the elastic principal stretches,  $g(\mathfrak{s})$  is a polynomial degradation function and  $\mathbf{n}_a$  and  $\mathbf{N}_a$  are the principal directions of the left and right stretch tensors.

# 1.1 Energetic response function

The stored energy function  $\widehat{\Psi}$  for the coupled problem takes the form

$$\widehat{\Psi} = \widehat{\Psi}^{\mathrm{e}}(\boldsymbol{F}, \boldsymbol{F}^{\mathrm{p}}, \mathfrak{s}, \theta) + \widehat{\Psi}^{\theta}(\theta) + \widehat{\Psi}^{\mathrm{p}}(\alpha, \nabla \alpha, \theta) + \widehat{\Psi}^{\mathrm{f}}(\mathfrak{s}, \nabla \mathfrak{s}, \Delta \mathfrak{s}),$$
(4)

which reflects a coupling of gradient thermoplasticity with gradient damage mechanics. The isotropic elastic contribution is decomposed

$$\widehat{\Psi}^{\rm e} = \widehat{\Psi}^{\rm e}_{\rm vol}(\widetilde{J}^{\rm e}(J, J^{\rm p}, \mathfrak{s}), \theta) + \widehat{\Psi}^{\rm e}_{\rm dev}(\widetilde{\widetilde{F}}^{\rm e}(F, F^{\rm p}, J, \mathfrak{s})),$$
(5)

into volumetric and deviatoric parts. As a representative constitutive law used for the numerical examples we introduce the thermomechanically extended Neo-Hookean material model

$$\widehat{\Psi}_{\rm vol}^{\rm e}(\tilde{J}^{\rm e},\theta) = \frac{\kappa}{2} \left( \frac{(\tilde{J}^{\rm e})^2 - 1}{2} - \ln[\tilde{J}^{\rm e}] \right) - \frac{3}{2} \beta \kappa(\theta - \theta_0) \left( \tilde{J}^{\rm e} - \frac{1}{\tilde{J}^{\rm e}} \right)$$
(6)

and

$$\widehat{\Psi}_{\text{dev}}^{\text{e}}(\tilde{\vec{F}}^{\text{e}}) = \frac{\mu}{2} (\tilde{\vec{F}}^{\text{e}} : \tilde{\vec{F}}^{\text{e}} - 3).$$
(7)

Therein,  $\mu > 0$  and  $\kappa > 0$  denote the shear modulus and the bulk modulus, respectively.  $\theta_0$  is a reference temperature and  $\beta$  is the linear thermal expansion coefficient.

The purely thermal contribution to the stored energy (4) is assumed to have the simple form

$$\widehat{\Psi}^{\theta}(\theta) = c \left(\theta - \theta_0 - \theta \ln\left(\frac{\theta}{\theta_0}\right)\right),\tag{8}$$

where  $c \ge 0$  is a constant parameter representing the specific heat capacity. Moreover, the Piola-Kirchhoff heat flux vector can be defined as

$$\boldsymbol{Q}(\boldsymbol{F},\mathfrak{s},\theta,\nabla\theta) := -\boldsymbol{K}(\boldsymbol{F},\mathfrak{s},\theta)\nabla\theta \tag{9}$$

to account for the heat transfer. This is known as Duhamel's law of heat conduction, where K is the material thermal conductivity tensor

$$\boldsymbol{K}(\boldsymbol{F},\mathfrak{s},\theta) := [K_0(1 - w_{\mathrm{K}}(\theta - \theta_0))(1 - \mathfrak{s}) + K^{\mathrm{conv}}\mathfrak{s}]\boldsymbol{C}^{-1}.$$
(10)

Note that in case of fracture, the conduction degenerates locally such that we achieve a pure convection problem and the heat transfer depends on the crack opening width. Here, we formulate the conductivity tensor K in terms of the phase-field parameter  $\mathfrak{s}$ . Moreover,  $w_{\rm K}$  is a thermal softening parameter,  $K_0$  is a conductivity parameter related to the reference temperature,  $K^{\rm conv}$  is a convection parameter and  $C = \mathbf{F}^{\rm T} \mathbf{F}$  denotes the right Cauchy-Green tensor.

We focus on the equivalent plastic strain  $\alpha$  and its gradient  $\nabla \alpha$  with the particular form for the energetic contributions

$$\widehat{\Psi}^{\mathbf{p}}(\alpha, \nabla \alpha, \theta) = \int_{0}^{\alpha} \widehat{y}(\tilde{\alpha}, \theta) \,\mathrm{d}\tilde{\alpha} + y_{0}(\theta) \frac{l_{\mathbf{p}}^{2}}{2} \|\nabla \alpha\|^{2} \,.$$
(11)

Here,  $l_{\rm p}$  is a plastic length scale related to a strain-gradient hardening effect and accounts for size effects to overcome the nonphysical mesh sensitivity of the localized plastic deformation in softening materials. Moreover,  $\hat{y}(\alpha, \theta)$  is a temperature dependent isotropic local hardening function obtained form experimental data.

The variational derivative of  $\widehat{\Psi}^{\mathbf{p}}$  with respect to  $\alpha$  yields

$$r^{\mathbf{p}} := \delta_{\alpha} \widehat{\Psi}^{\mathbf{p}} = \partial_{\alpha} \widehat{\Psi}^{\mathbf{p}} - \operatorname{Div}[\partial_{\nabla \alpha} \widehat{\Psi}^{\mathbf{p}}]$$
(12)

reflecting the characteristics of the gradient-extended model under consideration.

Eventually, the phase-field fracture contribution has to be formulated. Therefore, the sharp-crack surface topology  $\Gamma$  is replaced by a regularized functional

$$\Gamma_{1}(\mathfrak{s}) = \int_{\mathcal{B}_{0}} \widehat{\gamma}(\mathfrak{s}, \nabla \mathfrak{s}, \Delta \mathfrak{s}) \, \mathrm{d}V \quad \text{with} \quad \widehat{\gamma}(\mathfrak{s}, \nabla \mathfrak{s}, \Delta \mathfrak{s}) = \frac{1}{4l_{\mathrm{f}}} \mathfrak{s}^{2} + \frac{l_{\mathrm{f}}}{2} \|\nabla \mathfrak{s}\|^{2} + \frac{l_{\mathrm{f}}^{3}}{4} (\Delta \mathfrak{s})^{2}. \tag{13}$$

The functional is based on the crack surface density function  $\hat{\gamma}$  per unit volume of the solid and the fracture length scale parameter  $l_{\rm f}$  that governs the regularization. Note that in the limit  $l_{\rm f} \to 0$ , the regularized crack surface functional  $\Gamma_{\rm l}(\mathfrak{s})$  converges to the sharp crack surface  $\Gamma$ . For ductile fracture, we require additionally that  $l_{\rm p} \geq l_{\rm f}$ . For the given fracture surface functional introduced in (13), we define the critical energy required to create a diffusive fracture topology by

$$W^{\rm cr} = \int_{\mathcal{B}_0} \widehat{g}_{\mathbf{c}}(\alpha) \,\widehat{\gamma}(\mathfrak{s}, \nabla \mathfrak{s}, \Delta \mathfrak{s}) \,\mathrm{d}V,\tag{14}$$

in terms of the Griffith-type critical energy release rate  $\hat{g}_c$ , which is decomposed additively into elastic and plastic contributions  $\hat{g}_c(\alpha) = g_{c,p} + g_{c,e} \exp[-\omega_f \alpha]$ , using the modeling parameters  $\{g_{c,e}, g_{c,p}, \omega_f\}$ . Summarized, the phase-field fracture contribution is given in terms of the crack-density function as

$$\widetilde{\Psi}^{\mathrm{f}}(\mathfrak{s}, \nabla \mathfrak{s}, \Delta \mathfrak{s}) = \widehat{g}_{\mathrm{c}}(\alpha) \,\widehat{\gamma}(\mathfrak{s}, \nabla \mathfrak{s}, \Delta \mathfrak{s}) 
= \frac{\widehat{g}_{\mathrm{c}}(\alpha)}{4l_{\mathrm{f}}} \mathfrak{s}^{2} + \frac{\widehat{g}_{\mathrm{c}}(\alpha) \, l_{\mathrm{f}}}{2} \nabla \mathfrak{s} \cdot \nabla \mathfrak{s} + \frac{\widehat{g}_{\mathrm{c}}(\alpha) \, l_{\mathrm{f}}^{3}}{4} (\Delta \mathfrak{s})^{2}$$
(15)

which defines the crack resistance force via the variational derivative with respect to  $\mathfrak{s}$ 

$$r^{\mathrm{f}} := \delta_{\mathfrak{s}} \widehat{\Psi}^{\mathrm{f}} = \partial_{\mathfrak{s}} \widehat{\Psi}^{\mathrm{f}} - \mathrm{Div}[\partial_{\nabla \mathfrak{s}} \widehat{\Psi}^{\mathrm{f}}] + \Delta[\partial_{\Delta \mathfrak{s}} \widehat{\Psi}^{\mathrm{f}}].$$
(16)

# 1.2 Dissipative response function

Regarding the plastic material behavior, we postulate a modified Gurson model for porous plasticity as

$$\widehat{\Phi}^{\rm p}(\boldsymbol{\tau}, r^{\rm p}) = \frac{\sigma_{\rm eq}^2}{r^{\rm p2}} + 2q_1 f \cosh\left[\frac{3}{2}q_2\frac{p}{r^{\rm p}}\right] - \left(1 + (q_1 f)^2\right) \tag{17}$$

in terms of the Kirchhoff stress which is related to the Cauchy stress by  $\boldsymbol{\sigma} = \boldsymbol{\tau}/J$  and the dissipative resistance force  $r^{\rm p}$ . Here,  $\sigma_{\rm eq} = \sqrt{3/2} \|\boldsymbol{\tau}_{\rm dev}/J\|$  represents the von Mises equivalent stress, whereas  $p = \frac{1}{3} \operatorname{tr}[\boldsymbol{\tau}/J]$  denotes the local pressure along with the growth-based void volume fraction f and fitting parameters  $q_1 \approx 1.5$  and  $q_2 \approx 1.0$ .

On the fracture part, we define a crack threshold function  $\widehat{\Phi}^{f}$  based on the constitutive representation

$$\widehat{\Phi}^{\mathrm{f}}(\mathcal{H} - r^{\mathrm{f}}) = \mathcal{H} - r^{\mathrm{f}},\tag{18}$$

where the energetic driving force  $\mathcal{H}$  is bounded by the crack resistance force  $r^{f}$  dual to the fracture phase-field  $\mathfrak{s}$ .

The associated plastic evolution equations are defined as  $d^{\rm p} = \lambda^{\rm p} \frac{\partial \widehat{\Phi}^{\rm p}}{\partial \tau}$  and  $\dot{\alpha} = -\lambda^{\rm p} \frac{\partial \widehat{\Phi}^{\rm p}}{\partial r^{\rm p}}$ , whereas the evolution equation for the crack phase-field reads  $\dot{\mathfrak{s}} = \lambda^{\rm f} \frac{\partial \widehat{\Phi}^{\rm f}}{\partial (\mathcal{H} - r^{\rm f})}$ .

Eventually, we define the internal dissipation density function  $\mathcal{D}_{int} := \nu_p \tau : d^p + \nu_f \mathcal{H} \dot{s}$ , where  $\nu_p$  is a constant dissipation factor typically chosen in the range of 85% to 95% in the context of thermoplasticity. In addition,  $\nu_f$  is introduced as fracture dissipation factor based on the discussions related to an energy transfer into the thermal field in [4] and the references therein.

#### 2 Numerical Example

To illustrate the performance and applicability of the thermo-porous ductile fracture model to complex three-dimensional geometries, a numerical example is considered in this section. Therefore, we adopt CAD data from the third Sandia Fracture Challenge and apply the steel like material setting given. Within the quasi-static simulation setting, the lower end of the hollow body is fixed in space while the upper end is moved upwards. No heat in- or outflow is allowed. Figure 1 shows the von Misses residual stress distribution within the deformed configuration on fully ruptured state, where the fractured regions with g < 0.15 are removed from the contour plot for visualization purposes.



Figure 1. Third SFC. Von Mises stress distribution at fully ruptured state.

### Acknowledgments

Support for the present research was provided by the Deutsche Forschungsgemeinschaft (DFG) under grant HE5943/8-1 and DI2306/1-1.

### References

- [1] M. Dittmann, F. Aldakheel, J. Schulte, M. Krüger, P. Wriggers, and C. Hesch. Phase-field modeling of porous-ductile fracture in finite thermo-elasto-plastic solids. *submitted* (2018).
- [2] M. Dittmann, F. Aldakheel, J. Schulte, P. Wriggers, and C. Hesch. Variational Phase-Field Formulation of Non-Linear Ductile Fracture. *Computer Methods in Applied Mechanics and Engineering* 342 (2018.), pp. 71–94.
- [3] M. Dittmann, M. Krüger, F. Schmidt, S. Schuß, and C. Hesch. Variational modeling of thermomechanical fracture and anisotropic frictional mortar contact problems with adhesion. *Computational Mechanics* 63 (2019), pp. 571–591.
- [4] J. Schulte, M. Krüger, M. Dittmann, and C. Hesch. Multi-field modeling of thermomechanical coupled fracture problems. *Proceedings in Applied Mathematics and Mechanics* (2018). DOI: 10.1002/pamm. 201800348.