Phase-field Fracture with Representative Crack Elements for Non-linear Material Behaviour

Johannes Storm\textsuperscript{1,*} and Michael Kaliske\textsuperscript{1,**}

\textsuperscript{1} Institute for Structural Analysis, Technische Universität Dresden, 01062 Dresden, Germany

The mechanical energy potential of phase-field fracture models is subdivided into a portion which (actively) drives the crack and a passive portion. This decompositions depends further on the crack state (opened, closed) in order to consider the re-contact of the crack surfaces. The identification of the crack state and the decomposition is mostly approximated based on splits of the deformation or stress tensor. Stobel and Seelig \cite{Stobel}, and Steinke and Kaliske \cite{Steinke} have shown unrealistic predictions for the crack kinematic for those models in quasi-static and dynamic analyses. The approach proposed by these authors allows to predict the crack kinematic consistently. Nevertheless, this model is restricted to linear, isotropic elasticity and small deformations.

In Storm et al. \cite{Storm}, the underlying concept is generalised. The crack kinematics is consistently obtained from a representative, discrete crack model and coupled to the phase-field model by means of a variational homogenisation formulation. Thus, the crack driving force is a unique result of the framework of Representative Crack Elements. Analytical solutions for the mechanical problem of the representative crack element applied to linear, anisotropic elasticity and linear thermo-elasticity at small deformations are presented there.

In the current contribution to the method of phase-field fracture, the framework for Representative Crack Elements is applied to non-linear bulk materials. The iterative solution scheme for the representative crack element is presented and applied to elasticity with crack surface friction, visco-elastic and elasto-plastic materials.

1 Introduction

The framework of Representative Crack Elements (RCE) for phase-field fracture is used to derive regularised crack models where the crack kinematics follows those of a discrete crack model with contact. Therefore, a representative part of discrete crack is coupled to the phase-field model by means of computational homogenisation. This approach can be formulated in a fully variational framework and avoids artificial definitions for crack contact and the crack driving force.

The RCE framework for phase-field fracture allows to derive crack models, which successfully represent the crack kinematics of discrete cracks, and can, therefore, replace discrete crack models. This property is shown to be missing in the phase-field formulations with artificial splits so far, e.g. in Strobl and Seelig \cite{Strobl}, Schlüter \cite{Schluter} and Steinke and Kaliske \cite{Steinke}. Their important findings are ignored in further developments in phase-field fracture, which have yield to numerous models based on insufficient contact and crack driving formulations (splits). The crack propagation at a shear plate with different models for the initial crack in Fig. 1 demonstrates the importance of realistic crack kinematics.

![Fig. 1: Comparison of crack propagation at a single-edge notch specimen at shear load with a) a discrete initial crack, b) a phase-field initial crack applying phase-field fracture with spectral split \cite{5} and c) a phase-field initial crack applying phase-field fracture derived from RCE framework \cite{3}.

The extension of the variational RCE framework towards non-linear bulk material is presented in the following. The basic relations of computational homogenisation applied to phase-field fracture are introduced. The RCE problem for non-linear constitutives is formulated, linearised and an iterative solution scheme derived.

* Corresponding author: e-mail johannes.storm@tu-dresden.de

** Corresponding author: e-mail michael.kaliske@tu-dresden.de, phone +49 351 463 34386, fax +49 351 463 37086

© 2021 The Authors Proceedings in Applied Mathematics & Mechanics published by Wiley-VCH GmbH

Proceedings in Applied Mathematics & Mechanics

2020; 20:1 e202000207. www.gamm-proceedings.com

https://doi.org/10.1002/pamm.202000207 © 2021 The Authors Proceedings in Applied Mathematics & Mechanics published by Wiley-VCH GmbH

1 of 5
2 Application of Computational Homogenisation to Phase-field Fracture

The variational formulation for continuum solid mechanics can be given as Principle of Virtual Power. The total virtual power balances the virtual power of internal stresses and external forces. This first variation has to vanish for any admissible field of generalised virtual displacements \( \delta v \) and the corresponding generalised virtual strains \( D(\delta v) \)

\[
\delta P^{\text{int}} = P^{\text{int}}(\delta v, D(\delta v)) = P^{\text{int}}(D(\delta v)) - P^{\text{ext}}(\delta v) = 0, \quad \forall \delta v \in \text{Var}_v. \tag{1}
\]

For quasi-static phase-field fracture, the generalised displacements consist of the mechanical displacement vector and the phase-field variable

\[
v = \begin{bmatrix} u \\ p \end{bmatrix}. \tag{2}
\]

The generalised strains for small deformations are given by the linearised strain tensor, the phase-field variable and its gradient

\[
D(v) = \begin{bmatrix} E \\ p \\ \nabla p \end{bmatrix}. \tag{3}
\]

The dual products of generalised displacements and strains with the generalised external forces \( f \) and internal stresses \( \Sigma \) form the power terms

\[
P^{\text{int}}(D(\delta v)) = \int_B (\langle \Sigma, D(\delta v) \rangle) \, dV = \int_B [\sigma^E : \delta E + \sigma^p \delta p + \sigma^\nabla \cdot \delta p] \, dV, \tag{4}
\]

\[
P^{\text{ext}}(\delta v) = \int_B (\langle f, \delta v \rangle) \, dV = \int_B f \cdot \delta u \, dV \tag{5}
\]

for the global minimisation task. The stresses follow the constitutive laws given in the form of a HELMHOLTZ free energy potential as

\[
\sigma^E = \frac{\partial \psi(E, p, \nabla p, \alpha)}{\partial E}, \quad \sigma^p = \frac{\partial \psi(E, p, \nabla p, \alpha)}{\partial p}, \quad \alpha = -\frac{\partial \psi(E, p, \nabla p, \alpha)}{\partial \alpha}, \tag{6}
\]

where \( \alpha \) are the internal variables.

In the following, parts of the constitutive behaviour are derived from a representative crack element by means of homogenisation. The RCE forms a classical, variational problem in the framework of CAUCHY-BOLTZMANN mechanics, where

\[
\tilde{v} = \begin{bmatrix} \tilde{u} \end{bmatrix}, \quad \tilde{D}(\tilde{v}) = \begin{bmatrix} \tilde{E} \end{bmatrix}. \tag{8}
\]

Both variational problems are coupled by the following kinematical insertion and homogenisation operators

\[
\Gamma^v(u|x, p|x) = \begin{bmatrix} u|x \end{bmatrix}, \quad \Gamma^D(v|\bar{E} | x, p, \nabla p|x) = \begin{bmatrix} E|x \cdot (\bar{x} - \bar{x}^{\text{eff}}) \end{bmatrix}, \tag{9}
\]

\[
\mathcal{H}^v(u) = \begin{bmatrix} \frac{1}{V} \int_B u \, dV \\ 0 \end{bmatrix}, \quad \mathcal{H}^D(v|\tilde{E}) = \begin{bmatrix} \frac{1}{V} \int_B \tilde{E} \, dV \\ 0 \end{bmatrix}. \tag{10}
\]

The thermo-dynamically conjugated internal stresses and external forces of the deformed RCE

\[
\sigma^E|_x = \frac{1}{V} \int_B [\sigma - \bar{f} \otimes^* (\bar{x} - \bar{x}^{\text{eff}})] \, dV, \quad f^u|_x = \frac{1}{V} \int_B \bar{f} \, dV \tag{11}
\]

are a direct result of the Principle of Multiscale Virtual Power [6], which balances the total virtual power of the two coupled variational problems.
### 3 Concept of Representative Crack Elements (RCE)

The constitutive behaviour for phase-field fracture is postulated as superposition of those of intact material $\psi^0$ and fully degraded (cracked) material $\psi^c$

$$
\psi(E, p, \nabla p, \alpha) = \psi^c(E, \alpha) + g(p) \left[ \psi^0(E, \alpha) - \psi^c(E, \alpha) \right] + \psi^{pb}(E, p, \nabla p, \alpha).
$$  \tag{12}

The quite simple model given in Fig. 2 is proposed to represent the deformation kinematics at a crack, i.e. $\psi^c$. Two blocks of homogeneous material ($B_1, B_2$) and equal size are separated by a discrete crack $B^\Gamma$, where crack surface contact is under consideration. A CARTESIAN coordinate system ($N_1, N_2, N_3$) is introduced for the RCE. The first axis $N_1$ coincides with the normal direction of the crack surface. Homogeneous deformations are postulated in the subdomains of the RCE.

![Fig. 2: Sketch of an RCE with a discrete crack and local coordinates in a) undeformed and b) deformed configuration.](image)

The strain through the crack

$$
\bar{E}^\Gamma \cdot N_1 = \frac{1}{l_1} \Delta \bar{u}^\Gamma
$$  \tag{13}

follows from the kinematic compatibility at the boundaries of the subdomains, where $l_1$ is the initial thickness of the crack and $\Delta \bar{u}^\Gamma$ the displacement discontinuity. A limit analysis for $l_1 \to 0$ via L'HÔPITAL's rule yields

$$
\bar{E}(\bar{x}) = E|_{x} + \sum_{i=1}^{3} \Gamma_i N_i \otimes^s N_1, \quad \forall \bar{x} \in \{B_1 \cup B_2\}
$$  \tag{14}

and the displacement field

$$
\bar{u}(\bar{x}) = u|_{x} + E|_{x} \cdot (\bar{x} - \bar{x}^\text{ref}) + \kappa(\bar{x}) \sum_{i=1}^{3} \Gamma_i N_i \quad \text{with } \kappa(\bar{x}) = \frac{1}{2} l_1 \text{sgn} \left( N_1 \cdot (\bar{x} - \bar{x}^\text{ref}) \right) - N_1 \cdot (\bar{x} - \bar{x}^\text{ref}).
$$  \tag{15}

This displacement field is defined and linear in terms of $u|_{x}, E|_{x}$ and $\Gamma$. The first two terms are prescribed by the phase-field problem to the RCE model via DIRICHLET conditions, whereas the crack deformations $\Gamma_i$ are unknown. The linearisation and discretisation of this minimisation task for the RCE, compare Eq. (1), yield the iterative NEWTON-RAPHSON scheme

$$
\left[ K^{\Gamma_i, \Gamma_i} \right] \times \left[ \Delta \Gamma_i \right] = \left[ R^{\Gamma_i} \right],
$$  \tag{16}

where

$$
K^{\Gamma_i, \Gamma_i} = (N_1 \otimes^s N_j) : \frac{\partial \sigma}{\partial E} : (N_i \otimes^s N_1), \quad R^{\Gamma_i} = (N_1 \otimes^s N_j) : \bar{\sigma}.
$$  \tag{17}

Then, the stress, the internal variables and material tangent for the phase-field formulations read

$$
\sigma^c|_{x} = \sigma, \quad \alpha^c|_{x} = \alpha, \quad \dot{\alpha}^c|_{x} = \dot{\alpha},
$$  \tag{18}

$$
\frac{\partial \sigma^c - u|_{x}}{\partial E|_{x}} = \frac{\partial \sigma}{\partial E} - \left( N_i \otimes^s N_1 \right) \cdot \left( N_i \otimes^s N_1 \right)^{-1} \left( N_1 \otimes^s N_j \right) : \frac{\partial \sigma}{\partial E}.
$$  \tag{19}
4 Applications

The usage of common material models given in implicit or explicit formulations for the bulk material of at the RCE is straightforward and do not require modifications or a special treatment. Basic properties and kinematical consistency are demonstrated at a pre-cracked compression plate shown in Fig. 3.

Linear visco-elasticity, compare [7], results in constant material tangents for constant time increments. Therefore, those problems can be covered by the linear RCE framework in [3]. However, the concept of thermo-dynamics with internal variables for irreversible and dissipative processes is first addressed in the formulation above. The compressive displacement and its release (starting at 60% and ending at 70% of the time) cause viscous deformations and, thus, crack opening during unloading as well as delayed crack closing. Both effects are correctly predicted by the simulation shown in Fig. 4.

\[
l_x = \begin{bmatrix} 0, 1, 0 \end{bmatrix}
\]

**Fig. 3:** Pre-cracked compression plate with clamped edges and DIRICHLET boundary condition for the initial phase-field crack.

**Fig. 4:** a) Displacements normal to the crack at 80% of the simulation time and b) the global energy balance of the system.

**Fig. 5:** Reaction forces of a pre-cracked compression plate for an elastic and an elasto-plastic bulk material.

**Fig. 6:** a) Tensile and shear strain history and b) reaction forces at a pre-cracked plate with periodic boundary conditions a for phase-field crack model with crack surface friction.

For the bulk material using MOHR-COU aquant ela-plasticity with isotropic hardening, the permanent deformation induced during compression causes an early crack opening. This can be seen in Fig. 5 comparing the normal reaction force to those of a pure elastic simulation, where the compression is fully released after 80% of time.

The presented framework allows also to handle further deformation mechanisms which directly act at the crack surface, e.g., friction, corrosion etc. Crack surface friction of COU aquant type is considered at a pre-cracked plate applied to tension and shear strains by means of periodic boundary conditions. The normal and tangential reaction force is shown in Fig. 6 for different friction coefficients. Sticking and sliding states can be clearly distinguished. The corresponding deformation states of the compressed plate, at the end of the sticking state and during the plate sliding are shown in Fig. 6b.

Acknowledgements The authors gratefully acknowledge the financial support by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under contract 352324592 (KA1163/40-1) within the Priority Programme 2020. Open access funding enabled and organized by Projekt DEAL.

Correction added on 19 February 2021, after first online publication: Johannes Storm was designated as corresponding author.

References

[1] M. Strobl and T. Seelig, Proceedings in Applied Mathematics and Mechanics 15, 155–156 (2015).
[2] C. Steinke and M. Kaliske, Computational Mechanics 63, 1019–1046 (2018).
[3] J. Storm, D. Supriatna, and M. Kaliske, International Journal for Numerical Methods in Engineering 121, 779–805 (2020).
[4] A. Schlüter, Phase Field Modeling of Dynamic Brittle Fracture, PhD Thesis, Technische Universität Kaiserslautern, (2018).
[5] C. Miehe, F. Welschinger, and M. Hofacker, International Journal for Numerical Methods in Engineering 83, 1273–1311 (2010).
[6] P. J. Blanco, P. J. Sánchez, E. A. Souza Neto, and R. A. Feijóo, Archives of Computational Methods in Engineering 23, 1–63 (2014).
[7] B. Yin, J. Storm, and M. Kaliske, International Journal of Fracture (submitted).