Goal-oriented error estimation and mesh adaptivity for phase-field-based fracture propagation

T. Wick [a] [b],*

[a] Fakultät für Mathematik, Lehrstuhl M17, Technische Universität München,
Boltzmannstr. 3, D-85747 Garching bei München, Germany

[b] Johann Radon Institute for Computational and Applied Mathematics (RICAM), Austrian Academy of Sciences,
Altenberger Str. 69, 4040 Linz, Austria

*thomas.wick@ricam.oeaw.ac.at

Abstract. *In this study, we consider phase-field-based fracture propagation in solid mechanics. The phase-field model is based on a thermodynamically-consistent version proposed by Miehe, Welschinger, Hofacker. The main focus is on goal-oriented functional evaluations using a partition-of-unity dual-weighted residual estimator for accurate measurement of, for example, stresses or fluxes over parts of the boundary. Our developments are substantiated with a numerical test.*

Keywords: fracture; phase-field; dual-weighted residual method; goal-oriented error estimation

1 INTRODUCTION

The purpose of this study is on a posteriori error analysis accompanied with local mesh adaptivity for quasi-static phase-field-based fracture propagation problems. Specifically, we concentrate on goal-oriented error estimation with the dual-weighted residual (DWR) method [1, 2]. Here, a novel variational-based DWR localization technique is applied [3] that uses a partition-of-unity and avoids evaluation of strong forms (similar to [4]). A variational framework for brittle fracture was first proposed by Francfort and Marigo [5] (supplemented with numerical simulations in [6]) and later modified by Miehe et al. [7, 8] in order to obtain a thermodynamically-consistent phase-field model for brittle fracture. Numerical realization of such variational techniques for fracture are based on Ambrosio-Tortorelli approximations [9, 10] in which discontinuities in the displacement field across the lower-dimensional crack surface are approximated by an auxiliary function φ. The latter one can be viewed as an indicator function, which introduces a diffusive transition zone between the broken and the unbroken material. This zone has half bandwidth ε, the so-called model regularization parameter. Specifically, the resulting problem is a variational inequality because of a fracture irreversibility constraint. Consequently, while combining phase-field fracture with the DWR method, we borrow ideas from Rannacher and Suttmeier [11, 12, 13] who formulated DWR techniques for elasto-plasticity with similar challenges. The outline is as follows: In Section 2, the forward problem is formulated. Next in Section 3, the DWR estimator is derived. Finally in Section 4, a numerical example substantiates the algorithmic developments. This example is coded in deal.II [14].

2 THE FORWARD AND ADJOINT PROBLEMS

We are interested in the following system: Let the function spaces we work with be

$$V := H_0^1(\Omega) \quad \text{and} \quad W_{in} := \{w \in H^1(\Omega) \,|\, w \le \varphi^{n-1} \le 1 \text{ a.e. on } \Omega\},$$

where φ^{n-1} denotes the previous time step solution. For later purposes we also need $W := H^1(\Omega)$. For simplicity we consider in this entire study scalar-valued displacements (i.e., a modified version of Poisson's problem as displacement equation).

Formulation 1 (Euler-Lagrange system of phase-field fracture propagation) *Find scalar-valued displacements* u *and a scalar-valued phase-field variable* φ, *i.e.,* $(u, \varphi) \in V \times W$ *such that*

$$\Big(\big((1 - \kappa)\varphi^2 + \kappa\big) \, \sigma(u), e(w) \Big) = 0 \quad \forall w \in V, \tag{1}$$

and

$$(1 - \kappa)(\varphi \, \sigma(u) : e(u), \psi - \varphi) + G_c \Big(-\frac{1}{\varepsilon}(1 - \varphi, \psi - \varphi) + \varepsilon(\nabla\varphi, \nabla(\psi - \varphi)) \Big) \geq 0 \quad \forall \, \psi \in W_{in} \cap L^\infty(\Omega), \tag{2}$$

and the crack irreversibility constraint

$$\partial_t \varphi \leq 0.$$

The time t might enter through time-dependent boundary conditions, e.g., $u = u(t) = g(t)$ on $\partial\Omega_D$ with a pre-scribed boundary function $g(t)$ of Dirichlet-type or time-dependent traction conditions (Neumann).
In Formulation 1, κ is a positive regularization parameter for the elastic energy, with $\kappa \ll \varepsilon$, and G_c is the critical energy release rate. Linear elasticity with the standard stress-strain relationship is defined as

$$\sigma := \sigma(u) = 2\mu e(u) + \lambda \, \mathrm{tr}(e(u))I.$$

Here, μ and λ are material parameters, $e(u) = \frac{1}{2}(\nabla u + \nabla u^T)$ is the strain tensor, and I the identity matrix.
The primal problem is then formulated in terms of a semi-linear form:

Formulation 2 (Primal form of coupled elasticity phase-field) *Find* $U := \{u, \varphi\} \in V \times W$ *such that*

$$A(U)(\Psi) = 0 \quad \forall \Psi := \{w, \psi\} \in V \times W. \tag{3}$$

Here, $A(U)(\Psi)$ *is obtained as usually by summing up* (1) *and* (2). *In addition, the variational inequality is treated with a penalization term (a discussion as well as suggestion of a more sophisticated scheme are provided in [15]).*

The dual form (that is required for DWR error estimation) is obtained by switching test and ansatz functions in the linearized Formulation of 2:

Formulation 3 (Dual form of coupled elasticity phase-field) *Find* $Z := \{z^u, z^\varphi\} \in V \times W$ *such that*

$$A'(U)(\Phi, \delta Z) = J'(U)(\Phi) \quad \forall \Phi := \{\varphi^u, \varphi^\varphi\} \in V \times W, \tag{4}$$

where $J(\cdot)$ *is the goal functional under consideration.*

3   GOAL-ORIENTED ERROR ESTIMATION WITH THE DUAL-WEIGHTED RESIDUAL METHOD

A relevant example for $J(\cdot)$ is a flux evaluation, i.e., $J(U) = \int_{\Gamma_{top}} \partial_n u \, ds$. Employing the dual problem, the a posteriori error estimator to such a functional reads [2]:

$$|J(U) - J(U_h)| \leq \sum_{T \in \mathbb{T}_h} \rho_T(U_h) \omega_T(Z),$$

with the local residuals $\rho_T(U_h)$ and sensitivity weights $\omega_T(Z)$. Here, h denotes as usually the spatial discretization parameter. The above dual solution $Z \in V$ cannot be determined analytically but must be solved numerically as the primal problem, i.e, we search for $Z_h \in V_h$ by solving Formulation 3.
To localize the error, we use a recently introduced variational localization formulation [3] that only needs a partition-of-unity (PU), $\sum_i \chi_i \equiv 1$. Specifically as PU, we consider the space of piece-wise bilinear elements $V_h^{(1)}$ (without restrictions on Dirichlet boundaries) with usual nodal basis $\{\chi_h^i, \ i = 1, \ldots, N\}$. The reason is that the local influence of neighboring cells is collected via the PU rather than integration by parts and face-term evaluation as originally suggested [1, 2]. The latter (well-known) classical technique becomes computationally expensive and intractable for multiphysics problems (such as coupled elasticity phase-field) with many equations.
Taking into account that the phase-field variable φ is an auxiliary variable determining the crack path, we formulate the error estimator 'only' in terms of the physical displacements. Furthermore, we restrict ourselves to study estimates for varying h while keeping the regularization parameters ε and κ fixed.

Proposition 1 *Let U_ε be the continuous solution for fixed ε and $U_{\varepsilon,h}$ the corresponding discretized solution. We have the (reduced) a posteriori error estimate for the displacement-phase-field problem:*

$$|J(U_\varepsilon) - J(U_{\varepsilon,h})| \le \sum_i^N |\eta_i| = \sum_i^N \left| \left(-\left((1-\kappa)\tilde\varphi^2 - \kappa\right)\sigma(u), e(w) \right) \right|,$$

where η_i are the local (nodal-based) error indicators and their absolute value $|\eta_i|$ is used for mesh refinement. The weighting function (composed of the dual problem) [2] is defined as $w := (w_{2h}^{(2)} - w_h)\chi_h^i$. Furthermore, $\tilde\varphi$ is an extrapolation of the true φ as suggested and discussed in [16].

4 A NUMERICAL EXAMPLE: FLUX EVALUATION ON A BOUNDARY

In this section, a numerical example is used to substantiate our developments. We consider the slit domain in $\Omega := (-1,1)^2$ with a displacement discontinuity (i.e., the crack). In [17, 18], a manufactured solution for the displacement field has been constructed. The initial square domain is first five times globally refined; this mesh level is to be considered as the coarse mesh.
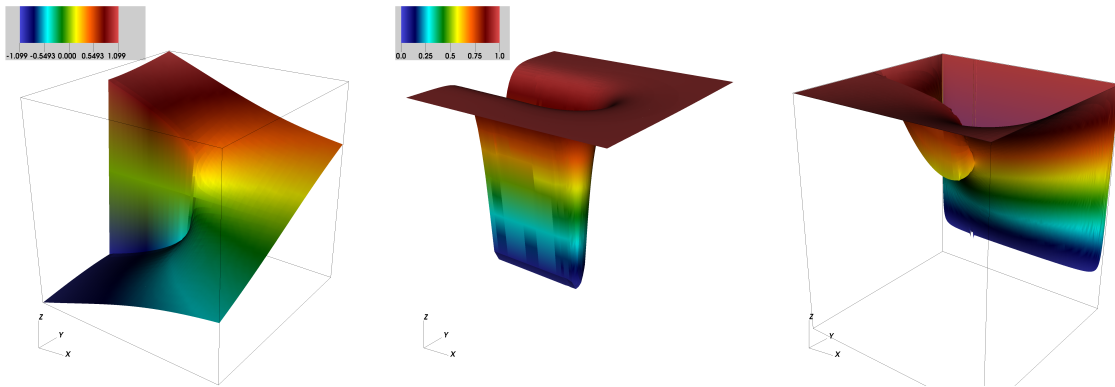

Figure 1: Numerical example: phase-field fracture approximation in the slit domain. In the left sub-figure the displacement field is shown in a three-dimensional view in order to highlight the displacement discontinuity. In the middle, the phase-field function is observed; with values 0 in the fracture and 1 outside and smooth interpolation in between. At right, the dual functional, here a flux evaluation on the top boundary $\{(x,y)|y = 1\}$ is displayed.

The analytical solution on the slit domain $\Omega \setminus \{(x,0)|-1 \le x \le 0\}$ is given by [18] as $(\lambda r^{1/2}\sin\varphi/2; \{(x,0)|-\infty \le x \le 0\})$ where polar coordinates with $r^2 = x^2 + y^2$ are used. Employing the boundary function $g = \lambda\sin\varphi/2$ on $\partial\Omega$, we prescribe non-homogeneous Dirichlet conditions on all parts. Specifically, transforming g into Cartesian coordinates we deal with

$$x \le 0 \text{ and } y \ge 0 : g(x,y) = \lambda/\sqrt(2) * \sqrt{\sqrt{x^2+y^2} - x}, \qquad x \le 0 \text{ and } y \le 0 \quad : g(x,y) = -\lambda/\sqrt(2) * \sqrt{\sqrt{x^2+y^2} - x},$$

$$x \ge 0 \text{ and } y \ge 0 : g(x,y) = \lambda/\sqrt(2) * \sqrt{\sqrt{x^2+y^2} - x}, \qquad x \ge 0 \text{ and } y \le 0 \quad : g(x,y) = -\lambda/\sqrt(2) * \sqrt{\sqrt{x^2+y^2} - x}.$$

These conditions introduce a discontinuity on the boundary at $(-1,0)$ and consequently a crack with displacement discontinuity as displayed in Figure 1. Here, ε is fixed by $h_{coarse} = 8.84e-2$. The other model and material parameters are given as: $\kappa = 10^{-14}$, $G_c = \lambda_{G_c}^2 \times \sqrt{\pi/2}$, $\lambda_{G_c} = 1.0$, $\mu = 1.0$. The goal functional is defined as

$$J(u_\varepsilon) = \int_{\Gamma_{top}} \partial_n u_\varepsilon \, ds,$$

and the error $J(u_\varepsilon) - J(u_{\varepsilon,h})$ (for fixed ε) is subject to our investigation. A related example has been considered in [19]. The primal problem is computed with Q_1^c (continuous bilinears) finite elements for both the displacement as well as the phase-field approximation. The dual problem is computed with finite elements of higher order; namely Q_2^c (continuous biquadratic); other options for discretizing the dual problem are outlined in [2].

Our findings are displayed in Figure 2. First, we observe that the error and the DWR estimate converge with the same order. Secondly, the effectivity index (fraction of true error with respect to DWR estimate) yield relative good results for such a problem. The corresponding primal and dual solutions are displayed in Figure 1.
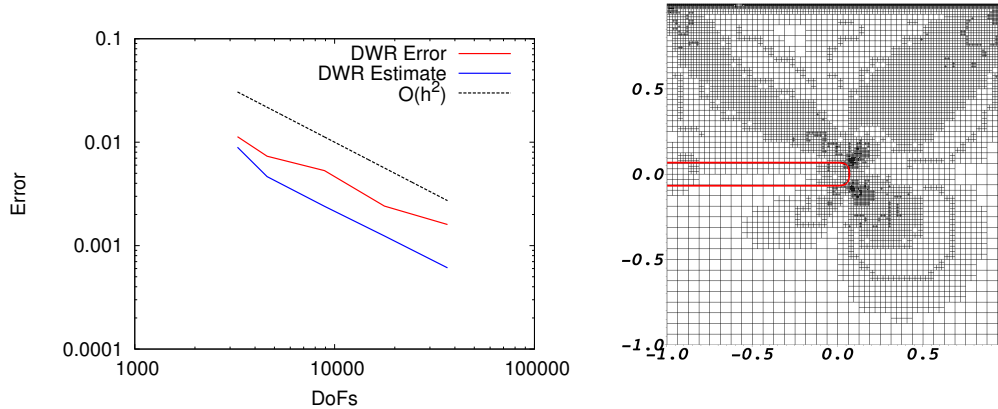

Figure 2: Numerical example: phase-field fracture approximation in the slit domain. At left the error and the DWR estimate are displayed including a comparison of the convergence order. Observing the error and the DWR estimate yield a relative good effectivity index while both show the similar convergence order. In the right sub-figure, the resulting locally adapted mesh and the crack contour $\varphi = 0.1$ (colorized in red) are shown. Here, the mesh is refined primarily around the top boundary (where the goal functional is evaluated) but also at the tip of the fracture in $(0,0)$.

5   CONCLUSIONS

In this study, we combined the dual-weighted residual method with phase-field fracture propagation. Using phase-field, two solution variables, for the displacements and a smoothed indicator function must be solved. In the dual-weighted residual estimator only the displacement equation is considered for the error approximation. The developments are substantiated with a numerical test in which the error and the DWR estimator converge with the same order and secondly, the effectivity is relatively satisfactory, while observing slight underestimation of the true error.

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