An Efficient Treatment of the Laplacian in a Gradient-Enhanced Damage Model

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As is well-known, softening effects that are characteristic for damage models are accompanied by ill-posed boundary value problems. This arises from non-convex and non-coercive energies and results in mesh-dependent finite element results. For that reason, regularization strategies, which somehow take into account the non-local behavior, have to be applied in order to prevent ill-posedness and to achieve mesh-independence. Hereto, most commonly gradient-enhanced formulations \([1,2]\) are considered, but also integral-type \([3,4]\) and viscous \([5,6]\) regularization are well-known.

Gradient-enhanced damage models such as \([1,2]\), to what group our new model \([7]\) basically belongs, come along with a field function acting on the non-local level. Two variational equations are resulting and, however, usually the number of nodal unknowns is increased and consequently the numerical effort is increased as well.

In contrast, we present an improved algorithm for brittle damage \([7]\) combining finite element and meshless methods resulting in a quick update of the field. Thereby, an efficient evaluation of the Laplace operator is adopted as introduced in \([8]\). In the end, the numerical effort of the novel approach is almost comparable with an elastic problem while maintaining well-posedness and therefore mesh-independent results.

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1 Material Model

The underlying Helmholtz free energy \(\Psi\), describing the isotropically damaging material, is given by

\[
\Psi := \Psi_m + \Psi_t = f \Psi_0 + \frac{1}{2} \beta |\nabla f|^2,
\]

with \(\Psi_0 = 1/2 \varepsilon \in \mathbb{E}_0 : \varepsilon\) representing the undamaged material state and \(f := f(d) = \exp(-d)\) with \(d \in [0,\infty)\) describing the damage function. Hamilton’s principle with the independent variations \(\delta u\) and \(\delta d\), indicated by \(\delta \mathcal{H}\), contains the Gibbs energy \(\mathcal{G}\) and the rate-independent dissipation function \(\mathcal{D} = r|\dot{d}|\). Consequently

\[
\delta \mathcal{H} = \delta_u \mathcal{G} + \delta_d \mathcal{G} + \int_{\Omega} \frac{\partial \mathcal{D}}{\partial \dot{d}} \delta d \, dV = 0 \quad \forall \delta u, \delta d \quad \text{with} \quad \mathcal{G} := \int_{\Omega} \Psi(\varepsilon, d) \, dV - \int_{\Omega} b \cdot u \, dV - \int_{\partial \Omega} t \cdot u \, dA.
\]

The individual evaluation of \(\delta u\) provides the stationarity condition for the displacement field \(u\) as follows

\[
\int_{\Omega} \sigma : \delta \varepsilon \, dV - \int_{\Omega} b \cdot \delta u \, dV - \int_{\partial \Omega} t \cdot \delta u \, dA = 0 \quad \forall \delta u,
\]

with \(\sigma = \partial \Psi_m/\partial \varepsilon = f \mathbb{E} : \varepsilon\). Moreover, the individual evaluation of \(\delta_d \mathcal{H}\) provides the stationarity condition for the internal variable \(d\) including a set-valued sub-differential \(\partial \mathcal{D}\) handling the non-differentiability, thus

\[
\int_{\Omega} \Psi_0 f' \delta d \, dV + \int_{\Omega} \beta \nabla f \cdot \nabla (f' \delta d) \, dV + \int_{\partial \Omega} \partial \mathcal{D} \delta d \, dV = 0 \quad \forall \delta d.
\]

Integration by parts of the second term yields the Laplace operator \(\nabla^2\) according to

\[
\int_{\Omega} \beta \nabla f \cdot \nabla (f' \delta d) \, dV = \int_{\partial \Omega} \beta n \cdot \nabla f f' \delta d \, dA - \int_{\Omega} \beta \nabla^2 f f' \delta d \, dV \quad \text{with} \quad \nabla^2 f := \nabla \cdot \nabla f = \sum_{i=1}^{3} \frac{\partial^2 f}{\partial x_i^2}.
\]

Herewith, the strong form of the stationarity condition of \(d\) including the Neumann boundary condition is obtained by

\[
f' \Psi_0 - \beta f' \nabla^2 f + \partial \mathcal{D} \ni 0 \quad x \in \Omega \quad \text{and} \quad \nabla f \cdot n = 0 \quad x \in \partial \Omega.
\]

In order to achieve an indicator function \(\Phi\) deciding on the damage evolution \(\dot{d}\), a Legendre transformation is performed

\[
\mathcal{D}^* = \sup_d \left\{ pd - \mathcal{D} \right\} = \sup_d \left\{ |d|(p \text{sgn} \dot{d} - r) \right\} \quad \forall x,
\]
yielding $\Phi := p - r \leq 0$ on the assumption of no healing by $\sgn \dot{d} = \{0, 1\}$ and including the driving force $p$ derived by

$$p := -f' \Psi_0 + \beta f' \nabla^2 f = f \Psi_0 - \beta f \nabla^2 f \quad \text{since} \quad f' = -f.$$ 

Finally, the damage evolution is completely described by

$$d \geq 0, \quad \Phi := f \Psi_0 - \beta f \nabla^2 f - r \leq 0, \quad \dot{d} \Phi = 0.$$ 

2 Algorithmic Procedure for Displacement Field

The displacement field $u$ can easily be solved by means of the respective stationarity condition for $\delta u$ and application of the finite element method. According to typical procedure, shape functions $S$ and the B-operator matrix $B$ are applied as follows

$$\int_{\Omega} B^T : \sigma \, dV = \int_{\Omega} S^T \cdot b \, dV + \int_{\partial \Omega} S^T \cdot t \, dA.$$ 

A first operator split is introduced by using the damage functions $f^n$ from the previous time step $n$, whereby their current values are uncoupled from the calculation of the displacement field. Thus, the stresses $\sigma$ are only depending on the current displacements and the tangent $K$ becomes constant for each time step. A simple and fast numerical handling follows by

$$\sigma = f^n \mathbb{E} \cdot e^{n+1} \quad \text{and} \quad K = \int_{\Omega} f^n B^T : \mathbb{E} \cdot B \, dV,$$

but a minimum number of loading steps is required to overcome the influences due to the operator split.

3 Algorithmic Procedure for Damage Function

The damage function $f_i$ is defined at the center of mass of each element $i$ and thus the indicator function $\Phi_i$ is element-wise formulated including the respective element-wise averaged elastic energy $\Psi_{0,i}$ with volume $\Omega_i$. Therefore

$$\Phi_i := f_i \Psi_{0,i} - \beta f_i \nabla^2 f - r \leq 0 \quad \text{with} \quad \Psi_{0,i} = \frac{1}{\Omega_i} \int_{\Omega_i} \Psi_0 \, dV.$$ 

A second operator split is introduced by using the neighbored damage functions $f^k_i$ from the previous iteration step $k$ within the Newton scheme. This simplifies the system of coupled inequalities with a coefficient matrix $n_e \times n_e$ into uncoupled inequalities of number $n_e$. Again, a minimum number of loading steps is required. The indicator function $\Phi$ becomes

$$\Phi^k_i := f^k_i \Psi^{n+1}_{0,i} - \beta f^k_i \nabla^2 f^k - r \leq 0.$$ 

At this point, the Taylor series expansion for a central element $x_i$ and nine neighbors $x_j$ (in 3D, five in 2D) is presented by

$$\Delta f_{i,j} := f_j - f_i = \sum_{k=1}^{3} \left( \frac{\partial f_i}{\partial x_k} \Delta x_{j,k} + \frac{1}{2} \sum_{p=1}^{3} \frac{\partial^2 f_i}{\partial x_k \partial x_p} \Delta x_{j,k} \Delta x_{j,p} \right) \Rightarrow \Delta f_i = D \cdot \partial f_i,$$

considering the spatial increments $\Delta x_{j} := x_i - x_j$ between the central and neighbored elements. The linear system of equations by $\Delta f_i = D \cdot \partial f_i$ includes the $9 \times 1$ vector of known increments of the damage function $\Delta f_i = (\Delta f_{i,j})_{e_j}$, the $9 \times 9$ matrix of known spatial increments $D$ with the following entries for each neighbor $j$

$$D_{j,1} = \Delta x_{j,1}, \quad D_{j,4} = \Delta x_{j,1} \Delta x_{j,2}, \quad D_{j,7} = (\Delta x_{j,1})^2/2,$$
$$D_{j,2} = \Delta x_{j,2}, \quad D_{j,5} = \Delta x_{j,1} \Delta x_{j,3}, \quad D_{j,8} = (\Delta x_{j,2})^2/2,$$
$$D_{j,3} = \Delta x_{j,3}, \quad D_{j,6} = \Delta x_{j,2} \Delta x_{j,3}, \quad D_{j,9} = (\Delta x_{j,3})^2/2,$$

and the $9 \times 1$ vector of unknown partial derivatives

$$\partial f_i := \left( \frac{\partial f_i}{\partial x_1}, \frac{\partial f_i}{\partial x_2}, \frac{\partial f_i}{\partial x_3}, \frac{\partial^2 f_i}{\partial x_1 \partial x_2}, \frac{\partial^2 f_i}{\partial x_1 \partial x_3}, \frac{\partial^2 f_i}{\partial x_2 \partial x_3}, \frac{\partial^2 f_i}{\partial x_1^2}, \frac{\partial^2 f_i}{\partial x_2^2}, \frac{\partial^2 f_i}{\partial x_3^2} \right)^T.$$ 

Solving for the unknown partial derivatives $\partial f_i = D^{-1} \cdot \Delta f_i$ and introducing the constant $3 \times 9$ matrix $B^{\nabla^2}$

$$B^{\nabla^2}_{i,j} := D^{-1}_{i+4,j}, \quad l \in \{1, 2, 3\}, \quad j \in \{1, \ldots, 9\}.$$

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allows to capture all necessary unmixed second derivatives for the Laplace operator $\Lambda_f$ and its derivative $D\Lambda_f$, consequently

$$\Lambda_f := (\Lambda_f)_i e_i = \sum_{l=1}^{3} (B^2 \cdot \Delta f_i) e_i, \quad i = 1, \ldots, n_e$$

$$D\Lambda_f := \frac{\partial(\Lambda_f)}{\partial f_i} e_i = \sum_{l=1}^{3} (B^2 \cdot \partial f_i) e_i = -\sum_{l=1}^{3} (B^2 \cdot 1) e_i.$$

Finally, the damage evolution for $\Phi^k_i = f^k_i \bar{\Psi}^{n+1}_{0,i} - \beta f^k_i (\Lambda_f)_i - r > 0$ is calculated by the Newton method with

$$f^{k+1}_i = f^k_i - \frac{\Phi^k_i}{\Phi^{n+1}_{0,i} - \beta (\Lambda_f)_i - \beta f^k_i (D\Lambda_f)_i}.$$

### 4 Numerical Results

Finite element calculations are performed in order to investigate the behavior of the model with respect to different loading rates as well as discretizations. Hereto, the double-notched plate (see right-hand side) is loaded by a displacement $u = 0.015$ mm and two sets of regularization are considered: a slight one with $\beta = 0.002$ MPa mm$^2$ for a localized and a stronger one with $\beta = 0.015$ MPa mm$^2$ for a diffusive characteristic. Further parameters are $E = 210$ GPa, $\nu = 0.33$ and $r = 1$ MPa. The results are provided by Figure 2 presenting the zoomed damage distribution by means of the damage function $f(d)$ and by Figure 3 for the corresponding global structural response by means of force-displacement diagrams.

The variation of the loading rate is realized by different number of time steps. Both the damage distribution as well as the global structural response demonstrate a converging behavior of the results with an increasing number of time steps. Obviously, in case of 1000 time steps hardly any effects due to the operator splits are included anymore. Consequently, this loading rate is considered to be suitable for further investigations. Accordingly, the variation of the discretization is realized by different number of elements. The results certify a mesh-independent behavior of the calculations by very similar damage distributions and well-agreeing force-displacement curves. Besides, these curves are characterized by very steep drops which fall to zero. This fall occurs more quickly in case of the stronger regularization described by the diffusive characteristic.

![Fig. 1: Geometry, discretization and boundary conditions for the double-notched plate with representatively 10161 unstructured elements.](image1)

![Fig. 2: Zoomed plots of damage function $f(d)$ for the double-notched plate for localized/diffusive (top/bottom) characteristic with different number of time steps $= \{200, 600, 1000\}$ for 10161 unstructured elements (from left to center) and with different number of unstructured elements $= \{10161, 5064, 986\}$ for 1000 time steps (from center to right).](image2)
Fig. 3: Force-displacement diagrams for the double-notched plate for localized/diffusive (top/bottom) characteristic with different number of time steps = \{200, 400, 600, 800, 1000\} for 10161 unstructured elements (left-hand side) and with different number of unstructured elements = \{986, 5064, 10161\} for 1000 time steps (right-hand side).

5 Conclusion

A novel approach for gradient-enhanced damage modeling based on a very efficient evaluation of the Laplace operator is presented. For the purpose of efficiency, two operator splits are applied and possible influences on the results are prevented by application of a suitable loading rates as investigated. Numerical examples for localized as well as diffusive damage characteristics provided mesh-independent results by very similar distributions of the damage function and well-agreeing global structural responses. Also, the computation times are very fast and for each load step close to purely elastic calculations.

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