

Une approche micromorphe de l'endommagement de matériaux quasi-fragiles : implémentation numérique et lien avec la méthode par champ de phase

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Micromorphic damage behaviours for quasi-brittle materials: link with phase-field approach to fracture and numerical implementations.

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Abstract — This paper describes discusses a class of micromorphic damage behaviours for quasi-brittle materials which approximates the classical AT1 and AT2 models of the phase-field approach to fracture in a variationnaly consistent framework.

This approximation allows a local treatment of the irreversibility constraint at the integration points. The balance equations are standard partial derivative equations which can readily be solved by most FEM or FFT solvers.

We show that the variational framework allows the derivation of (at least) three alternate minimisation schemes.

Numerical experiments performed using mgis.fenics show that the results are very close to the one obtained by AT2 model [1, 2].

Introduction

The variational approach to fracture takes its grounds in the work of Francfort and Marigo which recasted the Griffith theory into an enery minimization problem [3, 4]. This revisted approach of the Griffith theory is however not tractable with standard numerical methods [5, 6], in particular the commonly used finite element method. For this reason, Bourdin *et al.* developped regularised versions [5] following the works of Ambrosio and Tortorelli [7].

The so-called phase-field approaches to fracture have since become widely popular. As pointed by Gerasimov and De Lorenzis in their excellent review [8], one of the main difficulties in the implementation of those approaches is the treatment of the irreversibility constraint (the damage can only increase), a question on which a considerable amount of works has been published. Most of the proposed solutions are not directly implemented in standard FEM or FFT solvers. An noticeable exception to this statement is the Miehe' alternative based an the so-called history variable [9]. However, Miehe' alternative is not variationally consistent.

Following Forest' micromorphic framework [10], we propose in Section 1 a class of micromorphic brittle behaviours which can approximate the classical AT1 and AT2 phase-field models in a variationnaly consistent way. Those behaviours treat the irreversibility constraint locally, at the integration points. The balance equations are standard partial derivative equations which can readily be solved by most FEM or FFT solvers.

Such models were also recently investigated by Bharali *et al.* [11] using a monolithic resolution strategy. In this paper, we exploit the variational basis of the behaviour to derive in Section 2 three alternate minimisation schemes whose convergence is garanteed. Numerical experiments,

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described in Section 3 and performed using the mgis.fenics package, show that the results are very close to the one obtained by AT2 model.

1 Description of the micromorphic behaviours

In this paper, we consider the quasi-static evolution of a body Ω made of a brittle material.

The state of this material is characterized, at each time step, by:

- A displacement field \vec{u} .
- A micromorphic damage field d_{χ} .
- A local damage field d

In the view of generalized standard materials, the micromorphic model is defined by the following incremental Lagrangian [12]:

$$\mathcal{L}\left(\vec{u}^{\star}, d^{\star}, d^{\star}_{\chi}\right) = \int_{\Omega} \left[\psi\left(\underline{\epsilon}^{\star}, d^{\star}, d^{\star}_{\chi}, \nabla d^{\star}_{\chi}\right) + \Delta t \,\phi\left(\frac{d-d|_{t}}{\Delta t}\right)\right] \mathrm{d}V - \int_{\partial \Omega_{T}} \vec{T} \cdot \vec{u}^{\star} \,\mathrm{d}S$$

where:

- ψ is the free energy.
- ϕ is the dissipation potential.
- Δt is the time increment.
- $d|_t$ is damage at the beginning of the time step.
- \vec{T} is the imposed traction on the boundary $\partial \Omega_T$.
- $\vec{u}^{\star}, d^{\star}, d^{\star}_{\gamma}$ denotes any admissible displacement, damage and micromorphic damage field.

To satisfy the Ilyushin-Drucker postulate, the incremental Lagragian \mathcal{L} must be convex with respect to each variables $\vec{u}^{\star}, d^{\star}, d^{\star}_{\chi}$ taken independently. It can be shown that this condition is ensured if the ψ and the dissipation potential ϕ are convex with respect to their respective arguments.

Body forces and prescribed micromorphic tractions

The definition of the Lagragian \mathcal{L} can be enriched by adding body forces (such as gravity) and prescribed micromorphic tractions.

The state of the material minimises the incremental Lagragian:

$$\left(\left.\vec{u}\right|_{t+\Delta t}, \left.d_{\chi}\right|_{t+\Delta t}, \left.d\right|_{t+\Delta t}\right) = \operatorname*{argmin}_{\vec{u}^{\star} \in C.A.} \mathcal{L}\left(\left.\vec{u}^{\star}, \left.d^{\star}, \left.d^{\star}_{\chi}\right.\right)\right.$$

In pratice, this free energy is a differentiable function.

This is not the case of the dissipation potential ϕ for time independent mechanisms for which ϕ is assumed to be an homogeneous function of degree 1 which allows us to eliminate the time increment Δt from the definition of the Lagrangian as:

$$\Delta t \phi \left(\frac{d^{\star} - d|_t}{\Delta t} \right) = \phi(d^{\star} - d|_t)$$

In particular, the dissipation potential generally contains an indicator function imposing the *irreversibility of the damage evolution*.

1.1 Equilibrium

Deriving equilibrium equations from the principle of the minimum of the Lagrangian is non trivial due to the fact that the dissipation potentiel is not differentiable.

It is then convenient to separate the Lagrangian into two parts \mathcal{L}_1 and \mathcal{L}_2 as follows:

$$\mathcal{L}_1(\vec{u}^\star, d^\star, d^\star_\chi) = \int_{\Omega} \psi(\underline{\epsilon}^\star, d^\star, d^\star_\chi, \nabla d^\star_\chi) \,\mathrm{d}V - \int_{\partial \Omega_T} \vec{T} \cdot \vec{u}^\star \,\mathrm{d}S$$
$$\mathcal{L}_2(d^\star) = \int_{\Omega} \phi(d^\star - d|_t) \,\mathrm{d}V$$

In this report, we will admit the following mathematical result which characterize the minima of Lagrangian:

- The regular part of Lagrangian \mathcal{L}_1 is minimal with respect to the displacement field \vec{u} and the micromorphic damage field d_{χ} .
- At each point, the thermodynamic force Y associated with the damage, is in the subgradient of the dissipation potential:

 $Y\in\partial\phi$

where Y is defined by:

$$Y=-\frac{\partial \psi}{\partial d}$$

In this section, we only consider the condition on the regular part of the Lagrangian. The evolution of the damage is discussed in Section 1.2.

The variation of $\delta \mathcal{L}_1$ with respect to the displacement and micromorphic damage field is defined by:

$$\delta \mathcal{L}_1 = \mathcal{L}_1 \Big(\vec{u}|_{t+\Delta t} + \delta \vec{u}, d|_{t+\Delta t}, d_\chi|_{t+\Delta t} + \delta d_\chi \Big) - \mathcal{L}_1 \Big(\vec{u}|_{t+\Delta t}, d|_{t+\Delta t}, d_\chi|_{t+\Delta t} \Big)$$

where the variation $\delta \vec{u}$ is null on the part of the boundary where imposed displacements are prescribed, i.e. on $\partial \Omega \setminus \partial \Omega_T$.

By retaining only first order terms, this variation can be computed as follows:

$$\begin{split} \delta \mathcal{L}_1 &= \int_{\Omega} \left[\frac{\partial \psi}{\partial \underline{\epsilon}} : \ \delta \underline{\epsilon} + \frac{\partial \psi}{\partial d_{\chi}} \ \delta d_{\chi} + \frac{\partial \psi}{\partial \boldsymbol{\nabla} d_{\chi}} \cdot \boldsymbol{\nabla} \ \delta d_{\chi} \right] \mathrm{d}V - \int_{\partial \Omega_T} \vec{T} \cdot \delta \vec{u} \, \mathrm{d}S \\ &= \int_{\Omega} \left[\underline{\sigma} : \ \delta \underline{\epsilon} + a_{\chi} \ \delta d_{\chi} + \vec{b}_{\chi} \cdot \boldsymbol{\nabla} \ \delta d_{\chi} \right] \mathrm{d}V - \int_{\partial \Omega_T} \vec{T} \cdot \delta \vec{u} \, \mathrm{d}S \end{split}$$

where the following thermodynamic forces were introduced:

$$\underline{\sigma} = \frac{\partial \psi}{\partial \underline{\epsilon}} \qquad a_{\chi} = \frac{\partial \psi}{\partial d_{\chi}} \qquad \vec{b}_{\chi} = \frac{\partial \psi}{\partial \nabla d_{\chi}}$$

Applying the divergence theorem leads to:

$$\delta \mathcal{L}_{1} = \int_{\Omega} \left[-\boldsymbol{\nabla} \cdot \underline{\boldsymbol{\sigma}} \cdot \delta \vec{\boldsymbol{u}} + \left(\boldsymbol{a}_{\chi} - \boldsymbol{\nabla} \cdot \vec{\boldsymbol{b}}_{\chi} \right) \delta \boldsymbol{d}_{\chi} \right] \mathrm{d}\boldsymbol{V} + \int_{\partial \Omega_{T}} \left(\underline{\boldsymbol{\sigma}} \cdot \vec{\boldsymbol{n}} - \vec{\boldsymbol{T}} \right) \cdot \delta \vec{\boldsymbol{u}} \, \mathrm{d}\boldsymbol{S} + \int_{\partial \Omega} \left(\vec{\boldsymbol{b}}_{\chi} \cdot \vec{\boldsymbol{n}} \right) \delta \vec{\boldsymbol{d}}_{\chi} \, \mathrm{d}\boldsymbol{S}$$

where we took into account the fact that the variation of the displacement is null on $\partial \Omega \setminus \partial \Omega_T$. Classical arguments shows that this variation can characterize a minimum only if all the integrands are zero. The integrands associated with variation of the displacement field gives the classical mechanical equilibrium equation in Ω and boundary conditions on $\partial \Omega_T$:

$$\begin{cases} \boldsymbol{\nabla} \cdot \underline{\sigma} = 0 & \text{in } \Omega \\ \underline{\sigma} \cdot \vec{n} = \vec{T} & \text{on } \partial \Omega_T \end{cases}$$
(1)

The integrands associated with variation of the micromorphic damage field leads to the following balance equation and boundary conditions:

$$\begin{cases} \boldsymbol{\nabla} \cdot \vec{b}_{\chi} = a_{\chi} & \text{in } \Omega \\ \vec{b}_{\chi} \cdot \vec{n} = \vec{0} & \text{on } \partial \Omega \end{cases}$$
(2)

1.2 Constitutive equations

The free energy ψ is additively decomposed as follows:

$$\psi(\underline{\epsilon}, d, d_{\chi}, \boldsymbol{\nabla} \, d_{\chi}) = \psi^{el}(\underline{\epsilon}, d) + \psi^{d}(d) + \psi^{d, d_{\chi}}(d, d_{\chi}) + \psi^{\boldsymbol{\nabla} \, d_{\chi}}(\boldsymbol{\nabla} \, d_{\chi})$$

where:

- $\psi^{el}(\underline{\epsilon}, d)$ describes the mechanical part of the free energy.
- $\psi^d(d)$ defines an stored energy du to damage.
- $\psi^{d,d_{\chi}}(d,d_{\chi})$ defines the coupling between the damage d and the micromorphic damage d_{χ}
- $\psi^{\nabla d_{\chi}}(\nabla d_{\chi})$ defines the a micromorphic force.

1.2.1 Choices of ψ^{el} and expression of the stress

 ψ^{el} determines the expression of the stress and contributes to the thermodynamic force driving the damage evolution.

A classical choice is to multiply the free energy of an undamaged elastic material $\psi_0^{el}(\underline{\epsilon})$ by a degradation function g(d) as follows:

$$\psi^{el}(\underline{\epsilon},d) = g(d)\,\psi_0^{el}(\underline{\epsilon}) = \frac{g(d)}{2}\,\underline{\epsilon}:\,\underline{\underline{\mathbf{D}}}:\,\underline{\epsilon}$$

where $\underline{\mathbf{D}}$ is the stiffness matrix of the sound material.

The stresss $\underline{\sigma}$ is thus given by:

$$\underline{\sigma} = g(d) \underline{\underline{\mathbf{D}}} : \underline{\epsilon}$$

Another classical choice popularised by Miehe [9] is to use a spectral decomposition of the strain to split the free energy into a positive and negative part. The degradation function is only applied to the positive part of the free energy.

1.2.2 Evolution of the micromorphic damage

1.2.2.1 Choice of $\psi^{d,d_{\chi}}$

$$\psi^{d,d_{\chi}}(d,d_{\chi}) = \frac{H_{\chi}}{2} \left(d-d_{\chi}\right)^2$$

which leads to the following expression of a_{χ} :

$$a_{\chi} = -H_{\chi} \left(d - d_{\chi} \right) \tag{3}$$

1.2.2.2 Choice of $\psi^{\nabla d_{\chi}}$

$$\psi^{\nabla d_{\chi}}(\nabla d_{\chi}) = \frac{A}{2} \nabla d_{\chi} \cdot \nabla d_{\chi}$$

which leads to the following expression of \vec{b}_{χ} :

$$\vec{b}_{\chi} = A \, \boldsymbol{\nabla} \, d_{\chi} \tag{4}$$

Combining Equations (3) and (4) shows that the micromorphic damage follows the equation:

$$A\nabla^2 d_\chi + H_\chi \left(d - d_\chi\right) = 0 \tag{5}$$

where ∇^2 denotes the Laplacian operator.

1.2.3 Evolution of the damage

The thermodynamic forces Y associated with the damage is given by:

$$Y = -\frac{\mathrm{d}g}{\mathrm{d}d}\psi_0^{el}(\underline{\epsilon}) - \frac{\mathrm{d}\psi^d}{\mathrm{d}d} - \frac{\partial\psi^{d,d_{\chi}}}{\partial d} = -\frac{\mathrm{d}g}{\mathrm{d}d}\psi_0^{el}(\underline{\epsilon}) - \frac{\mathrm{d}\psi^d}{\mathrm{d}d} - H_{\chi}(d-d_{\chi})$$

$$= -\frac{\mathrm{d}g}{\mathrm{d}d}\psi_0^{el}(\underline{\epsilon}) - \frac{\mathrm{d}\psi^d}{\mathrm{d}d} + a_{\chi}$$
(6)

A simple choice of the dissipation potential is:

$$\phi\left(\dot{d}\right) = Y_0 \,\dot{d} + \mathbf{I}_{\mathbb{R}_+}\left(\dot{d}\right)$$

which is equivalent to define the following damage surface:

$$Y = Y_0 \tag{7}$$

The evolution of damage is thus driven by the following equations:

$$\begin{cases} \Delta d (Y - Y_0) = 0\\ \Delta d \ge 0\\ Y - Y_0 \le 0 \end{cases}$$
(8)

Combining Equations (5), (6) and (7), the yield surface may also be written:

$$-\frac{\mathrm{d}g}{\mathrm{d}d}\psi_0^{el}(\underline{\epsilon}) = Y_0 + \frac{\mathrm{d}\psi^d}{\mathrm{d}d} + A\nabla^2 d\chi$$

1.3 Link with phase field approaches to fracture

For high values of the H_{χ} coefficient, the contribution to the $\psi^{d,d_{\chi}}$ may be seen as a penalisation term which ensures that the damage d and the micromorphic damage d_{χ} are close. If this coefficient tends to infinity, those variables must become equal to ensure a finite energy.

Table 1: Parameters of the AT1 and AT2 models.

	AT1	AT2
g(d)	$(1-d)^2$	$(1-d)^2$

	AT1	AT2
$\psi^d(d)$	$rac{8G_c}{3l_0}d$	$\frac{G_c}{2l_0}d^2$
A	$\frac{4}{3}G_c l_0$	$G_c l_0$
Y_0	0	0

Classical phase-field models to fracture can then be recovered by appropriate choices of g(d), $\psi^d(d)$ and A. The case of AT1 and AT2 models, originating from the work of Ambrosio and Tortorelli (AT) [13], is treated in Table 1 where the following quantities were introduced:

- G_c is the fracture energy.
- l_0 is a characteristic length.

2 Alternate minimisation schemes

2.1 A first alternate minimization scheme

The Lagrangian \mathcal{L} is not convex, but convex with respect to each variables taken independently.

Thus, in the spirit of the alternate minimization scheme proposed by Bourdin et al. [5], the following iterative scheme can be proposed:

$$\begin{cases} \vec{u}|^{(n+1)} = \underset{\vec{u}^{\star} \in C.A.}{\operatorname{argmin}} \mathcal{L}\left(\vec{u}^{\star}, d|^{(n)}, d_{\chi}|^{(n)}\right) \\ \vec{d_{\chi}}|^{(n+1)} = \operatorname{argmin} \mathcal{L}\left(\vec{u}|^{(n+1)}, d|^{(n)}, d_{\chi}^{\star}\right) \\ d|^{(n+1)} = \operatorname{argmin} \mathcal{L}\left(\vec{u}|^{(n+1)}, d^{\star}, d_{\chi}|^{(n+1)}\right) \end{cases}$$

where $\vec{u}|^{(n)}$, $\vec{d_{\chi}}|^{(n)}$ and $d_{\chi}|^{(n)}$ denote respectively the estimates of the displacement field, micromorphic damage field and damage field at the nth iteration of the algorithm.

The displacement field is updated first because this problem takes into account the change in imposed boundary conditions. The mechanical problem at constant damage and constant micromorphic damage is a linear elastic problem with variable mechanical coefficients. This problem becomes non linear if unilateral effects are taking into account.

Each steps of the algorithm diminishes the value of the Lagrangian, ensuring the convergence of the scheme.

2.1.1 Evolution of damage in the AT2 model

The evolution of damage is given by Equation (8). In the case of damage increase, we directly impose that the new damage estimate $d|^{(n+1)}$ is such that Equation (7) is satisfied. In the case of the AT2 model, Equation (6) can be rewritten as follows:

$$2\left(1-d|^{(n+1)}\right)\psi_0^{el}\left(\underline{\epsilon}|^{(n+1)}\right) - \frac{G_c}{l_0} d|^{(n+1)} - H_{\chi}\left(d|^{(n+1)} - d_{\chi}|^{(n+1)}\right) = 0$$

The new damage $d|^{(n+1)}$ is thus given:

$$d|^{(n+1)} = \frac{2\psi_0^{el}\left(\underline{\epsilon}|^{(n+1)}\right) + H_{\chi} d_{\chi}|^{(n+1)}}{2\psi_0^{el}\left(\underline{\epsilon}|^{(n+1)}\right) + \frac{G_c}{l_0} + H_{\chi}}$$
(9)

Since the damage can only increase, a closed-form expression of $d|^{(n+1)}$ is finally given by:

$$d|^{(n+1)} = \min\left(\max\left(\frac{2\psi_0^{el}(\underline{\epsilon}|^{(n+1)}) + H_{\chi} d_{\chi}|^{(n+1)}}{2\psi_0^{el}(\underline{\epsilon}|^{(n+1)}) + \frac{G_c}{l_0} + H_{\chi}}, d|_t\right), 1\right)$$
(10)

Equation (10) can be adapted to take into account unilateral effects through tthe spectral decomposition by replacing ψ_0^{el} by its positive part.

2.2 A second alternate minimization scheme

Since an update of the damage variable is computationally inexpensive, compared to the computation of the displacement and micromorphic damage, one may consider evaluating its value twice, as follows:

$$\begin{aligned} \vec{u}|^{(n+1)} &= \underset{\vec{u}^{\star} \in C.A.}{\operatorname{argmin}} \mathcal{L}\left(\vec{u}^{\star}, d|^{(n)}, d_{\chi}|^{(n)}\right) \\ d|^{(n+1/2)} &= \operatorname{argmin} \mathcal{L}\left(\vec{u}|^{(n+1)}, d^{\star}, d_{\chi}|^{(n)}\right) \\ \vec{d_{\chi}}\Big|^{(n+1)} &= \operatorname{argmin} \mathcal{L}\left(\vec{u}|^{(n+1)}, d|^{(n+1/2)}, d_{\chi}^{\star}\right) \\ d|^{(n+1)} &= \operatorname{argmin} \mathcal{L}\left(\vec{u}|^{(n+1)}, d^{\star}, d_{\chi}|^{(n+1)}\right) \end{aligned}$$

The damage estimates $d|^{(n+1/2)}$ is given by an appropriate modification of Equation (10).

2.3 A third alternate minimization scheme

The third alternate minimization scheme is based on the fact that the minimisation with respect to d and d_{χ} is convex:

$$\begin{cases} \vec{u} \big|^{(n+1)} = \underset{\vec{u}^{\star} \in C.A.}{\operatorname{argmin}} \mathcal{L}\left(\vec{u}^{\star}, d\big|^{(n)}, d_{\chi}\big|^{(n)}\right) \\ \left(d\big|^{(n+1)}, \vec{d_{\chi}}\big|^{(n+1)}\right) = \operatorname{argmin} \mathcal{L}\left(\vec{u}\big|^{(n+1)}, d^{\star}, d_{\chi}^{\star}\right) \end{cases}$$

The evolution of d_{χ} is still given by Equation (2) but the determination of the conjugated force a_{χ} relies locally on the resolution of Equation (10). As this equation is only linear by part, Equation (2) is indeed non linear and its resolution is performed in this work using a Newton algorithm.

To be more specific, the computation of the stiffness matrix associated with Problem (2) requires the derivative $\frac{\partial a_{\chi}}{\partial \Delta d_{\chi}}$ which is piece-wise constant. In our numerical experiments, this Newton algorithm usually converges in less than 10 iterations.

2.4 Choice of the convergence criterion of the staggered schemes

In this paper, the staggered schemes are stopped when the damage becomes stationnary, i.e. when the absolute difference between two estimates of the damge is below a given threshold ε_d at each integration point.

This criterion is not totally satisfying as it does not ensure that a true minimum of the Lagrangian is found. We carefully checked that this is the case for each steps of the numerical experiments described in Section 3.

3 Numerical experiments

We consider in this section three classical test cases:

- a fiber reinforced matrix in tension [5],
- a precracked specimen loaded by applying a tangential displacement on the top boundary [9],
- a precracked specimen loaded by applying a normal displacement on the top boundary [9].



Figure 1: Damage patterns at the end of the unit tests.

Those tests are performed using the AT2 model and its micromorphic counterparts using a spectral decomposition of the elastic free energy. The damage patterns at the end of those tests are reported on Figure 1.

The python scripts are available in this repository: https://github.com/thelfer/micromorphic-damage-giens-2022.

Those scripts contains the geometry, material properties and loadings required to reproduce those tests.

For those tests, the penalisation parameter H_{χ} is chosen of the form:

$$H_{\chi} = \beta \, \frac{G_c}{l_0}$$

where β is a normalised penalisation parameter [11].

Those three tests lead to similar conclusions:



Figure 2: Evolution of the force as a function of the imposed displacement for the fiber reinforced matrix test for the third scheme with $\beta = 150$ and the standard phase-field schemes based on the resolution of the variational inegality or based on Miehe' history function



Figure 3: a) Evolution of the force as a function of the imposed displacement for $\beta = 50$, $\beta = 100$, $\beta = 150$ for the shear test using the third staggered scheme. b) Evolution of the dissipated energy as a function of the imposed displacement for $\beta = 50$, $\beta = 100$, $\beta = 150$ for the shear test using the third staggered scheme.



Figure 4: Number of iterations of the fixed point algorithm for the shear test as a function of the step number for the standard AT2 model and the third scheme for $\beta = 150$ and $\beta = 300$.

- The two first schemes converges very slowly (several thousand of fixed point iterations) even in the quasi-elastic range. A threshold as small as 10^{-5} is required to ensure converged results. Those schemes are considered unsuable in pratice.
- The second scheme converges much faster. A threshold value of 10^{-3} is sufficient to have converged results. The same threshold value is used for the standard AT2 model.
- As illustrated by Figure 2, the force-displacement curve of the third scheme is very similar to the standard AT2 model.
- As illustrated by Figure 3, the penalisation factor plays a major role on the overall force-displacement curve. Our experiments shows that a value of 150 leads to results undistinguishable with the one of the AT2 model for every tests. However, an higher value of 300 is required to reproduce closely the evolution of the fracture energy.
- The number of iteration of the fixed point algorithm is roughly similar between the standard AT2 model and the third scheme, altough a bit higher in general, as depicted on Figure 4.

4 Conclusions and perspectives

This work has investigated the use of micromorphic behaviours for the description of quasi-brittle materials and has shown that those micromorphic behaviours can be considered as varitionaly consistent approximations of standard phase-field models.

Three alternate minimisation schemes, which is straightforward to implement in standard FEM or FFT solvers, have been proposed.

Convergence of those schemes is guaranteed but requires a large number of fixed-point iterations. With respect to this observation, the third scheme appears to be more efficient.

The proposed approach can be extended to more complex damage behaviours and ductile failure.

However, as a future work, acceleration schemes could also be investigated to reduce the number of fixed-point iterations.

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