On a Computational Smeared Damage Approach to the Analysis of Strength of Quasi-Brittle Materials

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Abstract: Computational analysis of strength of quasi-brittle materials, crucial for the durability of building structures and industrial components, needs typically a smeared damage approach, referring to the Eringen theory of nonlocal elasticity. Unfortunately its ad hoc constitutive relations cannot avoid potential divergence of sequences of approximate solutions, exploiting some extended finite element techniques, as well as questionable or missing existence results for corresponding boundary value problems. Introducing a simple static partially linearized model problem of such type, this article demonstrates some relevant remedies and their limitations, with numerous references to desirable generalizations.

Key-Words: Quasi-brittle materials, smeared damage, nonlocal elasticity, boundary value problems for partial differential equations, extended finite element method (XFEM).

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1 Introduction

Behaviour of some materials widely used in engineering applications, typically of cementitious composites, supplied by various types of stiffening fibres, can be characterized as quasi-brittle ones. In such materials certain loss of strength in comparison of their expected reversible elastic deformation can be observed, caused by the presence of complicated systems of irreversible microcracks, whose mutual interaction cannot be analzyed properly, as recommended by [38], p. 100, thus its computational evaluation needs some homogenization or regularization approach, as demonstrated by [12], [16] or [44]. However, parallel to development of such microfractured zones, or even separately, also initiation and propagation of macroscopic cracks should be respected; for much more details, together with the sketch of history of such numerical modelling and simulation, see [21] and [39].

Although most theoretical considerations can be performed with initial and / or boundary value problems corresponding to special elliptic, parabolic or hyperbolic systems of partial differential equations (PDEs), in appropriate infinite-dimensional spaces of (abstract) functions, practical algorithms work with sparse finite systems of algebraic equations, coming from certain finite-dimensional approximations of such spaces, typically from the extended finite element method (XFEM), as evident from [24], [25] and [40]. Potential formal linearity of such systems (if possible) stops with the first occurrence of micro- or macrocracking, thus special adaptive enlargements of different types at crack tips and along crack paths (extrinsing XFEM) or modifications (intrinsic XFEM), as motivated by [38], pp. 31 and 36, are needed; for classification peculiarities cf. [42].

The existence of cracks is able to destroy the integrity of both building structures and industrial components, which normally results in the serious fracture accidents. Thus it is significant to investigate the formation mechanism of cracks, such that the fracture-critical structures can be rationally designed to prolong their service lives. Nevertheless, no detailed deterministic quantitative analysis of micromechanics of fracture is available for most building materials; the same can be addressed to some hypothetical large sets of reliable empiric characteristics for complicated models of material fracture. Thus in this article we shall present a rather inexpensive algorithm for the evaluation of damage of such materials without high requirements to special laboratory and / or in situ measurements, open to proper generalizations in several research directions.

After these introductory remarks, numbered as Section 1 formally, Section 2 introduces a static model problem of smeared damage, presenting an original iterative algorithm for its numerical analysis, together with some its theoretical and practical limitations. Section 3 can be seen as a careful analysis in which sense such iterative al-

gorithm, working with selected results from the Eringen nonlocal theory of elasticity, can converge to some solution of an original problem, referring to some non-discussed difficulties in former ad hoc analyses. Section 4 contains an incomplete list of possible generalizations, including references to software implementations with numerical results. Brief concluding remarks with plans for future research can be then found in Section 5.

2 A model problem

Let us consider a deformable body Ω in the 3-dimensional Euclidean space R^3, occupying a domain with Lipschitz boundary (cf. [34], p. 15) $\partial\Omega = \Theta \cup \Gamma$; its disjoint parts Θ of non-zero measure and Γ are distinguished to prepare the implementation of both Dirichlet (support) and Neumann (surface load) boundary conditions. A Cartesian coordinate system $x = (x_1, x_2, x_3)$ is used to describe all phenomena in R^3. Some of these (and the following) assumptions will be weakened, namely in Section 4, but we shall respect them now to avoid technical difficulties in proofs.

We shall use the simplified notation of Lebesgue, Sobolev, etc. function spaces, compatible with [34], p. 10: namely $V = \{v \in W^{1,2}(\Omega)^3 : v = o \text{ on } \Theta\}$ where o means the zero-valued vector in R^3, $H = L^2(\Omega)^3$, $Z = L^2(\Gamma)^3$ and $M = L^2(\Omega)^{3\times3}_{\rm sym}$. Let us consider some prescribed volume loads $f \in H$ and surface loads $g \in Z$ (inhomogeneous Neumann boundary conditions), together with some stresses $\sigma \in M$, dependent on unknown displacements $u \in V$, related to an initial geometric configuration; this forces $u = o$ on Θ (homogeneous Dirichlet boundary conditions).

Let us introduce a model static problem, based on the linear elasticity, whose Galerkin formulation (including all required boundary conditions) reads

$$(\varepsilon(v), \sigma) = (v, f) + \langle v, g\rangle \qquad (1)$$

for any $v \in V$. Here $(.\,,.)$ refers to the scalar product in H or in M, due to applied arguments, whereas $\langle .\,,\rangle$ refers to such product in Z. Moreover $\varepsilon(v)$ denotes the linear strain tensor from M with components $\varepsilon_{ij}(v) = (\partial v_i/\partial x_j + \partial v_j/\partial x_i)/2$ for all $i, j \in \{1, 2, 3\}$ and any $v \in V$. To support the reader-friendliness of the following text, for the evaluation of $\sigma \in M$ in (1) we shall come out from most mathematical formulations of [16], supplied with numerous remarks to useful modifications and generalizations.

The announced evaluation of σ can be performed using an empirical 6-step constitutive law with $\tilde\sigma \in M$, $\sigma_{\rm I}, \sigma_{\rm II}, \sigma_{\rm III} \in H$, $\tilde\varepsilon \in L^2(\Omega)$, $\bar\varepsilon \in L^2(\Omega)$ and $\delta \in L^\infty(\Omega)$, evaluated in particular steps, can be presented as

$$\begin{aligned}
&\tilde\sigma = C{:}\varepsilon(u)\,, \qquad (2)\\
&0 = \det(\tilde\sigma - \tilde\sigma_{\rm I}) = \det(\tilde\sigma - \tilde\sigma_{\rm II}) = \det(\tilde\sigma - \tilde\sigma_{\rm III})\,,\\
&\tilde\varepsilon = \mathcal{F}(\tilde\sigma_{\rm I}, \tilde\sigma_{\rm II}, \tilde\sigma_{\rm III})\,,\\
&\bar\varepsilon(x) = \int_\Omega \mathcal{K}(x,\xi)\,\tilde\varepsilon(\xi)\,{\rm d}\xi \ \text{ for any } x \in \Omega\,,\\
&\delta = \mathfrak{D}(\bar\varepsilon)\,, \quad \sigma = \delta\tilde\sigma\,.
\end{aligned}$$

Thus we can take $\sigma = \delta\, C{:}\varepsilon(u)$ formally, which enables us to present (3) as

$$(\varepsilon(v), \delta\, C{:}\varepsilon(u)) = (v, f) + \langle v, g\rangle \qquad (3)$$

for any $v \in V$ again.

The 1st relation (2) is the standard empirical Hooke law with some given material characteristics $C \in L^\infty(\Omega)^{(3\times3)\times(3\times3)}_{\rm sym}$; thus we need (according to the symmetry) 21 independent characteristics in general, reducible to 2 such characteristics, well known as the Young modulus E and the Poisson number μ, in an isotropic case; for more details see [15], p. 129.

The 2nd relation (2) refers to the evaluation of eigenvalues, corresponding to principal stresses, due to the natural requirement of objectivity. Such stresses belong to H only and are suitable inputs for further computations.

The 3rd relation (2) is suggested as

$$\mathcal{F}(\sigma_{\rm I}, \sigma_{\rm II}, \sigma_{\rm III}) = \sqrt{\left(\sigma_{\rm I}^2 + \sigma_{\rm II}^2 + \sigma_{\rm III}^2\right)/E} \qquad (4)$$

by [16], using no material characteristics except E for isotropic materials; clearly $\mathcal{F}(\sigma_{\rm I}, \sigma_{\rm II}, \sigma_{\rm III}) = 1$ represents an ellipsoid in R^3 (the drawing in [16] shows an ellipse in R^2 under the plane stress condition). For materials like cementitious composites with quite different behaviour under tension and compression, a more careful formulation is needed, including additional experimentally identified parameters for both (4) and (6) (see lower), as reflected by [31]; for fibre concrete with crucial distribution of i) volume fraction and ii) orientation of stiffening particles cf. [44].

The 4th relation (2) comes from the Eringen theory of nonlinear elasticity by [6] and [7], whose mathematical formulations (including existence and convergence results) by [1] have been revised by [9] substantially. It contains certain regularization kernel $\mathcal{K}$, mapping $L^2(\Omega)$ to $L^2(\Omega)$, as introduced by [12]; its basic form for arbitrary

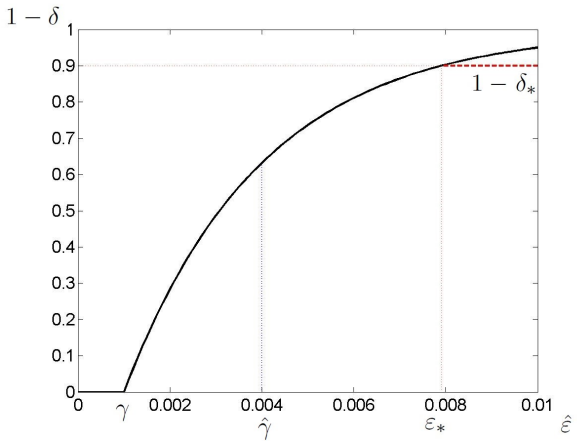

Figure 1: Dependence of $1-\delta$, declared as a "damage variable" by [16], for $\delta = \mathfrak{D}(\hat{\varepsilon})$ on $\hat{\varepsilon}$ by (6), utilizing a priori known parameters γ and γ_* (full black line). An artificial correction, relying on an additional parameter δ_*, discussed below (7), is supplemented (dashed red line). A unique solution ε_* of an equation $\mathfrak{D}(\varepsilon_*) = \delta_*$ was obtained by the Newton iterative method.

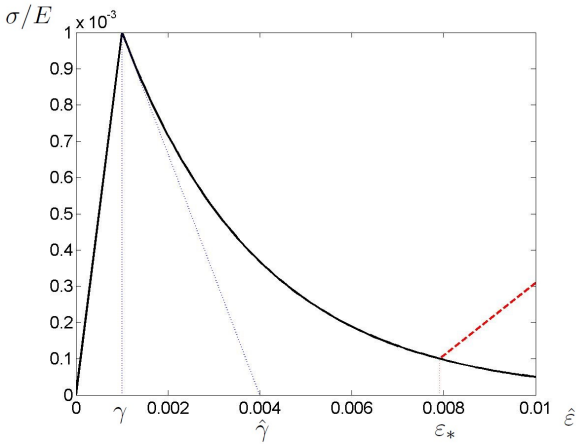

Figure 2: Graphical interpretation of (6), i. e. σ/E as a function of $\hat{\varepsilon}$, in a hypothetical one-dimensional constitutive relation $\sigma = \delta E\hat{\varepsilon}$ (thus no μ is needed), as presented by [16] (full black line), motivated by the 1st and last equations (2). An artificial correction from Fig. 1 (dashed red line) forces a non-realistic description of material behaviour for sufficiently large damage.

$x, \xi \in \Omega$ by [16] is

$$\phi(x,\xi) = \exp\left(-|x-\xi|^2\right)\,, \qquad (5)$$
$$\mathcal{K}(x,\xi) = \frac{\phi(x,\xi)}{\int_\Omega \phi(x,\tilde{\xi})\,\mathrm{d}\tilde{\xi}}\,;$$

here $|\,.\,|$ means the Euclidean norm in R^3. Such mapping is always compact, i. e. it transforms weakly convergent sequences to strongly convergent ones; for 2 independent proofs of this useful result see [5], p. 80. Certain modification of (5), taking a distance of ξ from $\partial\Omega$ (computationally rather expensive) into account, as well as its linear simplification, can be found in [16], too; still other approximations working with radial basis functions may be inspired by [36]. Unlike such approaches, [30] incorporates some knowledge on dislocations (usually not available for building composites in some simple deterministic form), solving an auxiliary bi-Helmholtz equation to get $\mathcal{K}(.\,,.)$ comparable with that coming from (5).

The design of some reasonable (typically non-explicit) formulation of the 5th relation (2), respecting the irreversibility of damage, is the most delicate step. The 2st substep by [16] relies on the evaluation of $\mathfrak{D}(\bar{\varepsilon}) = \mathcal{D}(\hat{\varepsilon})$ (including its graphical interpretation, showing a 1-dimensional stress-strain curve with softening) where $\mathcal{D}(\hat{\varepsilon}) = 1$ for $\hat{\varepsilon} \le \gamma$, otherwise

$$\mathcal{D}(\hat{\varepsilon}) = \frac{\gamma}{\hat{\varepsilon}}\exp\left(-\frac{\hat{\varepsilon}-\gamma}{\gamma_*-\gamma}\right); \qquad (6)$$

here γ and $\gamma_* > \gamma$ are certain positive constants obtained from experiments and $\hat{\varepsilon}$, called "history variable", comes from the 1st substep as the historical maximum of $\bar{\varepsilon}$, starting from an initial time with an unloaded body, without proper introduction of any evolutionary problem. Fig. 1 and Fig. 2 illustrate the utilization of (6) in an idealized strain - stress relation, as presented in [16]; its expected limitation will be discussed later. Unlike such access, induced by (6), we intend to come to $\mathfrak{D}(.)$ in the last relation (2) using appropriate successive iterations; this will be specified later. The last relation following the 5th one is a final simple evaluation only.

The course analysis of a continuous function $\delta(.)$, as prepared by (6), yields $0 \le \delta(.) \le 1$; more tight upper and lower bounds are impossible. Thus we are not able to exclude a priori, for example, the following case: let Ω_0 be certain subdomain of Ω with Lipschitz boundary, thus the whole interface Λ between Ω_0 and $\Omega_1 = \Omega\backslash\Omega_0$ belong to the closure of Ω in R^3; moreover let us set $\delta = 0$ on Ω_0 and Λ Consequently (3) degenerates to

$$(\varepsilon(v), \delta\, C{:}\varepsilon(u))_1 = (v,f)_1 + \langle v, g\rangle\,, \qquad (7)$$
$$0 = (v,f)_0\,;$$

here indices 0 a 1 refer to the integration over Ω_0 and Ω_1 instead of Ω. The 2nd equation (7) can be satisfied only with $f = o$ and indeterminable u on Ω_0. This manifests a shortcoming

of our linearized static formulation (3), not ready to simulate final stages of potential destruction of Ω. Thus we are obliged to implement a non-physical computational remedy: for some prescribed small positive δ_* take $\delta = \delta_*$ instead of any calculated "dangerous" result $\delta < \delta_*$. For illustration, our artificial correction can be then interpreted as switching between the full black and and the dashed red lines on Fig. 1 and Fig. 2.

Thanks to the trace theorem by [28], using the Cauchy - Schwarz inequality (cf. [34], p. 4), we can see that the right-hand side of (3) is a linear functional in the dual space to V. Consequently, following [8], applying the Korn inequality by [27], p. 244, V can be supplied with an alternative scalar product $(\varepsilon(v), C : \varepsilon(\tilde{v}))$ for all $v, \tilde{v} \in V$ and with a corresponding norm for any $v \in V$, utilizing the brief notation

$$\|v\| = \sqrt{(\varepsilon(v), C{:}\varepsilon(v))}\,. \tag{8}$$

The Riesz representation theorem (cf. [5], p. 50) then enables us to define a unique $w \in V$ satisfying

$$(\varepsilon(v), \delta\, C{:}\varepsilon(w)) = (v, f) + \langle v, g\rangle \tag{9}$$

for any $v \in V$.

For certain positive integer r (the limit passage $r \to \infty$ can be expected) let us now set $u_0 = o$ on Ω and certain constant load factors $\beta_0, \beta_1, \dots \beta_r$ such that $0 = \beta_0 \le \beta_1 \le \ldots \le \beta_r \le 1$, in particular $\beta_s = 1/2 + 1/2^2 + \ldots + 1/2^s$ for $s \in \{1, \dots, r\}$ (a geometric sequence), together with some constant positive relaxation factor α. We shall evaluate $u_1, \dots, u_r$, working with a computational modification of (3)

$$\begin{aligned}&\alpha(\varepsilon(v), C{:}(\varepsilon_s - \varepsilon_{s-1})) \\ &+ (\varepsilon(v), \delta_{s-1} C{:}\varepsilon_s) = \beta_s(\varepsilon(v), C{:}\varepsilon_*)\,,\end{aligned} \tag{10}$$

using the brief notation $\varepsilon_s = \varepsilon(u_s)$ for any $s \in \{1, \dots, r\}$, $\delta_{s-1} = \min(\delta_{s-2}, \mathcal{D}(\hat{\varepsilon}_{s-1}))$ with $\hat{\varepsilon}_{s-1}$ derived from u_{s-1} similarly to $\hat{\varepsilon}$ from u by by (2), $\delta_{-1} = \delta_0$ formally and $\varepsilon_* = \varepsilon(w)$, as introduced by (9); ε_0 is the zero element of M formally. The detailed analysis of properties of a sequence $\{u\}_{r=1}^{\infty}$ will be needed evidently.

3 Existence and convergence properties

Let us derive some a priori upper bounds. Choosing $v = u_s - u_{s-1}$ in (10), we obtain

$$\begin{aligned}&\alpha(\varepsilon_s - \varepsilon_{s-1}, C{:}(\varepsilon_s - \varepsilon_{s-1})) \\ &+ (\varepsilon_s - \varepsilon_{s-1}, \delta_{s-1} C{:}\varepsilon_s) = \beta_s(\varepsilon_s - \varepsilon_{s-1}, C{:}\varepsilon_*)\,.\end{aligned} \tag{11}$$

The 2nd left-hand-side additive term of (11) can be rewritten as

$$\begin{aligned}&(\varepsilon_s - \varepsilon_{s-1}, \delta_s C{:}\varepsilon_s) \\ &= (\varepsilon_s, \delta_{s-1} C{:}\varepsilon_s)/2 - (\varepsilon_{s-1}, \delta_{s-2} C{:}\varepsilon_{s-1})/2 \\ &+ (\varepsilon_s - \varepsilon_{s-1}, \delta_{s-1} C{:}(\varepsilon_s - \varepsilon_{s-1})/2 \\ &+ (\varepsilon_{s-1}, (\delta_{s-2} - \delta_{s-1}) C{:}\varepsilon_{s-1})/2\,,\end{aligned} \tag{12}$$

its right-hand-side similarly as

$$\begin{aligned}&\beta_s(\varepsilon_s - \varepsilon_{s-1}, C{:}\varepsilon_*) \\ &= \beta_s(\varepsilon_s, C{:}\varepsilon_*) - \beta_{s-1}(\varepsilon_{s-1}, C{:}\varepsilon_*) \\ &- (\beta_s - \beta_{s-1})(\varepsilon_{s-1}, C{:}\varepsilon_*)\,,\end{aligned} \tag{13}$$

Then (12) and (13) can be inserted into (11) and the sum over all $s \in \{1, \dots, r\}$ results

$$\begin{aligned}&\sum_{s=1}^{r} \alpha(\varepsilon_s - \varepsilon_{s-1}, C{:}(\varepsilon_s - \varepsilon_{s-1})) \\ &+ (\varepsilon_r, \delta_{r-1} C{:}\varepsilon_r)/2 \\ &+ \sum_{s=1}^{r} (\varepsilon_s - \varepsilon_{s-1}, \delta_{s-1} C{:}(\varepsilon_s - \varepsilon_{s-1})/2 \\ &+ \sum_{s=1}^{r} (\varepsilon_{s-1}, (\delta_{s-2} - \delta_{s-1}) C{:}\varepsilon_{s-1})/2 \\ &= \beta_r(\varepsilon_r, C{:}\varepsilon_*) - \sum_{s=1}^{r} (\beta_s - \beta_{s-1})(\varepsilon_{s-1}, C{:}\varepsilon_*)\,.\end{aligned} \tag{14}$$

Neglecting the always non-negative (and usually small) last left-hand-side additive term of (14) and applying the Cauchy - Schwarz inequality to both its right-hand-side additive terms, using the notation (8) we receive

$$\begin{aligned}&(\delta_*/2)\|u_r\|^2 + (\alpha + \delta_*/2) \sum_{s=1}^{r} \|u_s - u_{s-1}\|^2 \\ &\le \beta_r \|u_r\| \|w\| + \sum_{s=1}^{r} (\beta_s - \beta_{s-1}) \|u_{s-1}\| \|w\|\,,\end{aligned} \tag{15}$$

The form of (15) is now appropriate to the application of the Young inequality (cf. [34], p. 12)

$$\begin{aligned}\|u_r\|\|w\| &\le (\delta_*/4)\|u_r\|^2 + (1/\delta_*)\|w\|^2\,, \\ \|u_{s-1}\|\|w\| &\le (\delta_*/4)\|u_{s-1}\|^2 + (1/\delta_*)\|w\|^2\end{aligned} \tag{16}$$

where still $s \in \{1, \dots, r\}$, with the obvious consequence of the 2nd relation

$$\begin{aligned}&\sum_{s=1}^{r} (\beta_s - \beta_{s-1}) \|u_{s-1}\| \|w\| \\ &\le (\delta_*/4) \sum_{s=1}^{r} (\beta_s - \beta_{s-1}) \|u_{s-1}\|^2 + (1/\delta_*)\|w\|^2\end{aligned} \tag{17}$$

Thus (16) together with (17) imply

$$\|u_r\|^2 \le (4/\delta_*^2)\|w\|^2 + \sum_{s=1}^{r}(\beta_s - \beta_{s-1})\|u_s\|^2 . \quad (18)$$

Applying the discrete version of the Gronwall lemma by [17] in the form

$$\kappa_r \le \zeta_0 + \sum_{s=1}^{r}\zeta_s\kappa_{s-1} \Rightarrow \kappa_r \le \zeta_0 \exp\left(\sum_{s=1}^{r}\zeta_s\right) \quad (19)$$

where $\kappa_0 \ldots, \kappa_r$ and $\zeta_0 \ldots, \zeta_r$ are arbitrary non-negative real numbers, (18) guarantees

$$\|u_r\|^2 \le (2e/\delta_*^2)\|w\|^2 . \quad (20)$$

For some special choices of $\beta_1 \le \beta_2 \le \ldots \le 1$ the (rather rough) upper bound (20) could be improved: e. g. for $\beta_1 = \beta_2 = \ldots = 1$ the Gronwall inequality is not needed, thus $2e$ in (20) is allowed to be replaced by 2, as evident from (18) directly. Still other (less trivial) improvements are available with a well-considered modification of (16) and (17), together with some deeper analysis of implications like (19), inspired by [10].

An effect of suitable (non-obligatory) choice of a positive α can be then seen from the insertion of (20) into (15), neglectin g the positive 1st left-hand-side additive term, which gives

$$\sum_{s=1}^{r}\|u_s - u_{s-1}\|^2 \le \frac{4e}{(\alpha + \delta_*/2)\delta_*^2}\|w\|^2 . \quad (21)$$

Unfortunately, the limit passage from (10) to (3) cannot rely only on (21). Nevertheless, thanks to (20), a sequence $\{u\}_{r=1}^{\infty}$ is uniformly bounded in a reflexive Hilbert space V, thus the Eberlein - Shmul'yan theorem (see [5], p. 67) guarantees, up to a subsequence, its weak convergence to some $u \in V$.

Let us come back to (10). Let $\tilde{\sigma}_s$, $\tilde{\sigma}_{\mathrm{I}s}$, $\tilde{\sigma}_{\mathrm{II}s}$, $\tilde{\sigma}_{\mathrm{III}s}$, $\tilde{\varepsilon}_s$ and $\bar{\varepsilon}_s$ be applied to (10) instead of $\tilde{\sigma}$, $\tilde{\sigma}_{\mathrm{I}}$, $\tilde{\sigma}_{\mathrm{II}}$, $\tilde{\sigma}_{\mathrm{III}}$, $\tilde{\varepsilon}$ and $\bar{\varepsilon}$ similarly to the utilization of u_s replacing u and δ_s replacing δ for all $s \in \{1, \ldots, r\}$ and an arbitrary positive integer r.

Using the simplified notation $\to$ for the strong convergence in corresponding Banach spaces and $\rightharpoonup$ for the weak one, taking $r \to \infty$, in particular steps introduced by (2), thanks to the continuity of all applied functions, with respect to the discussion on compactness of kernels below (5), we come to

$$\begin{aligned}
&u_r \rightharpoonup u \text{ in } V , \quad (22)\\
&\varepsilon(u_r) \rightharpoonup \varepsilon(u) \text{ and } \tilde{\sigma}_r \rightharpoonup \tilde{\sigma} \text{ in } H ,\\
&\tilde{\sigma}_{\mathrm{I}r} \rightharpoonup \tilde{\sigma}_{\mathrm{I}} , \quad \tilde{\sigma}_{\mathrm{II}r} \rightharpoonup \tilde{\sigma}_{\mathrm{II}} \text{ and } \tilde{\sigma}_{\mathrm{III}r} \rightharpoonup \tilde{\sigma}_{\mathrm{III}} \text{ in } H ,\\
&\tilde{\varepsilon}_r \rightharpoonup \tilde{\varepsilon} \text{ in } L^2(\Omega) ,\\
&\bar{\varepsilon}_r \to \bar{\varepsilon} \text{ in } L^2(\Omega) ,\\
&\delta_r \to \delta \text{ in } L^{\infty}(\Omega) , \quad \sigma_r \rightharpoonup \sigma \text{ in } H
\end{aligned}$$

where i. a. a limit δ (as needed) corresponds just to u. Morevover the 1st left-hand-side additive term of (10) can be rewritten as

$$\begin{aligned}
&\alpha(\varepsilon(v), C\!:\!(\varepsilon_s - \varepsilon_{s-1})) \quad (23)\\
&= \alpha(\varepsilon(v), C\!:\!(\varepsilon_s - \varepsilon(u)))\\
&+ \alpha(\varepsilon(v), C\!:\!(\varepsilon(u) - \varepsilon_{s-1}(u))) .
\end{aligned}$$

Inserting (23) into (10), we can finish the required limit passage to (3) using (22).

4 Some modifications and generalizations

Although V is an infinite-dimensional space, we have performed no its approximation for practical computations yet, thus (10) should be discretized carefully now. Let us now consider, as usual in the finite element method (FEM) by [45], some approximation space V_n corresponding to V of a finite dimension n, in particular (but not obligatory) a subspace of V. Let us introduce a n-dimensional approximation

$$u_s(x) = U_{1s}\phi_1(x) + \ldots + U_{ns}\phi_n(x) \quad (24)$$

and subsequently $v(x) = \phi_1(x), \ldots, v(x) = \phi_n(x)$ for any $x \in \Omega$, working i) with some prescribed basis of V_n, created from functions with small compact supports $\{\phi_1(x), \ldots, \phi_n(x)\}$, ii) with some priori unknown real parameters (typically displacements in selected points), contained in a column vector $U_s = (U_{1s}, \ldots, U_{ns})^{\mathrm{T}}$.

For a regular family of such approximations, due to the limit passage $n \to \infty$, taking some length characteristic h corresponding to n, one can rewrite (10) to

$$h^2 M(U_s - U_{s-1}) + K(U_{s-1})U_s = h^2 F_s + hG_s \quad (25)$$

where $U_s, F_s, G_s \in R^n$ for $s \in \{1, \ldots, n\}$, U_0 being the zero vector of R^n, and $M, K(.) \in R^{n\times n}_{\mathrm{sym}}$. The symmetry and positive definiteness of sparse matrices M and $K(.)$ in (25) is inherited from C and α, whereas the argument of $K(.)$ comes just from the evaluation of a discretized nonlocal

damage factor $\delta(.)$, dependent on U_{s-1} in a complicated way. In particular, i) the 1st left-hand-side additive term vanishes in (25) for $\alpha = 0$, ii) all indices s on the right-hand side of (25) can be removed if $\beta_1 = 1$, iii) K is independent of U_{s-1} if $\mathfrak{D} = 1$ on Ω everywhere but this switches our problem to standard linear elastostatics.

Since (3) and (10) are not applicable to the prediction of creation and propagation of macroscopic cracks, a second model problem covering such phenomena could be useful, starting with the slight modification of a first one. As an illustrative example, we can take $\Omega = \Omega_0 \cup \Omega_1$ similarly to (7), but because of the absence of $\mathfrak{D}$ (formally $\mathfrak{D} = 1$ on Ω everywhere) instead of (7) we obtain

$$(\varepsilon(v), C{:}\varepsilon(u))_1 = (v, f)_1 + \langle v, g\rangle\,, \qquad (26)$$
$$(\varepsilon(v), C{:}\varepsilon(u))_0 = (v, f)_0\,.$$

In the more general context let us consider $\mathfrak{D} = 1$ in (10), but with Ω composed from a finite number of domains with Lipschitz boundaries, separated by their mutual interfaces, supplied by unit normals $\nu = (\nu_1, \nu_2, \nu_3)$ with some prescribed orientation, whose union will be denoted by Λ.

A delicate task is now some reasonable detection of active parts of Λ, i. e. those with discontinuous normal displacement components $u_\nu = u_1\nu_1 + u_2\nu_2 + u_3\nu_3$, applying some nonlocal stress evaluation again, because of the singularity on the crack tip. In such formulation no additional terms in (3) and (10) are needed, as respected by (26), too. However, more realistic models, inspired by [32] and [23], incorporate some cohesion on Λ, accompanied with tangential frictional slip along Λ; this brings always new additional terms analogous to $\langle v, g\rangle$ in (3), but integrated over just active parts of Λ instead of Γ and taking some experimentally validated functions of u_ν and $u_\tau = u - u_\nu\nu$ with values in $L^2(\Lambda)$ and $L^2(\Lambda)^3$ into consideration instead of $g \in Z$. Consequently such terms can be seen as contributions to $K(U_{s-1})$ in (25), preserving its formal linearity. This enables us to combine both micro- and macrocracking computations. Nevertheless, their limitations are obvious: a hypothetical extension of active cracks beyond an a priori prescribed set Λ, coming from certain prearranged list of potential cracks, coinciding with selected boundaries of finite elements to facilitate the composition of $K(.)$ in the analogue of (25) typically, can lead to total destruction at least of some parts of Ω again, similarly to that mentioned below (7).

For most practical computations the direct application of (25) in not acceptable because of the need of a priori knowledge of the location both of all microfractured zones and of all active macroscopic cracks, to cover them by a sufficiently detailed decomposition of Ω, together with its boundary and interfaces Θ, Γ and Λ. This was the basic motivation for the development of various improved adaptive techniques, namely those known as the partition of unity method (PUM, see [26]), the generalized finite element method (GFEM, see [37]) and the extended finite element method (XFEM, see [2] and [29] for its extrinsic version and [11] for the intrinsic one); for more comments to their 25 years old history and current progress cf. [43].

Applying the most frequent extrinsic XFEM approach, in an arbitrary s-th step of (25) some specialized additional basis functions are used adaptively, which for a finite number m of such functions reads

$$\begin{aligned} &h^2 \begin{bmatrix} M & M_s^* \\ M_s^{\star T} & M_s^\times \end{bmatrix} \cdot \begin{bmatrix} U_s - U_{s-1} \\ U_s^\times - U_{s-1}^\times \end{bmatrix} \qquad (27)\\ &+ \begin{bmatrix} K(U_{s-1}) & K_s^*(U_{s-1}) \\ K_s^\star(U_{s-1})^T & K_s^\times(U_{s-1}) \end{bmatrix} \cdot \begin{bmatrix} U_s \\ U_s^\times \end{bmatrix} \\ &= h^2 \begin{bmatrix} F_s \\ F_s^\times \end{bmatrix} + h \begin{bmatrix} G_s \\ G_s^\times \end{bmatrix}; \end{aligned}$$

here $M_s^\star$ and $K_s^\star(.)$ take values from $R^{n\times m}$ and $M_s^\times$ and $K_s^\times(.)$ from $R^{m\times m}_{\rm sym}$, forced extensions $F_s^\times$ and $G_s^\times$ are column vectors from R^m, as well as additional unkonwns $U_s^\times$. However, in practical implementations the form of (27) may be much less transparent because of the enrichment of the basis on a priori unpredicted locations, not on those referring just to the last m unknowns. Moreover the intrinsic XFEM approach tries to modify the original basis without an increase of the dimension of an approximation space from n to $n+m$; therefore (25) should be rewritten only with M_s instead of M and with K_s instead of K, including some possible modification of U_s, forced by crack development.

An illustrative example of appropriate types of enrichment functions for the original approximation by (24) both i) near crack tips and ii) along active cracks for a plane stress problem can be found in [43]. Certain nonlocal computational approach cannot be avoided here again, because of the presence of geometrical singularities, frequently also due to some specific choice of $\{\phi_1(x), \ldots, \phi_n(x)\}$ for (24), as in the simplest case of linear Lagrange splines, whose numerical derivatives cannot be assigned to particular FEM nodes directly. Other examples of cracking simulations under various conditions, received

from user-defined functions in the Abaqus software package, can be found in [41] and [42]. More general types of enrichment functions and integration strategies can be inspired by [22], [18] and [14].

Hitherto we have tried to treat microcracking (in details) and macrocracking (as sketched above) as a stationary problem, with some final stage determined by certain boundary value problem, for an originally linear elliptic system of partial differential equations of evolution of 2nd order, where potential sources of nonlinearities are only i) some values of $\mathfrak{D}(.) \neq 1$ and ii) interface phenomena on Λ. However, this may be not true for fracture propagation in real materials. The first step of generalization should convert such formulation to parabolic PDEs of evolution, supplied with homogeneous Cauchy initial conditions formally. However, this is rather easy: it is sufficient to take some $\alpha/\mathcal{H}$ instead of a positive constant α in (10), or even $\alpha/\mathcal{H}$ with $\alpha \in L^\infty(\Omega)$ such that $\alpha \geq \alpha_*$ for some positive α_* (then α must be located inside the corresponding scalar product) with $s \in \{1, \ldots, p\}$, p being some positive integer, and with $\mathcal{H} = \tau$ where τ means a finite length of certain fixed time interval, starting from zero, i. e. we intend to work with time t from a closed interval $I = [0, \tau]$ and with equidistant time steps $t = 0$, $t = \mathcal{H}$, ..., $t = p\mathcal{H} = \tau$. It is now reasonable to admit an explicit time-dependence of f and g, thus also of w and ε_*, as well as of an unknown solution u. Let an upper dot symbol refer to partial derivatives with respect to t. Then $(\varepsilon_s - \varepsilon_{s-1})/\mathcal{H}$ in (10) can be understood as a relative time difference at $t = s\mathcal{H}$, approximating $\varepsilon(\dot{u})$ there if $(s-1)\mathcal{H} < t \leq s\mathcal{H}$ in all other cases we can take only values at $t = s\mathcal{H}$ for $(s-1)\mathcal{H} < t \leq s\mathcal{H}$ everywhere, including those unknown ones for u, except those for $\mathfrak{D}$ at $t = (s-1)\mathcal{H}$. Using the notation of various Bochner - Sobolev spaces by [34], p. 187, and 3 types of Rothe sequences of abstract functions (namely linear splines, standard simple functions and retarded simple functions), mapping I to corresponding Lebesgue and Sobolev spaces (cf. [34], p. 201), we are able to derive $u \in V$ by (3) as $u(.\,\tau)$ here, provided that $\tau \to \infty$, with $\dot{u} \in V$ tending to o everywhere. Moreover the occurrence of the 1st left-hand-side additive term in (10) enable us to extend (3) to its non-stationary version to handle a simple linear form of the Kelvin parallel viscoelastic model (cf. [13]).

Such considerations are more significant as a rough introduction to time-dependent problems than as a competing (more complicated) procedure how to derive the same results as in Section 3. As verified by [41] properly, the above sketched approach can be applied to much more general time-dependent loads f and g, thus its usability in fracture mechanics is not limited to stationary cracks, even if no limit passage $\tau \to \infty$ is available. Resulting systems of sparse linearized systems of algebraic equations, corresponding to (25) and (27), are generated naturally applying the combination of XFEM with the method of discretization in time, based on the weak and strong convergence properties of Rothe sequences.

However, for the analysis of fully dynamical processes, as required by [4], such idealization is not acceptable. Some Kelvin-like or even more advanced material model, combining elasticty, plasticity, damage, interface phenomena, etc., must be supplied by inertia forces and a suitable mechanism of energy dissipation. Consequently we come to hyperbolic PDEs of evolution instead of parabolic ones. A still partially linearized problem of this type has been analyzed in details by [42].

In numerical modelling of fast dynamical processes, like cracking forced by mutual contacts / impacts of particular bodies, still other difficulties occur, like i) cracking forced by mutual contacts / impacts of particular bodies, with the need of advanced search of potential contact candidates using the graph theory and parallel / distributed computing, as sketched by [33], and ii) necessity of frequent ad hoc (rather expensive) resets of initial configuration, to suppress the effect of geometrical linearization, or even the implementation of arbitrary Lagrangian-Eulerian approach, well-tried in computational fluid dynamics, as recommended by [19]. Development of explicit parallable time integration methods for such problems becomes an important research direction in the last decade, as documented by [3].

Derivation of weak and strong convergence properties of $\{u\}_{r=1}^{\infty}$, as well as of all sequences used in (2) and generated by $\{u\}_{r=1}^{\infty}$, is rather intuitive, regardless of a proposed non-trivial 6-step algorithm of their evaluation. Technical difficulties caused by possible implementation of more advanced constitutive models can be overcome using selected results on Nemytskiĭ operators, as introduced by [5], p. 134, satisfying some additional requirements, e. g. on coerciveness with pseudomonotony or with weak continuity (see [34], pp. 46 and 58). Nevertheless, knowledge of standard Korn, trace, etc. theorems on domains with sufficiently smooth (in particular Lipschitz) boundary seems to be already insufficient for the proper analysis and implementa-

tion of complicated dynamical models handling micro- an macrocracking. This stimulates further progress in mathematical analysis, which can be documented on relevant results of [20] and [35].

5 Conclusion

The detailed analysis of Section 3 demonstrates that some useful existence and convergence results for an algorithm induced by (10), as the final formulation of Section 2, can be derived. Such algorithm can be extended naturally to the analysis of both micro- and macrocracking, to time-dependent problems, etc. In general, it is open to new ideas overcoming limitations of its presented preliminary version, as sketched by Section 4.

Still open questions, both i) in physical and mathematical analysis of cracking formation and ii) in corresponding numerical methods and their robust and effective software implementations, occur. They can be seen as a research challenge for the near future.

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