

COMPUTATIONAL SMEARED DAMAGE IN THE MACROSCOPIC ANALYSIS OF QUASI-BRITTLE MATERIALS AND STRUCTURES

JIŘÍ VALA*

Abstract. Computational modelling of behaviour of composite materials and structures is based on principles of classical thermodynamics, supplied by appropriate constitutive relations. In the case of quasi-brittle materials like ceramics, rocks and building composites including concrete, the initiation and development of micro-fractured zones, up to the formation of systems of macroscopic cracks, can be handled using the nonlocal smeared damage factors, respecting different behaviour in tension and compression, whose characteristics must be determined from well-designed experiments. This contribution shows the mathematical background of such modelling approach, needed for practical computational experiments.

Key words. Quasi-brittle materials, smeared damage, cohesive interfaces, computational modelling, method of discretization in time, finite element method.

AMS subject classifications. 74R10, 65M60

1. Introduction. Initiation and development of material damage, including the qualitative change of such damage from the local to the global one, belongs to the most dangerous processes in engineering structures. Namely in cementitious composites, utilized widely in building structures, dangerous tensile stresses in their matrices, leading to formation and propagation of crack systems, can be expected; this is usually suppressed by certain reinforcement by (nearly) elastic rods or fibres. The prediction of mechanical, thermal, etc. behaviour of such composite structures is rather difficult because of complicated material structure and assessment of physical processes at several scales: even for a macroscopic analysis, from the point of view of a typical size, we have to deal with i) matrix particles [10^{-3} m], ii) hardening fibres [10^{-2} m] and iii) laboratory samples [10^{-1} m] or iv) complete structures [m]; for several available approaches to non-destructive identification of such structures see [58].

The classification of fracture, in its roughest form, can be done due to usual fraction manifestation: a) by discrete crack discontinuities, as in *brittle* materials like glass or welds in metal structures, b) by shear localization bands, as in elasto-plastic *ductile* metal or similar materials, c) by fracture process zones, as in *quasi-brittle* materials like rocks or concrete; for much more detailed classifications cf. [35], [52] and [53]. Namely for c) it is difficult to distinguish between particular cracks by reasonable deterministic computations; nonlocal evaluations are needed typically because of the presence of many irregular parts boundaries and interfaces.

In this conference paper we shall pay attention to the deterministic approaches to the strain and stress analysis of quasi-brittle composites, based on the principles of classical thermodynamics, supplied by appropriated constitutive equations with material characteristics, identifiable from laboratory experiments. After this introductory *Section 1*, in *Section 2* we shall continue with brief comments to problem history, to obtain the basic orientation in various physical, mathematical and computational approaches. Then in *Section 3* we shall discuss the classical simplified quasi-static approach, utilizing the Kelvin parallel viscoelastic strain-stress relation, generalizing the

*Institute of Mathematics and Descriptive Geometry, Faculty of Civil Engineering, Brno University of Technology, CZ-60200 Brno, Veveří 331/95 (Jiri.Vala@vut.cz).

fully static and purely elastic Hooke relation in a direct way, but implementing certain (scalar or matrix) damage factor reducing the material stiffness, whose nonlocal evaluation relies on [17], upgraded by [18]. Possible ways to direct generalization of this approach to the fully dynamic one will be presented in *Section 4*. However, this can cover only the initiation and propagation of microfractured zone, not the creation and development of particular macroscopic cracks and their systems. Coupling of both such processes will be sketched in *Section 5*, with a key reference to [31], based on the detailed description of cohesive interfaces. Moreover, [31] can be seen as certain continuation of this paper: it shows numerical results of illustrative problems, useful for the comparison of various methods discussed here, too. *Section 6* will demonstrate how the potential removal of non-physical simplifications modifies all formulations of *Sections 3, 4, 5*, resulting in still unclosed mathematical and computational problems. *Section 7* sketches computational algorithms related to all preceding considerations, based i) on the method of Rothe sequences (of discretization in time) and ii) on the extended finite element method (XFEM), or some similar one. Let us notice that the development of algorithms ii) and the related convergence analyses, coming from [40], [46], [20], [6] and [23], form a separate research area during two last decades; e.g. the review article [11] contains 317 relevant references. The concluding *Section 8* contains the brief summary of presented results together with some research priorities for the near future.

2. Problem history. The early problem analysis is connected with the local study of behaviour of material samples, simulating to simple 3-point, 4-point, etc. flexural tests with a special geometrical configuration and a sufficiently simple material structure, as motivated by [21] and documented by [15], [4], [48], [50] and [54]. First attempts to develop more complex mathematical models date back to the last decade of the 20th century. A rather simple quasi-static isotropic model for damaged materials with microscopic cracks and other defects, applicable even to a significant class of anisotropic media, was suggested by [26]. More general isotropic models need to respect bi-modularity, i.e. degradation in tension vs. compression, as analyzed by [25] and [22], corresponding to principles of classical thermomechanics. The usual triple of reference models, used by numerous recent studies for comparison, is (in the historical order) [38], Chaps. 7, 8 of [34] and [13].

Let us notice that [39], using strain tensor invariants and control loading functions by [10] which can be seen as an upgrade of [38], has been implemented in many later analyses just for concrete and similar composites. Recent computational approaches still refer to certain simplified quasi-static or dynamic formulations in most cases, with potential coupling of smeared damage with cohesive interfaces like [37]. Regardless of the implementation of their computational algorithms into both research and commercial software codes, significant open question occur both in their formal verification and practical validation, as required by [3]. Partial existence, uniqueness, convergence, etc. results can be found in [24], [9], [60] and [61], in contrast with the serious non-existence examples of [2] and [16].

Recently several attempts to avoid non-physical assumptions with the aim of more realistic damage predictions must be appreciated. Some disadvantages of the above presented approaches can be suppressed using a proper evaluation of phase-field fracture energy by [65] and [7]. Unlike this, [66] tries to overcome the randomness and irregularity of concrete cracking using the fractal dimension. Another thermodynamically improved approach, suggested by [28] and [63], relies on the implementation of matrix damage characteristics via Helmholtz and Gibbs energies, including an appro-

appropriate set of internal variables; its basic idea can be traced back to [43]. Nevertheless, i) some additional analysis of non-trivial inverse problems (setting of material parameters from experiments) is always required and ii) all mathematical modelling is then switched to special strongly nonlinear initial and boundary hyperbolic problems for systems of partial differential equations and / or inequalities, with a lot of expectable difficulties in both theoretical and numerical analyses.

3. Smearred damage: a quasi-static simplified approach. For the introduction of a model problem, open to later modifications, let us consider a deformable body occupying a domain Ω in the 3-dimensional Euclidean space \mathcal{R}^3 with Lipschitz boundary $\partial\Omega$, consisting of 2 disjoint parts Θ (for homogeneous Dirichlet boundary conditions) and Γ (for Neumann boundary conditions, inhomogeneous in general). A Cartesian coordinate system $x = (x_1, x_2, x_3)$ is implemented in \mathcal{R}^3 ; in *Sections 4, 6* we shall need the gradient operator $\nabla = (\partial/\partial x_1, \partial/\partial x_2, \partial/\partial x_3)$. For the brevity of notation, we shall have $(\cdot)_{,i}$ instead of $\partial/\partial x_i$ with $i \in \{1, 2, 3\}$; all displacements u_i of x_i will be related to a reference configuration of Ω , in the initial time $t = 0$ formally. The time redistribution of $u = (u_1, u_2, u_3)$ will be studied for $t \in \mathcal{I}$ for certain time interval $\mathcal{I} = [0, \tau]$, τ being a given positive time. The dot symbols will be used instead of $\partial/\partial t$ everywhere for brevity. We shall consider the zero-valued Cauchy initial conditions, i. e. $u_1(0) = u_2(0) = u_3(0) = 0$. The Sobolev space of test functions can be then defined in as $\mathcal{V} = \{w \in W^{1,2}(\Omega)^3 : w = (0, 0, 0) \text{ on } \Theta\}$. A symmetric strain tensor $\varepsilon(w)$ can be introduced for each $w \in \mathcal{V}$ by its components $\varepsilon_{ij}(w) = (w_{i,j} + w_{j,i})/2$ for $i, j \in \{1, 2, 3\}$, as usual in the small deformation theory.

All approaches presented in this paper refer to conservation principles of classical thermodynamics, as mass, (linear and angular) momentum and energy, compatible with [44], and to an appropriate choice of material characteristics. In a quasi-static simplification we can work with conservation of linear momentum in its weak form

$$[\varepsilon(w), \sigma(u, \dot{u})] = (w, f) + \langle w, g \rangle, \quad (3.1)$$

valid for any $w \in \mathcal{V}$, $t \in \mathcal{I}$ and some unknown $u(t)$ from \mathcal{V} for any fixed $t \in \mathcal{I}$. The brief notations (\cdot, \cdot) , $[\cdot, \cdot]$ and $\langle \cdot, \cdot \rangle$ are used for the scalar products defined in $L^2(\Omega)^3$, $L^2(\Omega)^{3 \times 3}$ and $L^2(\Gamma)^3$; $\sigma(u, \dot{u})$ denotes a symmetric stress matrix. The time development of $u(t)$ for $t \in \mathcal{I}$ is driven by the time development of prescribed volume loads $f \in L^2(\Omega \times \mathcal{I})^3$ and surface loads $g \in L^2(\Gamma \times \mathcal{I})^3$.

To be able to evaluate u and v from (3.1), constitutive stress-strain equations for $\sigma(u, v)$ are needed. Namely $\sigma = C\varepsilon(u)$ in linear elasticity, with a 4-th order tensor $C \in L^\infty(\Omega)_{\text{sym}}^{(3 \times 3) \times (3 \times 3)}$, containing 21 independent characteristics in general, reducible up to 2 (the Young modulus, the Poisson ratio) in the isotropic case. We need to include some energy dissipation, using e. g. the Kelvin parallel viscoelastic model $\sigma = C\varepsilon(u) + \alpha C\varepsilon(\dot{u})$ with certain structural damping factor $\alpha \in L^\infty(\Omega)$. Let us notice that such simple model is considered to avoid various technical difficulties here; for much more general classes of the Kelvin chains see [49] and [56], for the formal existence and uniqueness considerations cf. [30].

The last ingredient of such model is a couple of damage characteristics \mathcal{D} , \mathcal{D}^T , in general from $L^\infty(\Omega)_{\text{sym}}^{(3 \times 3) \times (3 \times 3)}$ again: C is replaced by certain $\mathcal{D}C\mathcal{D}^T$ such that the original symmetry of C is preserved. However, it is not easy to identify these rather complicated material characteristics, thus \mathcal{D} is taken as $\sqrt{1 - \mathfrak{D}} I$ frequently, I being an identity operator, where a scalar factor \mathfrak{D} with values between 0 and 1 is used, to express the loss of material stiffness due to microfracture. Thus, for

simplicity with a scalar \mathfrak{D} only, we have

$$\sigma(u, \dot{u}) = \alpha(1 - \mathfrak{D})C\varepsilon(\dot{u}) + (1 - \mathfrak{D})C\varepsilon(u). \quad (3.2)$$

The most difficult task, both from the mathematical end engineering points of view, is than to design a reasonable dependence of \mathfrak{D} on some regularized versions of appropriate strain and / or stress invariants. Typically some $\bar{\varsigma}$ replaces an original scalar invariant ς , both from $L^2(\Omega)$, using certain kernel operator $\mathcal{K} \in L^2(\Omega \times \Omega)$ by [14], Part 2.2, inspired by [18], in the form

$$\bar{\varsigma}(x) = \int_{\Omega} \mathcal{K}(x, \tilde{x}) \varsigma(\tilde{x}) d\tilde{x} \quad (3.3)$$

for any $x \in \Omega$. A lot of different variants of \mathcal{K} for (3.3) have been tested in last 2 decades: various ad hoc functions, as exponential or polynomial ones, Gaussian distributions, exact or approximated radial basis functions, Green functions for a bi-Helmholtz ordinary differential equation of fourth order (based on certain microstructural considerations), etc. The more extensive discussion on the derivation of such functions can be found in [33], [51] and [57]. Let us remind that even the design of invariants for concrete-like materials is not easy because of the need of different values of characteristics under tension and compression.

In all cases (3.1), supplied with (3.2), generates a nearly linear equation, whose nonlinearity is caused only by the rather delicate evaluation of \mathfrak{D} . Clearly the removal of \mathfrak{D} from the first right-hand-side additive term of (3.1) would be helpful computationally, but this has no transparent physical justification. For a rather wide classes i) of \mathcal{K} in (3.3) and ii) of the choice of above sketched invariants, the existence of both u and \dot{u} in the Bochner-Sobolev space $L^2(\mathcal{I}, \mathcal{V})$ can be verified using the theory of Rothe sequences; for the details see [60]. One can expect reasonable outputs from the related computations for engineering application with a relatively small damage, i. e. $\mathfrak{D} \ll 1$, not for the study of behaviour of a structure up to its total destruction. Moreover, the absence of a proper formulation of kinetic energy does allow to study any fast dynamic processes.

4. Smearred damage: a dynamic simplified approach. Fortunately, for the simplified study of dynamic processes, most arguments from *Section 3*, including the Kelvin viscoelastic model and the damage factor, can be adopted. Instead of (3.1) we have

$$(w, \rho \ddot{u}) + (w, \beta \rho \dot{u}) + [\varepsilon(w), \sigma(u, \dot{u})] = (w, f) + \langle w, g \rangle \quad (4.1)$$

where $\rho \in L^2(\Omega)$ is material density and $\beta \in L^2(\Omega)$ is a new material factor, referred as mass damping one; moreover an acceleration \ddot{u} occurs here. The Cauchy initial condition from *Section 3* must be replaced by a couple of such conditions for both $u(0)$ and $\dot{u}(0)$. Thus we have a hyperbolic equation (4.1) instead of a parabolic equation (3.1) with comparable initial and boundary conditions, without any additional nonlinearity.

Also (3.1), supplied with (3.2), can be handled using the theory of Rothe sequences. Following [61], it is possible to find both u and \dot{u} in $L^2(I, V)$, whereas \ddot{u} belongs only to $L^2(\mathcal{I} \times \Omega)$. Some motivations for useful generalizations can be found in [64]. However, the fully dynamic model should cover also contacts and impacts of particular deformable bodies with possible damage, which bring serious additional problems, connected with the advanced search algorithms for potential contacts, as

discussed by [47] and [62]. open to parallel and distributed computational strategies, following [12]. Still other difficulty can be caused by practical violation of expected small deformation; a (at least partial) remedy relies on computational restarts with upgraded reference configurations.

Selected generalizing terms can be added both to (3.1) and to (4.1) without substantial difficulties. As a frequently presented example, introducing a prescribed thermal expansion coefficient γ , we can add $\gamma\nabla(\vartheta - \vartheta^{\text{ref}})$ to $\varepsilon(u)$ in (3.2), as well as $\gamma\nabla\dot{\vartheta}$ to $\varepsilon(\dot{u})$ there, ϑ being the absolute Kelvin temperature, ϑ^{ref} some its reference value. However, such simplified formulae cannot substitute a proper thermodynamic formulation, as sketched by *Section 6*.

5. Incorporation of cohesive interfaces. Initiation and development of visible cracks of macroscopic size, described as internal interfaces with possible discontinuities in u , v and a , do not agree with the smeared damage approach, but the incorporation of this process may be necessary, due to certain values of nonlocal strain or stress invariants: such criteria as strange energy density, crack driving force, special nonlocal integrals, related to the stress and strain at possible crack tip, can be found in the literature. The development of cohesive models is connected e. g. with [45], [32] and [36]; for much more information see [31].

In this paper we shall present only a simple way how these considerations can be coupled with the smeared damage approach. This can be done both for (3.1) and for (4.1) similarly, thus we are allowed to pay attention to (4.1) here only. For illustration, let us consider a system of potential cohesive interfaces Λ inside Ω ; $\langle \cdot, \cdot \rangle_*$ will refer to the scalar product in $L^2(\Lambda)$. Using the symbol δ for the jump in values in the normal direction $\nu = (\nu_1, \nu_2, \nu_3)$ of the unit length in \mathcal{R}^3 almost everywhere on Λ , preserving some predefined orientation of ν , we can rewrite (4.1) in the form

$$(w, \rho\ddot{u}) + (w, \beta\rho\dot{u}) + [\varepsilon(w), \sigma(u, \dot{u})] + \langle w, \mathcal{T} \rangle_* = (w, f) + \langle w, g \rangle; \quad (5.1)$$

here, instead of g on Γ , we have $\mathcal{T} = \omega(\delta u_\nu)$ where u_ν denotes the normal component of u with respect to ν , i. e. $u_\nu = u_1\nu_1 + u_2\nu_2 + u_3\nu_3$, evaluated from both sides of Λ separately. A new material characteristic ω is needed here, known as the traction separation law; for some its commonly used forms cf. [31] again. Let us remark that this formulation is only illustrative; in the more general context also jumps in values of u in tangential directions can be included. Since ω is not a linear function in reasonable engineering applications, the second type of nonlinearity, in addition to that first one caused by the smeared damage factor, occurs in (5.1), unlike (4.1).

6. A proper thermodynamic approach. For the detailed analysis of development of damage a less simplified model may be required. Such model can work with certain power of dissipation \mathcal{P} , avoiding non-physical assumptions if possible. Here we shall demonstrate basic ideas of such approach only; the related theory is still far from being complete and closed. Let us consider some heat q flow on Ω for particular $t \in \mathcal{I}$; ρ will be constant in time again, like *Section 4*. Now \mathcal{P} is supposed to come from specific Helmholtz free energy \mathcal{H} , taken specific entropy η into account, as induced by the formula

$$\mathcal{P} = -\rho\dot{\mathcal{H}} + \sigma : \dot{\varepsilon} - \rho\dot{\vartheta}\eta - \vartheta^{-1}\nabla\vartheta \cdot q \geq 0; \quad (6.1)$$

: and \cdot here mean the scalar products in $\mathcal{R}^{3 \times 3}$ and \mathcal{R}^3 , still on Ω locally. Alternatively \mathcal{P} can be expressed from specific Gibbs free energy $\mathcal{G} = \rho^{-1}\sigma \cdot \varepsilon - \mathcal{H}$, namely

$$\mathcal{P} = \rho\dot{\mathcal{G}} - \dot{\sigma} : \varepsilon - \rho\dot{\vartheta}\eta - \vartheta^{-1}\nabla\vartheta \cdot q \geq 0. \quad (6.2)$$

Now $\mathcal{G}(\mathcal{S})$ can be seen as a function of four state variables $\mathcal{S} = (\vartheta, \sigma, \mathcal{D}, \kappa)$: only one internal variable κ (is considered here for simplicity, together with the 2nd-order symmetric damage tensor \mathcal{D}). Four dissipative variables are $\mathcal{W} = (\dot{\vartheta}, q, \mathcal{D}^*, \kappa^*)$; here $\mathcal{D}^* = \rho \partial \mathcal{G} / \partial \mathcal{D}$ and $\kappa^* = -\rho \partial \mathcal{G} / \partial \kappa$. Using (6.1) and (6.2), this results

$$\mathcal{P} = \rho (\partial \mathcal{G} / \partial \vartheta - \eta) \dot{\vartheta} + \dot{\sigma} : (\rho \partial \mathcal{G} / \partial \sigma - \varepsilon) - \vartheta^{-1} \nabla \vartheta \cdot q + \mathcal{D}^* \dot{\mathcal{D}} - \kappa^* \dot{\kappa} \geq 0. \quad (6.3)$$

Whereas $\mathcal{G}(\mathcal{S})$ corresponds to the reversible part of material behaviour, its irreversible part can be characterized by some dissipative potential $\mathcal{E}(\mathcal{S}, \mathcal{W})$.

In the following evaluations, $D\mathcal{E}_\zeta$ with $\zeta \in \mathcal{W}$ can be considered as particular components of $\partial \mathcal{E} / \partial \mathcal{W}$ for sufficiently smooth \mathcal{E} (which is not guaranteed), otherwise as those of a subdifferential of \mathcal{E} , i. e.

$$\mathcal{P} = \dot{\vartheta} D\mathcal{E}_\vartheta + q \cdot D\mathcal{E}_q + \mathcal{D}^* : D\mathcal{E}_{\mathcal{D}^*} + \kappa^* D\mathcal{E}_{\kappa^*}. \quad (6.4)$$

Thus (6.3) and (6.4) yield the general condition

$$\begin{aligned} & (\rho (\partial \mathcal{G} / \partial \vartheta - \eta) - D\mathcal{E}_\vartheta) \dot{\vartheta} - (\vartheta^{-1} \nabla \vartheta + D\mathcal{E}_q) \cdot q + \dot{\sigma} : (\rho \partial \mathcal{G} / \partial \sigma - \varepsilon) \\ & + \mathcal{D}^* : (\dot{\mathcal{D}} - D\mathcal{E}_{\mathcal{D}^*}) - \kappa^* (\dot{\kappa} + D\mathcal{E}_{\kappa^*}) = 0, \end{aligned} \quad (6.5)$$

satisfied for any \mathcal{W} . In (6.5), $\varepsilon = \rho \partial \mathcal{G} / \partial \sigma$ is identifiable from a function \mathcal{G} , due to appropriate experimental setting, moreover $D\mathcal{E}_\vartheta = \rho (\partial \mathcal{G} / \partial \vartheta - \eta)$, $D\mathcal{E}_q = -\vartheta^{-1} \nabla \vartheta$, $D\mathcal{E}_{\mathcal{D}^*} = \dot{\mathcal{D}}$ and $D\mathcal{E}_{\kappa^*} = -\dot{\kappa}$.

Unfortunately, a complete physical and mathematical theory, based on (6.5), is still missing, unlike some computational results under substantial simplifications, coinciding with those from *Sections 3, 4, 5* in some aspects. For illustration, [63] assumes: i) Only the small strain theory is considered, with the fixed initial reference configuration, working with the additive decomposition $\mathcal{G}(\mathcal{S}) = \mathcal{G}_1(\vartheta) + \mathcal{G}_2(\sigma, \mathcal{D}) + \mathcal{G}_3(\kappa)$. ii) \mathcal{G}_2 needs careful design of appropriate invariants derived from σ and \mathcal{D} . iii) The non-local 4-parameter evaluation of κ for \mathcal{G}_3 relies on [27]. iv) \mathcal{E} is reduced to its simplest case, which is certain set of characteristic functions by [19]. Moreover, regardless of [63], some particular results are available, as an estimation technique for \mathcal{E} via crack tip velocity by [8], or the proof of local well-posedness for a model problem by [1], referring to [19] again.

7. Computational algorithms. Two numerical methods are crucial for the design of computational algorithms here: i) the method of discretization in time, supported by the results on properties of Rothe sequences of linear spline abstract functions, simple abstract functions and their appropriate modifications, including delayed ones, ii) the standard finite element method in \mathcal{R}^3 , or its some extended, generalized, etc. variant, namely for the incorporation of cohesive interfaces Λ in *Section 5*. However, numerical approaches connected with *Section 6* need substantial upgrade of i), ii), exceeding the introductory analysis presented in this paper. Therefore, for illustration, we shall come from one possible effective algorithm related to *Section 5*, based on the equidistant time discretization on \mathcal{I} . It will be presented for $u, \dot{u} \in L^2(I, \mathcal{V})$ and $\ddot{u} \in L^2(\Omega \times \mathcal{I})$, still with an infinite-dimensional Sobolev space V formally, although all practical calculations work with some finite-dimensional approximation of V . Thus, instead of $u(sh)$, $\dot{u}(sh)$ and $\ddot{u}(sh)$, we are searching for certain displacements $u^s \in \mathcal{V}$, their rates $v^s \in \mathcal{V}$ and accelerations $a^s \in L^2(\Omega)^3$ step-by-step for $s \in \{1, 2, \dots, m\}$, $h = \tau/m$ where m is an integer, admitting the limit passage $m \rightarrow \infty$. Let us remind that \mathcal{V} and $L^2(\Omega)^3$ are still Hilbert spaces where standard scalar products can be applied, as introduced in *Sections 3, 5*.

Clearly we are allowed to set $f^s = f(., sh)$ on Ω and $g^s = g(., sh)$ on Γ , or e. g. (if possible) f^s and g^s as mean values of f and g on $[(s-1/2)h, (s+1/2)h]$, in the sense of abstract functions mapping \mathcal{I} to $L^2(\Omega)^3$ and $L^2(\Gamma)^3$. We shall work with the discretization of the Newmark type, as introduced by [5], referring to the original idea of [42], for simplicity. Then (5.1) together with (3.2) can be discretized as

$$\begin{aligned} & (w, \rho(a^s + \beta v^s)) + [\varepsilon(w), (1 - \mathfrak{D}_\times^s)C(\alpha\varepsilon(v^s) + \varepsilon(u^s))] + \langle w, \omega(\delta u_{\nu\times}^s)\delta u_\nu^s \rangle_* \\ & = (w, f^s) + \langle w, g^s \rangle \end{aligned} \quad (7.1)$$

where, using the standard trapezoidal rule for numerical quadrature,

$$\begin{aligned} v^s &= v^{s-1} + \frac{h}{2}(a^s + a^{s-1}), \\ u^s &= u^{s-1} + \frac{h}{2}(v^s + v^{s-1}) = u^{s-1} + hv^{s-1} + \frac{h^2}{4}(a^s + a^{s-1}). \end{aligned} \quad (7.2)$$

Thus, for a priori known a^{s-1} , v^{s-1} and u^{s-1} and rough estimates $v_\times^s = v^{s-1}$ and $u_\times^s = u^{s-1}$, generating a damage factor \mathfrak{D}_\times^s , too, (7.1) with (7.2) can be seen as a linear elliptic equation for the evaluation of a^s with $s \in \{1, \dots, m\}$, as evident from its slightly modified form

$$\begin{aligned} & (w, \rho a^s) + \frac{h}{2}(w, \rho \beta a^s) \\ & + h[\varepsilon(w), (1 - \mathfrak{D}_\times^s)C\alpha\varepsilon(a^s)] + \frac{h^2}{4}[\varepsilon(w), (1 - \mathfrak{D}_\times^s)C\varepsilon(a^s)] + \frac{h^2}{4}\langle w, \omega(\delta u_{\nu\times}^s)\delta a_\nu^s \rangle_* \\ & = (w, f^s) + \langle w, g^s \rangle - (v, \rho \beta v^{s-1}) - \frac{h}{2}(v, \rho \beta a^{s-1}) \\ & - [\varepsilon(w), (1 - \mathfrak{D}_\times^s)C\alpha\varepsilon(v^{s-1})] - \frac{h}{2}[\varepsilon(w), (1 - \mathfrak{D}_\times^s)C\alpha\varepsilon(a^{s-1})] \\ & - [\varepsilon(w), (1 - \mathfrak{D}_\times^s)C\varepsilon(u^{s-1})] - h[\varepsilon(w), (1 - \mathfrak{D}_\times^s)Ch\varepsilon(v^{s-1})] \\ & - \frac{h^2}{4}[\varepsilon(w), (1 - \mathfrak{D}_\times^s)C\varepsilon(a^{s-1})] \\ & - \langle w, \omega(\delta u_{\nu\times}^s)\delta u_\nu^{s-1} \rangle_* - h\langle w, \omega(\delta u_{\nu\times}^s)\delta v_\nu^{s-1} \rangle_* - \frac{h^2}{4}\langle w, \omega(\delta u_{\nu\times}^s)\delta a_\nu^{s-1} \rangle_*. \end{aligned} \quad (7.3)$$

Since u^0 and v^0 are zero-valued thanks to the Cauchy initial conditions, a^0 can be calculated from (7.1), too, taking $s = 0$ formally. Using a suitable discretization in \mathcal{R}^3 , as XFEM-based one, (7.3) generates a finite sparse system of linear algebraic equations.

Instead of the above introduced rough estimates of u_\times^s and v_\times^s , one can insert the values of v^s and u^s in any s -th time step, repeat the same calculations and apply an appropriate error estimator. This can be understood as a basis for an adaptive iteration process inside particular time steps. However, a less complicated computational scheme than this semi-implicit one might be preferred especially for some fast dynamic processes, because of the necessary choice of very small h from another reason, such as the detailed analysis of dissipation energy on contact surface areas by [55] and [41]; for the possible implementation of explicit integration schemes cf. [29] and [59].

8. Conclusion. We have sketched several types of approaches to the evaluation of damage in composite materials and structures. The quality of such evaluation

determines the reliability of predictions of behaviour of engineering structures under various types of loads, involving the risk of their deterioration, up to total destruction, thus the careful verification and validation of all algorithms is needed. New trends in numerical modelling and simulation reflect the development of advanced materials, structures and technologies where the long-time experience of their designers, based on standard laboratory experiments and observations in situ, is missing.

This paper contains no computational examples intentionally; the reader can find them in [31] in the same 22nd *Algorithmic Proceedings*. However, in several parts of this paper still unclosed problems are mentioned, especially (but not only) in *Section 6*, devoted to potential removal of non-physical simplifications from engineering computations. This is a serious challenge for further research activities, whose support by the progress both in mathematical and numerical analysis and in computational hardware and software can be expected.

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REFERENCES

- [1] G. AKAGI AND G. SCHIMPERNA, *Local well-posedness for Frémond's model of complete damage in elastic solids*, Eur. J. Appl. Math., 33 (2022), pp. 309–327.
- [2] S. ALEXANDROV AND R. GOLDSTEIN, *On the nonexistence of certain solutions for damage mechanics models*, Int. J. Fract., 200 (2016), pp. 151–158.
- [3] I. BABUŠKA AND J. T. ODEN, *Verification and validation in computational engineering and science: basic concepts*, Comput. Methods Appl. Mech. Eng., 193 (2004), pp. 4057–4066.
- [4] G. I. BARENBLATT, *The mathematical theory of equilibrium of cracks in brittle fracture*, Adv. Appl. Mech., 7 (1962), pp. 55–129.
- [5] F. BAMER, N. SHIRAFKAN, X. CAO, A. OUESLATI, M. STOFFEL, G. DE SAXCÉ AND B. MARKERT, *A Newmark space-time formulation in structural dynamics*, Comput. Mech., 67 (2021), pp. 1331–1348.
- [6] T. BELYTSCHKO, R. GRACIE AND G. VENTURA, *A review of extended / generalized finite element methods for material modelling*, Modeling Simul. Mater. Sci. Eng., 17 (2009), pp. 043001 / 1–24.
- [7] R. BHARALI, F. LARSSON AND R. JÄNICKE, *A micromorphic phase-field model for brittle and quasi-brittle fracture*, Comput. Mech., 73 (2024), pp. 579–598.
- [8] T. Q. BUI, H. T. TRAN, X. HU AND CH.-T. WU, *Simulation of dynamic brittle and quasi-brittle fracture: a revisited local damage approach*, Int. J. Fract., 236 (2022), pp. 59–85.
- [9] M. CAPONI, *Existence of solutions to a phase-field model of dynamic fracture with a crack-dependent dissipation*, Nonlinear Differ. Equations Appl., 27 (2020), pp. 14 / 1–48.
- [10] I. CAROL, E. RIZZI AND K. WILLAM, *A unified theory of elastic degradation and damage based on a loading surfaces*, Int. J. Solids Struct., 31 (1994), pp. 2835–2865.
- [11] M. CERVERA, G. B. BARBAT, M. CHIUMENTI, J. Y. WU, *A comparative review of XFEM, mixed FEM and phase field models for quasi-brittle cracking*, Arch. Comput. Methods Eng., 29 (2022), pp. 1009–1083.
- [12] Y. CHEN, L. ZHOU, Y. TANG, J. P. SINGH, N. BOUGUILA, C. WANG, H. WANG AND J. DU, *Fast neighbor search by using revised k-d tree*, Inf. Sci., 472 (2019), pp. 145–162.
- [13] J. DE VREE, W. BREKELMANS AND M. VAN GILS, *Comparison of nonlocal approaches in continuum damage mechanics*, Comput. Struct., 55 (1995), pp. 581–588.
- [14] P. DRÁBEK AND I. MILOTA, *Methods of Nonlinear Analysis*, Birkhäuser, Basel, 2013.
- [15] D. S. DUGDALE, *Yielding of steel sheets containing slits*, J. Mech. Phys. Solids, 8 (1960), pp. 100–104.
- [16] A. EVGRAFOV AND J. C. BELLIDO, *From non-local Eringen's model to fractional elasticity*, Math. Mech. Solids, 24 (2019), pp. 1935–1953.
- [17] A. C. ERINGEN, *Theory of Nonlocal Elasticity and Some Applications*, Princeton University, technical report 62, 1984.
- [18] A. C. ERINGEN, *Nonlocal Continuum Field Theories*, Springer, Berlin, 2002.
- [19] M. FRÉMOND AND B. NEJDAR, *Damage, gradient of damage and principle of virtual power*, Int. J. Solids Struct., 33 (1996), pp. 1083–1103.

- [20] T.-P. FRIES AND T. BELYTSCHKO, *The intrinsic XFEM: a method for arbitrary discontinuities without additional unknowns*, Int. J. Numer. Methods Eng., 68 (2006), pp. 1358–1385.
- [21] A. A. GRIFFITH, *The phenomena of rupture and flow in solids*, Philos. Trans. R. Soc. A, 221 (1920), pp. 163–198.
- [22] P. HAVLÁSEK, P. GRASSL AND M. JIRÁSEK, *Analysis of size effect on strength of quasi-brittle materials using integral-type nonlocal models*, Eng. Fract. Mech., 157 (2016), pp. 72–85.
- [23] M. HIRMAND, M. VAHAB M. AND A. R. KHOEI, *An augmented Lagrangian contact formulation for frictional discontinuities with the extended finite element method*, Finite Elem. Anal. Des., 107 (2015), pp. 28–43.
- [24] C. IMBERT AND A. MELLET, *Existence of solutions for a higher order non-local equation appearing in crack dynamics*, Nonlinearity, 24 (2011), pp. 3487–2514.
- [25] M. JIRÁSEK, *Non-local damage mechanics with application to concrete*, Revue française de génie civil, 8 (2004), pp. 683–707.
- [26] J. W. JU, *Isotropic and anisotropic damage variables in continuum damage*, J. Eng. Mech., 116 (1990), pp. 2764–2770.
- [27] I. KACHANOV, *Effective elastic properties of cracked solids: critical review of some basic concepts*, Appl. Mech. Rev., 45 (1992), pp. 304–335.
- [28] I. KAMIŃSKA AND A. SZWED, *A thermodynamically consistent model of quasibrittle elastic damaged materials based on a novel Helmholtz potential and dissipation function*, Materials, 14 (2022), pp. 6323 / 1–30.
- [29] W. KIM, *Higher-order explicit time integration methods for numerical analyses of structural dynamics*, Lat. Am. J. Solids Struct., 16 (2019), pp. e201 / 1–29.
- [30] K. KOUMATOS, C. LATTANZIO, S. SPIRITO AND A. E. TZAVARAS, *Existence and uniqueness for a viscoelastic Kelvin–Voigt model with nonconvex stored energy*, J. Hyperbolic Differ. Equations, 20 (2023), pp. 433–474.
- [31] V. KOZÁK, *Crack propagation modelling using XFEM, building materials applications*, 22nd Algoritmy in Podbanské (2024), STU Bratislava, to appear.
- [32] V. KOZÁK AND Z. CHLUP, *Modelling of fibre-matrix interface of brittle matrix long fibre composite by application of cohesive zone method*, Key Eng. Mater., 465 (2011), pp. 231–234.
- [33] K. LANGENFELD, P. KURZEJA AND J. MOSLER, *How regularization concepts interfere with (quasi-)brittle damage: a comparison based on a unified variational framework*, Continuum Mech. Thermodyn., 34 (2022), pp. 1517–1544.
- [34] J. LEMAITRE AND J. CHABOCHE, *Mechanics of Solids Materials*, Cambridge University Press, 1990.
- [35] J. LEMAITRE AND R. DESMORAT, *Engineering Damage Mechanics: Ductile, Creep, Fatigue and Brittle Failures*, Springer, 2005.
- [36] X. LI, W. GAO AND W. LIU, *A mesh objective continuum damage model for quasi-brittle crack modelling and finite element implementation*, Int. J. Damage Mech., 28 (2019), pp. 1299–1322.
- [37] X. LU, X. M. GUO, V. B. C. TAN AND T. E. TAY, *From diffuse damage to discrete crack: A coupled failure model for multi-stage progressive damage of composites*, Comput. Methods Appl. Mech. Eng., 379 (2021), pp. 113760 / 1–23.
- [38] J. MAZARS AND G. PIAUDIER-CABOT, *Continuum damage theory – application to concrete*, J. Eng. Mech., 115 (1989), pp. 345–365.
- [39] J. MAZARS, F. HAMON AND S. GRANGE, *A new 3D damage model for concrete under monotonic, cyclic and dynamic loadings*, Mater. Struct., 48 (2015), pp. 3779–3793.
- [40] N. MOËS AND T. BELYTSCHKO, *Extended finite element method for cohesive crack growth*, Eng. Fract. Mech., 69 (2002), pp. 813–833.
- [41] I. NĚMEC, J. VALA, H. ŠTEKBAUER, M. JEDLIČKA AND D. BURKART, *New methods in collision of bodies analysis*, 21st Programs and Algorithms of Numerical Mathematics (PANM) in Jablonec n. N. (2022), Institute of Mathematics CAS, Prague, 2023, pp. 133–148.
- [42] N. M. NEWMARK, *A method of computation for structural dynamics*, Trans. Am. Soc. Civ. Eng., 127 (1962), pp. 1406–1433.
- [43] N. OTTOSEN, *A failure criterion for concrete*, J. Eng. Mech., 103 (1977), pp. 527–535.
- [44] CH. PAPANFUSS, *Continuum Thermodynamics and Constitutive Theory*, Springer, Berlin, 2020.
- [45] K. PARK, G. H. PAULINO AND J. R. ROESLER, *Cohesive fracture model for functionally graded fiber reinforced concrete*, Cem. Concr. Res., 40 (2010), pp. 956–965.
- [46] M. G. PIKE AND C. OSKAY, *XFEM modeling of short microfiber reinforced composites with cohesive interfaces*, Finite Elem. Anal. Des., 106 (2005), pp. 16–31.
- [47] V. REK AND J. VALA, *On a distributed computing platform for a class of contact-impact problems*, Seminar on Numerical Analysis (SNA’21) in Ostrava (2021), Institute of Geonics CAS, Ostrava, 2021, pp. 64–67.

- [48] J. R. RICE, *A path independent integral and the approximate analysis of strain concentration by notches and cracks*, J. Appl. Mech., 35 (1968), pp. 379–386.
- [49] A. SERRA-AGUILA, J.M. PUIGORIOL-FORCADA, G. REYES AND J. MENACHO, *Viscoelastic models revisited: characteristics and interconversion formulas for generalized Kelvin–Voigt and Maxwell models*, Acta Mech. Sin., 35 (2019), pp. 1191–1209.
- [50] G. C. SIH, *Strain-energy density factor applied to mixed mode crack problems*, Int. J. Fract., 10 (1974), pp. 304–321.
- [51] M. SMOLÍK, V. SKALA AND Z. MAJDIŠOVÁ, *3D vector field approximation and critical points reduction using radial basis functions*, Int. J. Mech., 13 (2019), pp. 100–103.
- [52] Y. SUMI, *Mathematical and Computational Analyses of Cracking Formation.*, Springer, Tokyo, 2014.
- [53] Y. SUN, M. G. EDWARDS, B. CHEN AND C. LI, *A state-of-the-art review of crack branching*, Eng. Fract. Mech., 257 (2021), pp. 108036 / 1–33.
- [54] S. TAIRA, R. OHTANI AND T. KITAMURA, *Application of J-integral to high-temperature crack propagation, Part I – Creep crack propagation*, J. Eng. Mater. Technol., 101 (1979), pp. 154–161.
- [55] M. TRCALA, I. NĚMEC, A. VANĚČKOVÁ AND F. HOKEŠ, *Dynamic analysis of viscous material models*, 20th Programs and Algorithms of Numerical Mathematics (PANM) in Hejnice (2020), Institute of Mathematics CAS, Prague, 2021, pp. 139–148.
- [56] M. TRCALA, P. SUCHOMELOVÁ, M. BOŠANSKÝ, F. HOKEŠ AND I. NĚMEC, *The generalized Kelvin chain-based model for an orthotropic viscoelastic material*, Mech. Time. Depend. Mater., 28 (2024), pp. 163–183.
- [57] J. VALA, *Numerical approaches to the modelling of quasi-brittle crack propagation*, Arch. Math., 56 (2023), pp. 295–303.
- [58] J. VALA, L. HOBST AND V. KOZÁK, *Detection of metal fibres in cementitious composites based on signal and image processing approaches*, WSEAS Trans. Appl. Theor. Mech., 10 (2015), pp. 39–46.
- [59] J. VALA AND P. JAROŠOVÁ, *On computational stability of explicit schemes in nonlinear engineering dynamics*, 19th International Conference of Numerical Analysis and Applied Mathematics (ICNAAM) in Rhodes (2021), AIP Conf. Proc., 2849 (2023), pp. 370004 / 1–4.
- [60] J. VALA AND V. KOZÁK, *Computational analysis of quasi-brittle fracture in fibre reinforced cementitious composites*, Theor. Appl. Fract. Mech., 107 (2020), pp. 102486 / 1–8.
- [61] J. VALA AND V. KOZÁK, *Nonlocal damage modelling of quasi-brittle composites*, Appl. Math., 66 (2021), pp. 815–836.
- [62] J. VALA AND V. REK, *On a computational approach to multiple contacts/impacts of elastic bodies*, 21st Programs and Algorithms of Numerical Mathematics (PANM) in Jablonec n. N. (2022), Institute of Mathematics CAS, Prague, 2023, pp. 269–280.
- [63] J. VILPPO, R. KOUHIA, J. HARTIKAINEN, K. KOLARI, A. FEDOROFF AND K. CALONIUS, *Anisotropic damage model for concrete and other quasi-brittle materials*, Int. J. Solids Struct., 225 (2021), pp. 111048 / 1–13.
- [64] CH. D. VUONG, X. HU AND T. Q. BUI, *A dynamic description of the smoothing gradient damage model for quasi-brittle failure*, Finite Elem. Anal. Des., 230 (2024), pp. 104084 / 1–25.
- [65] T. WANG, H. HAN, Y. WANG, X. YE, G. HUANG, Z. LIU AND Z. ZHUANG, *Simulation of crack patterns in quasi-brittle materials under thermal shock using phase field and cohesive zone models*, Eng. Fract. Mech., 276 (2022), pp. 108889 / 1–17..
- [66] Y. YIN, Q. REN, S. LEI, J. ZHOU, L. XU AND T. WANG, *Mesoscopic crack pattern fractal dimension-based concrete damage identification*, Eng. Fract. Mech., 296 (2024), pp. 109829 / 1–17.