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MODELLING OF MICRO- AND MACRO-FRACTURE IN CEMENTITIOUS COMPOSITES

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Abstract. Frequent utilization of composites with a cementitious matrix, reinforced by fibres of different origin, as constructive parts in civil engineering motivates the reliable computational prediction of their mechanical properties, namely of the risk of initiation and development of micro- and macro-fracture. This paper demonstrates the possibility of deterministic prediction of such physical process, applying the dynamical approach with the modified Kelvin viscoelastic model and cohesive contacts together with the method of discretization in time, using 3 types of Rothe sequences, and the extended finite element method (XFEM).

Key words. Cementitious composites, quasi-brittle fracture, computational modelling, method of discretization in time, finite element method.

AMS subject classifications. 74R10, 35L20, 74S20, 74S05

1. Introduction. Mechanical properties of composites with a cementitious matrix and fibre reinforcement depend on characteristics of particular components, their interfaces and localization and directional distribution of fibres due to proposed loads. An increasing number of projects in civil engineering working with such composites as constructive parts motivates the development of reliable prediction of crack formation, expectable namely as consequences of concentration of tension stresses. Such prediction cannot be based on simple calculations well-known from linear elasticity and related fracture mechanics. Using the nomenclature of [24], the above introduced materials are from the class of quasi-brittle ones where two stages of damage can be recognized: i) formation of micro-fractured zones, reducing the stiffness of a structure, ii) creation of macro-cracks, whose later opening and closing is conditioned by the cohesive characteristics of new interfaces. As another serious problem, a reasonable setting of material parameters on the macroscopic scale, supported by appropriate experiments, can be seen; some (typically incomplete) data on material structure, as random or intentionally oriented fibre directions; problems of this kind, preferring non-destructive or low-invasive testing approaches (as direct photographic, radiographic and tomographic or indirect electromagnetic ones, working with stationary magnetic ar harmonic electromagnetic fields), are discussed in [27].

This paper will try to find a compromise between an above sketched multidisciplinary group of problems and the need to design and implement rather simple computations in the following sense:

- We shall come out from the principle of energy conservation from classical mechanics, incorporating the kinetic and deformation energy, together with certain energy dissipation, similarly to [16]. For the strain-stress relations we shall start with the linearized viscoelastic Kelvin law.
- The initiation of some micro-cracks will be incorporated using the approach of [20] and [10], working with the non-local Eringen model [7]. The recent result [8] on the ill-posedness of this model for boundary conditions significant

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in practical applications, is not addressed to our formulation fortunately; for the detailed analysis see [28].

- The matrix / fibre interfaces, as well as the interfaces inside the matrix, or even inside any fibre, depending on the process of activation of macro-cracks, will be assumed to satisfy the cohesive model by [19], [3], [13], [14] and [15].
- For effective practical computations we shall use the method of discretization in time, based on the Rothe sequences, end the extended finite element method (XFEM), working with the adaptive enrichment of the set of base functions near above mentioned geometric singularities. This method (including numerous modifications with their own names and special notations) has its own rich history; the progress in several decades can be traced from the comparison of pioneering works [1], [2] and [9] with the later monograph [12] and the recent articles [16] and [25]. However, we shall pay attention namely to the unconditional convergence properties of the method of discretization in time, i. e. those independent of the choice of XFEM adaptive strategies, as discussed by [11].

Some additional simplifications are motivated by the effort to avoid formally complicated, reader-unfriendly formulae and technical difficulties in proofs, with regard to the limited extent of this paper.

2. Physical and mathematical background. For simplicity, let us consider a material specimen occupying an open set Ξ with its boundary $\partial\Xi$ in the 3-dimensional Euclidean space R^3, compound from a finite number of domains $\Omega_\times$ with their boundaries $\partial\Omega_\times$ in the following sense:

- The union of all domains $\Omega_\times$ is identical with the closure of the domain Ω in R^3.
- Every boundary $\partial\Omega_\times$ consists of a part belonging to $\partial\Xi$ (external boundary) and from that non-belonging to $\partial\Xi$ (internal boundary); the 1st one will be denoted by $\Psi_\times$, the 2nd one by $\Lambda_\times$. (Some of them can be empty.) Cohesive interface conditions will be applied later on $\Lambda_\times$.
- Every boundary part $\Psi_\times$ is the union of its disjoint subsets $\Theta_\times$ and $\Gamma_\times$. (Some of them can be empty.) Homogeneous Dirichlet boundary conditions will be then prescribed on $\Theta_\times$ (supported boundary part), unlike Neumann boundary conditions (inhomogeneous in general) on $\Gamma_\times$ (unsupported boundary part).
- The unions of above introduced sets $\Theta_\times$, $\Gamma_\times$ and $\Lambda_\times$ are certain sets Ω, Γ and Λ. Similarly the union of all $\Omega_\times$ generates an open set Ω (i. e. Ξ without interior boundaries) with its boundary $\partial\Omega$.

A potential modification for another finite dimension than 3 (as 2 in the illustrative example of [29]) is left to the curious reader.

In the following text we shall work with the Cartesian coordinate system $x = (x_1, x_2, x_3)$ in R^3 and with the time t from the time interval $[0, T]$ of the prescribed positive length T; the limit passage $T \to \infty$ is possible, but not handled here explicitly. For simplicity we shall introduce the notation

$$(\varphi, \psi) = \int_\Omega \varphi(x) \cdot \psi(x)\,\mathrm{d}x$$

(in the Lebesgue sense) where the central dot refers to the scalar product of vectors $\varphi(x)$ and $\psi(x)$ from R^3, or (here always symmetric) matrices from $R^{3\times 3}_{\mathrm{sym}}$, as well as the notations

$$\langle\varphi, \psi\rangle_\Gamma = \int_\Gamma \varphi(x) \cdot \psi(x)\,\mathrm{d}s(x)\,, \qquad \langle\varphi, \psi\rangle_\Lambda = \int_\Lambda \varphi(x) \cdot \psi(x)\,\mathrm{d}s(x)$$

with the central dot applied to vectors from R^3 in both cases here (considering integration in the Hausdorff sense). For now we shall assume a sufficiently smooth boundary and such appropriate choice of $\varphi(x)$ and $\psi(x)$ that all above introduced integral exist. The upper dot symbol will be reserved for time derivatives, i. e. $\partial/\partial t$. For the brevity we shall use $\emptyset$ instead of $(0,0,0)$. For an arbitrary virtual displacement $v(x) = (v_1(x), v_2(x), v_3(x))$, related to the initial geometric configuration, i. e. for $t = 0$, such that $v(x) = \emptyset$ for any $x \in \Theta$ (in the sense of traces), we shall also consider a virtual strain $\varepsilon(v)$, introduced by the usual linearized relation $2\varepsilon_{ij}(v(x)) = \partial v_i \partial x_j + \partial v_j \partial x_i$ for any $i, j \in \{1,2,3\}$ and $x \in \Omega$. We shall also work with the notation $\delta v(x)$ for the differences of triples of values $v(x)$ from the neighbour domains $\Omega_\times$. The same notation is applicable to arbitrary $\tilde{v}(x,t)$, dependent also on $t \in I$, replacing $v(x)$ here.

Let us assume that the volume load $f(x,t) = (f_1(x,t), f_2(x,t), f_3(x,t))$ for any $x \in \Omega$ and $t \in I$ and the surface load $g(x,t) = (g_1(x,t), g_2(x,t), g_3(x,t))$ for any $x \in \Gamma$ and $t \in I$ is prescribed. Our aim is to find such displacement $u(x,t) = (u_1(x,t), u_2(x,t), u_3(x,t))$ for any $x \in \Omega$ and $t \in I$, related to the initial stationary geometric configuration, thus $u(x,0) = \emptyset$ and $\dot{u}(x,0) = \emptyset$ for any $x \in \Omega$, (which can be seen as the couple of Cauchy homogeneous initial conditions), that $u(x,t) = \emptyset$ for any $x \in \Theta$ and $t \in I$. Introducing the notation $\sigma(x,t)$ for a symmetric stress matrix from $R^{3\times 3}_{\mathrm{sym}}$ for any fixed $x \in \Omega$ and $t \in I$ and $\tau(x,t)$ for a vector of contact load from R^3 for any fixed $x \in \Lambda$ and $t \in I$, the weak form of the principle of conservation of energy from classical mechanics reads

$$(v, \rho\ddot{u}) + (\varepsilon(v), \sigma) = (v, f) + \langle v, g\rangle_\Gamma + \langle \delta v, \tau\rangle_\Lambda \quad \text{on } I \tag{2.1}$$

(a variable t is not highlighted here, this will be true even for x later) for any virtual displacement v; ρ here means the material density, variable in Ω in general. The classical differential formulation can be derived, using some facts from the theory of distributions, following [29], Sections 2 and 4 (handling 2 model problems of the quasi-static case in details). However, some appropriate properties of prescribed functions are needed, as well as of virtual displacements v, taken from some subspace of the Sobolev space $W^{1,2}(\Omega)$ – cf. Section 3 here.

To be able to compute u from (2.1), supplied by the above introduced boundary and initial conditions, we need to express σ and τ from appropriate constitutive relations containing u, in addition to a priori known material characteristics. Here we shall start with the Kelvin viscoelastic relation

$$\sigma = \gamma C\varepsilon(u) + \alpha C\varepsilon(\dot{u}) \quad \text{on } \Omega\times I \tag{2.2}$$

where C is the symmetric stiffness tensor with values from $R^{(3\times 3)\times(3\times 3)}_{\mathrm{sym}}$, as usual in the linear elasticity, containing (in general, for a non-polar continuum) 21 independent characteristics, whose number can be reduced to 2, well-known as the Lamé factors (or the Young modulus and the Poisson constant alternatively), in the isotropic case, and α means the structural damping factor; the damage factor $\gamma < 1$ then evaluates the loss of stiffness caused by micro-cracking. The evaluation of γ can be done using the formula

$$\gamma = 1 - \omega(|A(\sigma(.,\tilde{t})|_{3\times 3}) \quad \text{for } \tilde{t} \in [0,t] \text{ on } \Omega\times I \tag{2.3}$$

where $|.|_{3\times 3}$ refers to the norm in $R^{3\times 3}_{\mathrm{sym}}$; ω should incorporate the material characteristics obtained from laboratory experiments, e. g. the tensile strength. An operator $A(w(x))$, compatible with [10], must be defined carefully, to incorporate the damage history, for a appropriate function $w(x)$ of a variable $x \in \Omega$, as an integral

$$A(w(x)) = \int_\Omega K(x,\tilde{x})\, w(\tilde{x})\, \mathrm{d}\tilde{x} \tag{2.4}$$

where $K(x,\tilde{x})$ is an a priori given operator kernel. Selected possibilities of its practical constructions, supported by the radial basis functions from [17], are discussed in [28]. In particular, for a sufficiently low $|A(\sigma(.,\tilde{t})|_{3\times 3}$ in (2.3) we have always $\gamma = 1$, thus (2.2) refers to the standard linear parallel viscoelastic model; this may be true on some parts of Ω only (where no micro-cracking occurs yet).

Subsequently, every opening and closing of micro-cracks can be expressed using the relation

$$\tau = \lambda(\delta u) \quad \text{on } \Lambda \times I\,; \tag{2.5}$$

potential forms of a just introduced function λ can be found in [13] and [14]. Especially $\lambda(\delta u) = \lambda_0\, \delta u$ with a real constant $\lambda_0 \to \infty$ forces $\delta u \to \emptyset$ on Λ, i. e. the continuity of u without no active macro-cracking. Finally, inserting (2.5), (2.3) and (2.2) back to (2.1), we receive an integral form of a system of partial differential equations of evolution of hyperbolic type with only one vector-valued unknown function u

$$\begin{aligned} &(v,\rho\ddot{u}) + (\varepsilon(v),\alpha C\varepsilon(\dot{u})) + (\varepsilon(v),\gamma C\varepsilon(u)) \\ &= (v,f) + \langle v,g\rangle_\Gamma + \langle \delta v,\lambda(\delta u)\rangle_\Lambda \quad \text{on } I\,; \end{aligned} \tag{2.6}$$

γ is supposed (for brevity) to come from (2.3). There are only 2 sources of its non-linearity, uncovered by the classical book [21]: the evaluations of γ (for micro-cracking) and of λ (for macro-cracking). Especially the high nonlinearity of the 1st one must be handled carefully, both from the point of view of existence and convergence questions and from that of practical XFEM calculations – cf. [10] and [29], Section 6. The same comment can be addressed to (2.7), (2.8), etc., too.

Now we can sketch the heuristic time discretization, elaborated in the following section. Let us divide I into a finite number of m subintervals $I_s = \{t \in I : (s-1)h < t \le sh\}$ with $s \in \{1,\dots m\}$ where $h = T/m$ (the dependence of h, I_s and other quantities on m is not emphasized explicitly). Clearly this is prepared for the limit passage $m \to \infty$ (or $h \to 0_+$). Let us apply the approximation of u using a linear Lagrange spline on I, working with certain (a priori unknown) nodal values $u_0, u_1, \dots u_m$, which generates the piecewise linear function u^m on I, and the approximation of u using a simple function $\bar{u}^m$ on I, taking right-hand-side values on every I_s, or a simple function $\breve{u}^m$, taking left-hand side values (thus $\breve{u}^m$ can derived as h-retarded from $\bar{u}^m$ formally). Respecting the initial conditions, let us define the 1st and 2nd differences $\mathcal{D}u_s = u_s - u_{s-1}$ and $\mathcal{D}^2 u_s = \mathcal{D}u_s - \mathcal{D}u_{s-1}$ for each $s = \{1,\dots,m)$, taking $u_0 = \emptyset$ and $\mathcal{D}u_0 = \emptyset$. Therefore we have

$$u^m(t) = u_{s-1} + \frac{t-(s-1)h}{h}\,\mathcal{D}u_s\,, \qquad \bar{u}^m(t) = u_s\,, \qquad \breve{u}^m(t) = u_{s-1}$$

assuming $t \in I_s$, $s = \{1,\dots,m)$.

However, such simple discretization cannot be applied to (2.6) directly. For all integrable functions $\phi(t)$ on I let us introduce the additional notation $[\phi](t)$, referring to the integral of $\phi(\tilde{t})$ over all $\tilde{t}$ between 0 and t. Then (2.6) can be converted into its integro-differential form

$$\begin{aligned} &(v,\rho\dot{u}) + (\varepsilon(v),\alpha C\varepsilon(u)) + [(\varepsilon(v),\gamma C\varepsilon(u))] \\ &= [(v,f)] + [\langle v,g\rangle_\Gamma] + [\langle \delta v,\lambda(\delta u)\rangle_\Lambda] \quad \text{on } I\,; \end{aligned} \tag{2.7}$$

Then a natural approximation of (2.7), based on the slight modification of the Euler implicit method, taking 2 terms disturbing linearity from preceding time steps, is

$$(2.8)\qquad \begin{aligned}&(v,\rho\dot{u}^m)+(\varepsilon(v),\alpha C\varepsilon(\bar{u}^m))+[(\varepsilon(v),\breve{\gamma}^m C\varepsilon(\bar{u}^m))]\\&=[(v,f^m)]+[\langle v,g^m\rangle_\Gamma]+[\langle\delta v,\lambda(\delta\breve{u}^m)\rangle_\Lambda]\quad\text{on } I\,;\end{aligned}$$

here $\breve{\gamma}^m$ means γ coming from (2.3) and (2.2) evaluated for $\breve{u}^m$ replacing u (similarly γ_s, γ_{s-1}, etc., can be understood) and f^m and g^m are the results of the Clémens quasi-interpolation of f and g, implementing the mean values f_s^* and g_s^* on I_s, $s\in\{1,\dots,m\}$; for more details see [29]. In terms of the values $u_1,\dots,u_m$, for each $s\in\{1,\dots,m\}$ (2.8) gives

$$(2.9)\qquad \begin{aligned}&\frac{1}{h}(v,\rho\mathcal{D}u_s)+(\varepsilon(v),\alpha C\varepsilon(u_s))+h\sum_{r=1}^{s}(\varepsilon(v),\gamma_{s-1}C\varepsilon(u_r))\\&=h\sum_{r=1}^{s}(v,f_r^*)+h\sum_{r=1}^{s}\langle v,g_r^*\rangle_\Gamma+h\sum_{r=1}^{s}\langle\delta v,\lambda(\delta u_{r-1})\rangle_\Lambda\,.\end{aligned}$$

Subtracting 2 sequential s-th and $(s-1)$-th equations (2.9), we obtain

$$(2.10)\qquad \begin{aligned}&\frac{1}{h}(v,\rho\mathcal{D}^2u_s)+(\varepsilon(v),\alpha C\varepsilon(\mathcal{D}u_s))+h(\varepsilon(v),\gamma_{s-1}C\varepsilon(u_s))\\&=h(v,f_s^*)+h\langle v,g_s^*\rangle_\Gamma+h\langle\delta v,\lambda(\delta u_{s-1})\rangle_\Lambda\,,\end{aligned}$$

which is the desired formula for the step-by-step evaluation of u_s.

The computational scheme (2.10) refers to the numerical analysis of m elliptic problems of infinite dimension. In the following section, under some additional assumptions, we shall verify its convergence for $m\to\infty$, unconditioned by its discretization in R^3. In practical calculations, instead of v in (2.10) from an inifinite-dimensional spase V (cf. the following section), we consider a finite number n of test functions v_n; the approximation u_s^n of u_s from (2.10) with n unknown parameters can be constructed as their linear combinations. Consequently, step-by-step, we choose $v^n=\phi_i$ where functions ϕ_i with $i\in\{1,\dots,n\}$ generate a basis of certain finite-dimensional space V^n, approximating V (which can be a subspace of V in particular cases), and

$$u_s^n=\sum_{i=1}^{n}u_{si}^n\phi_i$$

with unknown parameters u_{si}^n. Typically ϕ_i are functions with small compact support, applicable in Ω, as well as on Θ, Γ and Λ, to create a sparse system of linear algebraic equations, and u_{si}^n refer to nodal displacement values. The guarantee of solvability of such system, together with the convergence properties for $n\to\infty$, depend on certain (semi-)regularity of such decomposition, including the XFEM adaptive enrichment functions; for much more details on XFEM strategies see [12], for several instructive numerical examples cf. [29].

3. Existence and convergence considerations. We shall use the standard notation of Lebesque, Sobolev, Bochner, etc. (abstract) function spaces, as introduced by [26], with numerous references to [22]. Namely we shall need the Hilbert spaces

$$(3.1)\qquad \begin{aligned}&H=L^2(\Omega)^3\,,\quad V=\{v\in W^{1,2}(\Omega)^3\colon\ v=\emptyset\ \text{ on }\Theta\}\,,\\&Z=L^2(\partial\Omega\cup\Lambda)^3\,,\quad Z_\Gamma=L^2(\Gamma)^3\,,\quad Z_\Lambda=L^2(\Lambda)^3\end{aligned}$$

with the corresponding scalar products (the same notation as above): $(.\,,.)$ both in H and $H\times H$, $\langle.\,.\rangle_\Gamma$ in Z_Γ and $\langle.,.\rangle_\Lambda$ in Z_Λ; the measure of Θ on $\partial\Omega$ must be non-zero. We shall utilize also some symbols for standard norms, namely $|\,.\,|$ both in H and

$H \times H$, $\|\,.\,\|$ in V, $|\,.\,|_\Gamma$ in Z_Γ and $|\,.\,|_\Lambda$ in Z_Λ. We shall use the upper star symbols for dual spaces, $\subset$ for continuous embeddings, $\Subset$ for compact embeddings and $\cong$ for the identification of a space with its dual (following the Riesz representation theorem). Consequently any $v \in V$ can be implemented into (2.6), (2.7), (2.8), (2.10), etc.

In our following considerations these special results from [22] are needed:

- In the Gelfand triple $V \subset H \cong H^* \subset V^*$ both inclusions are dense, with the guaranteed embedding $W^{1,2,2}(I,V,V^*) \subset C(I,H)$.
- $L^2(I,V)^* \cong L^2(I,V^*)$, thus $L^2(I,V)$ is reflexive.
- $H \Subset V$ (the Sobolev embedding theorem), thus every weakly convergent sequence in V converges in H strongly.
- $Z \Subset V$ (the trace theorem); this forces $|v|^2_\Gamma \le \mathfrak{T}\|v\|^2$ and $|v|^2_\Lambda \le \mathfrak{T}\|v\|^2$ for any $v \in V$ with a positive constant $\mathfrak{T}$ independent of v and also every weakly convergent sequence in V converges in Z strongly.
- $W^{1,2,2}(I,V,V^*) \Subset L^2(I,X)$ with $X \in \{H,Z\}$ (the Aubin - Lions lemma).
- $|\varepsilon(v)|^2 \ge \mathfrak{K}\|v\|^2$ with a positive $\mathfrak{K}$ independent of $v \in V$ (the Korn inequality); consequently $|\varepsilon(v)|$ is an alternatively norm in V is generated because $|\varepsilon(v)|^2 \le |\nabla v|^2 \le \|v\|^2 \le |v|^2 + |\nabla v|^2 = \|v\|^2$.

All these results are valid for domains $\Omega_\times$ (from the previous section) with Lipschitz boundaries literally; some more general domains (or open sets) could be handled (with non-negligible technical difficulties) following [4].

Some additional assumptions, respecting the notation (3.1), must be satisfied:

- *On the volume and surface loads:* $f \in L^2(I,H)$ and $g \in L^2(I,Z_\Gamma)$.
- *On the stiffness characteristics:* $C \in L^\infty(\Omega)^{(3\times3)\times(3\times3)}_{\text{sym}}$, $C(x)$ being positive definite in the sense $\sum_{i,j,k,l\in\{1,2,3\}} C_{ijkl}(x)a_{ij}a_{kl} \ge C_0 \sum_{i,j\in\{1,2,3\}} a_{ij}a_{ij}$ for any $x \in \Omega$ with a positive C_0 independent of x.
- *On the material density:* $\rho \in L^\infty(\Omega)$ and $\rho(x) \ge \rho_0$ for a positive ρ_0 independent of x.
- *On the damping factor:* $\alpha \in L^\infty(\Omega)$ and $\alpha(x) \ge \alpha_0$ for a positive α_0 independent of x.
- *On the cohesive characteristics:* λ is a Lipschitz continuous mapping from Z_Λ to Z_Λ; this yields $\lambda(\delta v) \le \lambda_\star|\delta v|_\Lambda \le \lambda_\star N\|v\|$ for any $v \in V$, a positive $\lambda_\star$ and a finite integer N independent of v; the existence of N comes from the careful definition od Ω and Λ in Section 2 (traces are related to any $\Omega_\times$ at most N-times, from corresponding cohesive boundary parts $\Lambda_\times$).
- *On the nonlocal damage factor:* there exists such positive constant ς (independent of t) that, for any fixed time t, γ is always a continuous mapping from V to $L^\infty(\Omega)$ satisfying $\gamma \le \varsigma$; this must be guaranteed from its construction by (2.3) (which may be complicated in practice).

Moreover, by its definition, as a function of t, γ cannot be increasing (the loss of stiffness due to micro-cracking is irreversible). We shall also need the following regularization (compactness) property of the kernel K, taken from $L^2(\Omega\times\Omega)$, following (2.4): if $\{w^k\}_{k=1}^\infty$ is some sequence converging weakly to w in H then, taking $\tilde{w} = A(w)$ and $\tilde{w}^k = A(w^k)$, up to a subsequence, $\{\tilde{w}^k\}_{k=1}^\infty$ converges strongly to $\tilde{w}$ in H. Indeed, $\tilde{w}^k(x)_{k=1}^\infty$ converges locally to $\tilde{w}(x)$ for almost every $x \in \Omega$; by the Lebesgue dominated convergence theorem is then sufficient to verify the boundedness of $\{\tilde{w}^k\}_{k=1}^\infty$ in H, which is guaranteed by the weak convergence (thus also the boundedness) of $\{w^k\}_{k=1}^\infty$, by the Fubini theorem (on multiple integrals) and by the Cauchy - Schwarz inequality; for all details see [5], p. 81. An important consequence is that for a continuous γ (cf. the assumptions above) and for any fixed $t \in I$ we are able to guarantee the strong convergence of $\{\gamma(u(.,t))\}_{k=1}^{\infty}$ to $\gamma(u(.,t))$ provided that $\{u^k(.,t)\}_{k=1}^{\infty}$ converges weakly to some $u(.,t)$ in V.

Let us now come back to (2.10) with $s \in \{1,\dots,m\}$, to derive some a priori bounds for the sequences $\{u^m\}_{m=1}^{\infty}$, $\{\dot{u}^m\}_{m=1}^{\infty}$, $\{\bar{u}^m\}_{m=1}^{\infty}$ and $\{\breve{u}^m\}_{m=1}^{\infty}$. Choosing $v = \mathcal{D}u_s/h$, we have

$$\begin{aligned}(3.2)\qquad &\frac{1}{h^2}(\mathcal{D}u_s,\rho\mathcal{D}^2u_s)+\frac{1}{h}(\varepsilon(\mathcal{D}u_s),\alpha C\varepsilon(\mathcal{D}u_s))+(\varepsilon(\mathcal{D}u_s),\gamma_{s-1}C\varepsilon(u_s))\\ &=(\mathcal{D}u_s,f_s^*)+\langle\mathcal{D}u_s,g_s^*\rangle_\Gamma+\langle\delta\mathcal{D}u_s,\lambda(\delta u_{s-1})\rangle_\Lambda\,,\end{aligned}$$

The same results hold with arbitrary $r \in \{1,\dots,s\}$ instead of s. The sum of all such equations derived from (3.2) is then

$$\begin{aligned}(3.3)\qquad &\frac{1}{2h^2}(\mathcal{D}u_s,\rho\mathcal{D}u_s)+\frac{1}{2h^2}\sum_{r=1}^{s}(\mathcal{D}^2u_r,\rho\mathcal{D}^2u_r)+\frac{1}{h}\sum_{r=1}^{s}(\varepsilon(\mathcal{D}u_r),\alpha C\varepsilon(\mathcal{D}u_r))\\ &+\frac{1}{2}(\varepsilon(u_s),\gamma_sC\varepsilon(u_s))+\frac{1}{2}\sum_{r=1}^{s}(\varepsilon(u_r),(\gamma_{r-1}-\gamma_r)\varepsilon(u_r))\\ &+\frac{1}{2}\sum_{r=1}^{s}(\varepsilon(\mathcal{D}u_r),\gamma_{r-1}C\varepsilon(\mathcal{D}u_r))\\ &=\sum_{r=1}^{s}(\mathcal{D}u_r,f_r^*)+\sum_{r=1}^{s}\langle\mathcal{D}u_r,g_r^*\rangle_\Gamma+\sum_{r=1}^{s}\langle\delta\mathcal{D}u_r,\lambda(\delta u_{r-1})\rangle_\Lambda\,.\end{aligned}$$

All left-hand-side additive terms are non-negative, thus the 2nd, 5th and 6th ones can be seen as bounded from below by zero, whereas the 1st, 3th and 4th ones admit the more careful estimates

$$\begin{aligned}(3.4)\qquad \frac{1}{2h^2}(\mathcal{D}u_s,\rho\mathcal{D}u_s)&\ge\frac{\rho_0}{2h^2}|\mathcal{D}u_s|^2\,,\\ \frac{1}{h}\sum_{r=1}^{s}(\varepsilon(\mathcal{D}u_r),\alpha C\varepsilon(\mathcal{D}u_r))&\ge\frac{\alpha_0C_0\mathfrak{K}}{h}\sum_{r=1}^{s}\|\mathcal{D}u_r\|^2\,,\\ \frac{1}{2}(\varepsilon(u_s),\gamma_sC\varepsilon(u_s))&\ge\frac{\varsigma C_0\mathfrak{K}}{2}\|u_s\|^2\,.\end{aligned}$$

Finally, using the Cauchy - Schwarz and the Young inequalities, 3 right-hand-side terms can be estimated as

$$\begin{aligned}(3.5)\qquad \sum_{r=1}^{s}(\mathcal{D}u_r,f_r^*)&\le\sum_{r=1}^{s}|\mathcal{D}u_r||f_r^*|\le\frac{\epsilon}{2h}\sum_{r=1}^{s}|\mathcal{D}u_r|^2+\frac{h}{2\epsilon}\sum_{r=1}^{s}|f_r^*|^2\\ &\le\frac{\epsilon}{2h}\sum_{r=1}^{s}\|\mathcal{D}u_r\|^2+\frac{h}{2\epsilon}\sum_{r=1}^{s}|f_r^*|^2\,,\\ \sum_{r=1}^{s}\langle\mathcal{D}u_r,g_r^*\rangle_\Gamma&\le\sum_{r=1}^{s}|\mathcal{D}u_r|_\Gamma|g_r^*|_\Gamma\le\frac{\epsilon}{2h}\sum_{r=1}^{s}|\mathcal{D}u_r|_\Gamma^2+\frac{h}{2\epsilon}\sum_{r=1}^{s}|g_r^*|_\Gamma^2\\ &\le\frac{\epsilon\mathfrak{T}}{2h}\sum_{r=1}^{s}\|\mathcal{D}u_r\|^2+\frac{h}{2\epsilon}\sum_{r=1}^{s}|g_r^*|_\Gamma^2\,,\\ \sum_{r=1}^{s}\langle\delta\mathcal{D}u_r,\lambda(\delta u_{r-1})\rangle_\Lambda&\le\lambda_\star\sum_{r=1}^{s}|\delta\mathcal{D}u_r|_\Lambda\delta u_{r-1}|_\Lambda\le\frac{\epsilon\lambda_\star}{2h}\sum_{r=1}^{s}|\delta\mathcal{D}u_r|_\lambda^2+\frac{h\lambda_\star}{2\epsilon}\sum_{r=1}^{s}|\delta u_r|_\Lambda^2\\ &\le\frac{\epsilon\lambda_\star N\mathfrak{T}}{2h}\sum_{r=1}^{s}\|\mathcal{D}u_r\|^2+\frac{h\lambda_\star N\mathfrak{T}}{2\epsilon}\sum_{r=1}^{s}\|u_r\|^2\end{aligned}$$

where ϵ is an arbitrary positive constant. Its appropriate setting enables us, implementing (3.5) together with (3.4) into (3.3) to conclude

$$\frac{1}{h^2}|\mathcal{D}u_s|^2 + \frac{1}{h}\sum_{r=1}^{s}\|\mathcal{D}u_r\|^2 + \|u_s\|^2 \le c + c_\star h \sum_{r=1}^{s}\|u_r\|^2 \,. \tag{3.6}$$

with certain positive constants c and $c_\star$ independent of h (as well as of m, s, etc.) where, in particular, $c_\star = 0$ if all u_r with $r \in \{1,\dots,s\}$ are continuous on Λ (i. e. $\delta u_r = \emptyset$ because no macro-cracks are active yet). In such special case (3.6) takes the simple form

$$\frac{1}{h^2}|\mathcal{D}u_s|^2 + \frac{1}{h}\sum_{r=1}^{s}\|\mathcal{D}u_r\|^2 + \|u_s\|^2 \le \bar{c}\,. \tag{3.7}$$

with $\bar{c} = c$. Nevertheless, (3.7) (with another value of $\bar{c}$) is true even with $c_\star > 0$, thanks to the discrete Gronwall lemma, applied to (3.6) – cf. [5], p. 99, and [22], p. 26.

Since $u^m(t)$ can be seen as piecewice linear abstract functions of $t \in I$ and $\bar{u}^m(t)$ and $\breve{u}^m(t)$ as simple ones for any $m \in \{1, 2, \dots\}$, the a priori estimate (3.7) guarantees some boundedness of the Rothe sequences by (2.8) directly:

$$\begin{aligned} \{\dot{u}^m(t)\}_{m=1}^{\infty} &\text{ is bounded in } H \text{ for any } t \in I\,,\\ \{\bar{u}^m(t)\}_{m=1}^{\infty} &\text{ is bounded in } V \text{ for any } t \in I\,,\\ \{\breve{u}^m(t)\}_{m=1}^{\infty} &\text{ is bounded in } V \text{ for any } t \in I\,,\\ \{\grave{u}^m\}_{m=1}^{\infty} &\text{ is bounded in } L^2(I,V)\,. \end{aligned} \tag{3.8}$$

Since all spaces in (3.8) are reflexive, the Eberlein - Shmul'yan theorem by [5], p. 67, yields, up to subsequences, that

$$\begin{aligned} \{\dot{u}^m(t)\}_{m=1}^{\infty} &\text{ converges weakly to } u' \text{ in } H \text{ for any } t \in I\,,\\ \{\bar{u}^m(t)\}_{m=1}^{\infty} &\text{ converges weakly to } \bar{u} \text{ in } V \text{ for any } t \in I\,,\\ \{\breve{u}^m(t)\}_{m=1}^{\infty} &\text{ converges weakly to } \breve{u} \text{ in } V \text{ for any } t \in I\,,\\ \{\grave{u}^m\}_{m=1}^{\infty} &\text{ converges weakly to } \hat{u} \text{ in } L^2(I,V) \end{aligned} \tag{3.9}$$

where u', $\bar{u}$, $\breve{u}$ and $\grave{u}$ are some elements of corresponding spaces. Let us also define

$$u(t) = \int_0^t u'(\xi)\,\mathrm{d}\xi \quad \text{for each } t \in I\,.$$

Now we are ready to exploit the inclusions and compactness lemmas from their list at the beginning of this section, to verify further convergence properties. Here we shall present (for brevity) only those crucial ones for the limit passage from (2.8) to (2.7) with $m \to \infty$. Namely

$$\begin{aligned} \{\grave{u}^m\}_{m=1}^{\infty} &\text{ converges strongly to } \hat{u} \text{ in } L^2(I,H)\,,\\ \{\lambda(\breve{u}^m)\}_{m=1}^{\infty} &\text{ converges strongly to } \lambda(\breve{u}) \text{ in } L^2(I,Z_\Lambda)\,, \end{aligned} \tag{3.10}$$

taking the continuity of λ into account. However, the 1st relation (3.10) must be true also with the strong limit u', thanks to the 1st relation (3.9), thus $u' = \hat{u}$. Moreover, following (3.7), for any $t \in I$ we have

$$\max\left(|u^m(t) - \bar{u}^m(t)|, |u^m(t) - \breve{u}^m(t)|\right) \le \max_{s\in\{1,\dots,m\}} |\mathcal{D}u_s| \le \sqrt{\bar{c}}h = \frac{\sqrt{\bar{c}}T}{m}\,,$$

which implies $u = \bar{u} = \breve{u}$ and $\grave{u} = u'$. Consequently u can be considered as a weak limit in the 2nd and 3rd relations (3.9) and and $\lambda(u)$ as a strong limit in the 2nd relation

(3.10), whereas $\dot{u}$ replaces a weak limit in the 1st and 4th relations of (3.9) and a strong limit in the 1st relation (3.10). The guarantee of the last needed convergence result

$$\{\gamma^m\}_{m=1}^{\infty} \text{ converges strongly to } \gamma \text{ in } t \in L^\infty(\Omega) \tag{3.11}$$

is the most delicate one: this needs the careful design of K, ω, etc., by the rather complicated formulae (2.3) and (2.4). Nevertheless, such design is not straightforward and contains still open questions for future work. Finally the convergence properties of the Rothe sequences by (3.9), (3.10) and (3.11) enables us the announced limit passage (2.8) to (2.7), which completes the constructive proof of the existence of u and $\dot{u}$ from $L^2(I, V)$ satisfying (2.7) for any virtual displacement $v \in V$.

4. Conclusions. Most computational algorithms predicting fracture of cementitious composites refer to some principles of classical mechanics, but apply ad hoc approaches in heir final stages. Queer and mutually incompatible results lead to their seeking for some heuristic macroscopic models with numerous parameters, coming from laboratory experiments, whose reasonable setting needs advanced statistical approaches or soft computing tricks like genetic programming techniques – cf. [23], [6] and [18]. Unlike them, this paper tries to demonstrate the possibility of well-posed formulation of a relevant deterministic problem, supported by the constructive design of convergent sequences of approximate solutions.

Some rather strong simplifications are involved here, not always caused by the necessity to avoid technical difficulties in the short conference paper. For example, some weaker assumptions on given loads and material characteristics could be handled by more precise embeddings, as $L^{6-\epsilon}(\Omega)^3 \Subset V$ (instead of $H \Subset V$) for a positive $\epsilon \leq 4$ and $L^{4-\epsilon}(\partial\Omega \cup \Lambda)^3 \Subset V$ (instead of $Z \Subset V$) for a positive $\epsilon \leq 2$, etc.; even the converegence of Rothe sequences does not need the boundedness of $\{\dot{u}^m\}$ in $L^2(I, V)$ and of $\{\dot{u}^m(t)\}$ in H for any $t \in I$, which can be replaced by the boundedness of $\{\dot{u}^m\}$ in $L^2(I, V^*)$, as evident from [26] (on parabolic problems). However, substantial restrictions in both nonlinear terms occur: i) the requirement $\varsigma > 0$ forbids any local total loss of stiffness due to micro-cracking, whose lifelikeness would be controversial because of the a priori strain / stress linearizations, ii) macro-cracks are allowed on a finite number of (potential) cohesive surfaces only, whereas some XFEM algorithms promise to predict them (nearly) everywhere. Together with the further development of relevant software (some preliminary crack simulation results can be found in [29]), these are significant motivations for further research in the near future.

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REFERENCES

[1] I. Babuška and J. M. Melenk, *The partition of unity method*, International Journal for Numerical Methods in Engineering 40 (1997), pp. 727–758.
[2] T. Belytchko and T. Black, Elastic crack growth in finite elements with minimal remeshing, International Journal for Numerical Methods in Engineering 45 (1999), pp. 601–620.
[3] L. Bouhala, A. Makradi, S. Belouettar, H. Kiefer-Kamal and P. Fréres, *Modelling of failure in long fibres reinforced composites by X-FEM and cohesive zone model*, Composites Part B 55 (2013), pp. 352–361.
[4] A. Cianchi and V. Mazýa, *Sobolev inequalities in arbitrary domains* Advances in Mathematics 293 (2016), pp. 644–696.
[5] P. Drábek and J. Milota, *Methods of Nonlinear Analysis*, Birkhäuser, 2013.

[6] J. Eliáš, M. Vořechovský, J. Skoček and Z. P. Bažant, *Stochastic discrete meso-scale simulations of concrete fracture: comparison to experimental data*, Engineering Fracture Mechanics 135 (2015), pp. 1–16.

[7] A. C. Eringen, *Theory of Nonlocal Elasticity and Some Applications*, Princeton University Press, 1984, technical report 64.

[8] A. Evgrafov and J. C. Belido, *From nonlocal Eringen's model to fractional elasticity*, Mathematics and Mechanics of Solids 24 (2019), pp. 1935–1953.

[9] T.-P. Fries and T. Belytschko, *The intrinsic XFEM: a method for arbitrary discontinuities without additional unknowns*, International Journal for Numerical Methods in Engineering 68 (2006), pp. 1358–1385.

[10] M. Jirásek, *Damage and smeared crack models*, in: Numerical Modeling of Concrete Cracking (G. Hofstetter and G. Meschke, eds), Springer: CISM International Centre for Mechanical Sciences 532, 2011, 1–49.

[11] M. Kaliske, H. Dal, R. Fleischhauer, C. Jenkel and C. Netzker, *Characterization of fracture processes by continuum and discrete modelling*, Computational Mechanics 50 (2012), pp. 303–320.

[12] A. R. Khoei, *Extended Finite Element Method: Theory and Applications*. J. Wiley & Sons, 2015.

[13] V. Kozák and Z. Chlup, *Modelling of fibre-matrix interface of brittle matrix long fibre composite by application of cohesive zone method*, Key Engineering Materials 465 (2011), pp. 231–234.

[14] V. Kozák, Z. Chlup, P. Padělek and I. Dlouhý, *Prediction of the traction separation law of ceramics using iterative finite element modelling*, Solid State Phenomena 258 (2017), pp. 186–189.

[15] X. Li and J. Chen, *An extensive cohesive damage model for simulation arbitrary damage propagation in engineering materials*, *Computer Methods in Applied Mechanics and Engineering* 315 (2017), pp. 744–759.

[16] X. Li, W. Gao and W. Liu, *A mesh objective continuum damage model for quasi-brittle crack modelling and finite element implementation*, International Journal of Damage Mechanics 28 (2019), pp. 1299–1322.

[17] Z. Majdišová and V. Skala, *Radial basis function approximations: comparison and applications*, Applied Mathematical Modelling 51 (2017), pp. 728–743.

[18] M. Moradi, A. R. Begherieh and M. R. Esfahani, *Constitutive modeling of steel fiber-reinforced concrete*, International Journal of Damage Mechanics 29 (2020), pp. 388–412.

[19] M. G. Pike and C. Oskay, *XFEM modeling of short microfiber reinforced composites with cohesive interfaces*, Finite Elements in Analysis and Design 106 (2005), pp. 16–31.

[20] Yu. Z. Povstenko, *The nonlocal theory of elasticity and its application to the description of deffects in solid bodies*. Journal of Mathematical Sciences 97 (1999), pp. 3840–3845.

[21] K. Rektorys, *The Method of Discretization in Time and Partial Differential Equations*, Springer, 1982.

[22] T. Roubíček, *Nonlinear Partial Differential Equations with Applications*. Birkhäuser, 2013.

[23] X. T. Su, Z. J. Yang and G. H. Liu, *Monte Carlo simulation of complex cohesive fracture in random heterogeneous quasi-brittle materials: a 3D study*, International Journal of Solids and Structures 47 (2010), pp. 2336–2345.

[24] Y. Sumi, *Mathematical and Computational Analyses of Cracking Formation*, Springer, 2014.

[25] R. F. Swati, L. H. Wen, H. Elahi, A. A. Khan and S. Shad, *Extended finite element method (XFEM) analysis of fiber reinforced composites for prediction of micro-crack propagation and delaminations in progressive damage: a review*, Microsystem Technologies 25 (2019), pp. 747–763.

[26] J. Vala, *Remarks to the computational analysis of semilinear direct and inverse problems of heat transfer*, Thermophysics – 24th International Conference in Smolenice (2019), AIP Conference Proceedings 2170, 2019, pp. 020023/1–6.

[27] J. Vala, *Structure identification of metal fibre reinforced cementitious composites*, Algoritmy – 20th Conference on Scientific Computing in Podbanské (2016), Proceedings, STU Bratislava, 2016, pp. 244–253.

[28] J. Vala, P. Jarošová and V. Kozák, *On the computational analysis of quasi-brittle fracture using integral-type nonlocal models*, International Journal of Applied Physics 4 (2019), pp. 8–13.

[29] J. Vala and V. Kozák, *Computational analysis of quasi-brittle fracture in fibre reinforced cementitious composites*, Theoretical and Applied Fracture Mechanics 107 (2020), pp. 102486/1–8.