An energy-conserving time-discretisation scheme for poroelastic media with phase-field fracture emitting waves and heat

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Abstract. The model of brittle cracks in elastic solids at small strains is approximated by the Ambrosio-Tortorelli functional and then extended into evolution situation to an evolutionary system, involving viscoelasticity, inertia, heat transfer, and coupling with Cahn-Hilliard-type diffusion of a fluid due to Fick's or Darcy's laws. Damage resulted from the approximated crack model is considered rate independent. The fractional-step Crank-Nicolson-type time discretisation is devised to decouple the system in a way so that the energy is conserved even in the discrete scheme. The numerical stability of such a scheme is shown, and also convergence towards suitably defined weak solutions. Various generalizations involving plasticity, healing in damage, or phase transformation are mentioned, too.

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1. **Introduction.** An efficient *approximation of transient problems* and *wave propagation problems* in mechanics of continua with inertial effects represents a computationally difficult problem which has deserved a wide attention during many decades. Various explicit or implicit methods have been devised with various phenomena accented. One important attribute (beside e.g. dispersion or wave length or causality etc.) to be followed is a possible *energy conservation*. Among other theoretically important effects, this prevents an artificial numerical attenuation which often destroys the practical applicability of numerical schemes.

It was observed in [49] that a combination of the Crank-Nicolson scheme with a fractional-step strategy for first-order systems allows for an energy-conserving implicit time-discretisation of a relatively wide class of mechanical systems at small strains governed by a separately quadratic free-energy functionals. Here we want to illustrate it on a quite complicated system coupling the classical force equilibrium equation with inertia at small strains with crack nucleation/propagation modelled in the spirit of Ambrosio-Tortorelli's approximation [1, 2] discussed in Remark 1 below, combined also with a diffusion driven by the gradient of a chemical potential, and eventually with a heat-transfer equation.

The state variables are the displacement u, the scalar damage z, the concentration c of a diffusant (typically some liquid, gas, or some solvent and, depending on specific applications, it may be hydrogen, deuterium, water, etc.), and the (absolute) temperature θ. The particular equations of the system considered in this paper are the momentum equilibrium, the flow rule for damage, the balance of mass of the diffusant, and the heat-transfer equation. The basic notation is summarized in Table 1.

u displacements	$e(u)=\frac{1}{2}(\nabla u)^\top+\frac{1}{2}\nabla u$ small strain tensor
v velocity	M Biot modulus
z damage scalar variable	β Biot coefficient
c concentration	κ coefficient for the ratio Fick/Darcy flow
θ temperature	$\varkappa$ capillarity coefficient
ϑ heat content	a energy released per unit volume by damage
σ stress	$\psi=\varphi+\phi$ free energy
μ chemical potential	φ,ϕ chemo-mechanical and thermal energies
$\mathbb{C}$ elastic-moduli tensor	$\mathfrak{u}$ internal energy
$\mathbb{D}$ viscous-moduli tensor	$c_{\rm E}$ equilibrium concentration
$\mathbb{M}$ the mobility matrix	g bulk force (gravity)
$\mathbb{K}$ the heat-conductivity matrix	f traction force
$c_{\rm v}$ heat capacity	$h_{\rm B}$ prescribed boundary heat flux
ϱ mass density	$j_{\rm B}$ prescribed boundary diffusant flux
r heat-production rate	$\varepsilon>0$ a fixed regularization parameter
$\mathfrak{s}$ entropy	$\tau>0$ a time step for discretisation

Table 1. Summary of the basic notation used through this paper.

More specifically, using the dot-notation $(\cdot)^{\boldsymbol\cdot}$ for the time derivative, the system of the mentioned four equations are:

$$\varrho\ddot{u} - \operatorname{div}\sigma = g \quad \text{with} \quad \sigma = (\varepsilon^2{+}z^2)(\mathbb{D}e(\dot{u}) + \mathbb{C}e(u)) + \beta M(\beta \operatorname{tr} e(u){-}c)\mathbb{I}, \tag{1a}$$

$$N_{\{\dot{z}\le 0\}}(\dot{z}) + \frac{a_0 z}{2\varepsilon} + z\mathbb{C}e(u){:}e(u) - 2a_0\varepsilon\Delta z \ni \frac{a}{2\varepsilon}, \tag{1b}$$

$$\dot{c} = \operatorname{div}\big(\mathbb{M}(z,c,\theta)\nabla\mu\big) \qquad \text{with} \quad \mu = \Big(M{+}\frac{\kappa}{c_{\rm E}}\Big)c - \beta M \operatorname{tr} e(u) - \kappa - \varkappa\Delta c, \tag{1c}$$

$$c_{\rm v}(\theta)\dot{\theta} - \operatorname{div}(\mathbb{K}(z,c,\theta)\nabla\theta) = r(z,c,\theta;e(\dot{u}),\dot{z},\nabla\mu)$$
$$\text{with} \;\; r(z,c,\theta;\dot{e},\dot{z},\nabla\mu) = (\varepsilon^2{+}z^2)\mathbb{D}\dot{e}{:}\dot{e} - \frac{a_1}{\varepsilon}\dot{z} + \mathbb{M}(z,c,\theta)\nabla\mu{\cdot}\nabla\mu, \tag{1d}$$

where N_C is the normal cone to the convex set C, i.e. here in (1b) the set of nonpositive functions on Ω. These equations/inclusions are to hold on a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$. In (1b), we denoted by

$$a = a_0 + a_1$$

the overall energy dissipated (up to the factor ε) by damaging a unit volume; note that we have distinguished a part a_0 which is stored (and does not contribute to heat production) and the remaining part a_1 which contributes to heat production. Actually, the additive constant $-\kappa$ in μ is not important in (1) itself but it could be relevant when general boundary conditions involving the value of μ were be considered.

The application of this model in the full generality is expectedly in tectonic earthquakes caused by ruptures of existing lithospheric faults in poroelastic rocks which emit seismic waves and exhibiting sometimes a so-called "flash heating" during rupture, combined with the possible water diffusion interacting with the rupture, or possibly even a nucleation of new faults [22, 33, 34, 54]; in particular then c is the water concentration. A similar model applies to heat and moisture transfer in concrete undergoing damage or fracture as in [30]. Particular simplified (or modified) models may serve for some other applications such as martensitic phase transformation in polycrystalline shape-memory alloys or metal/hydrid phase transformation during diffusion of hydrogen in specific intermetalics, cf. Remark 4 below; in particular then c is the hydrogen concentration.

Not surprisingly, we have to make a lot of various simplifications, some of them dictated by the desired energy conservation of the discretisation scheme. In particular, we neglect temperature-dependence of the stored energy (i.e. in particular thermal expansion), healing of damage, or allow for a possible interpenetration of cracks.

The energy conservation (needed in particular in thermally coupled problems) in the continuous system essentially requires the Kelvin-Voigt viscoelastic rheology. The convergence of the discrete schemes typically needs certain gradient theories, namely the strain gradient (so-called 2nd-grade nonsimple materials), or alternatively also some phase-field regularization (in addition to the z-variable, as considered in [51]), or the concentration gradient. Here in (1) we have adopted the last option, which leads to the Cahn-Hilliard [13] system coupled with damage [8, 23, 24], see also [25, Chap. 7], and with inertia [26], and coupled with heat transfer [27].

The goal of this article is to illustrate the discretisation strategy devised in [49] for a relatively simpler situation on a nontrivial system coupling many physical phenomena with many potential applications. The general model coupling dynamic visco-elasticity with damage and heat and fluid transfer is presented in Section 2. The time discretisation is devised in Section 3 where also existence of its energy-conserving solution is shown. Eventually, its numerical stability (certain a-priori estimates) and convergence towards weak solutions of the continuous system for time-step approaching zero is proved in Section 4. Recent nontrivial results from the theory of rate-independent processes are exploited for the damage model which otherwise seems to bring an essential trouble, cf. [37, Example 1.2.7].

Beside the already mentioned difference from this type of models in [51] consisting of not using any phase-field variable in the present paper, the viscosity here is subjected to damage by the same way as elastic response and, most importantly, the time discretization used in [51] is improved to be actually applicable for problems where vibrations and waves are pursued. The energy conservation of the discrete scheme also requires to avoid a regularization of the discrete heat-transfer equation, which then keeps the heat sources valued in L^1-spaces also in the discrete scheme and complicates the analysis at many spots. Also the Crank-Nicholson scheme requires many demanding modifications of the usual techniques used otherwise for backward-Euler schemes.

2. **The thermodynamics of the model.** Some boundary conditions for the system (1) should be still prescribed on the boundary $\Gamma = \partial\Omega$. There are a lot of options. Focusing rather on the bulk model,

let us choose quite a simple set of conditions:

$$\sigma\nu = f, \quad \frac{\partial z}{\partial \nu} = 0, \quad \frac{\partial c}{\partial \nu} = 0, \quad \mathbb{M}(z,c,\theta)\nabla\mu\cdot\nu = j_{\rm B}, \quad \mathbb{K}(z,c,\theta)\nabla\theta\cdot\nu = h_{\rm B} \tag{2}$$

where $\frac{\partial c}{\partial\nu} := \nabla c\cdot\nu$ and $\frac{\partial z}{\partial\nu} := \nabla z\cdot\nu$. The index "B" stands for a "boundary" data. We consider in addition the initial conditions:

$$u(0) = u_0, \qquad \dot u(0) = v_0, \qquad z(0) = z_0, \qquad c(0) = c_0, \qquad \theta(0) = \theta_0. \tag{3}$$

The energetics of the system (1)–(3) can be revealed by testing the particular equations (1a,b,c) respectively by $\dot u$, $\dot z$, and μ. It yields the *chemo-mechanical energy* balance

$$\underbrace{\mathscr{T}(\dot u(t))}_{\substack{\text{kinetic energy}\\ \text{at time } t}} + \underbrace{\mathscr{E}(u(t),z(t),c(t))}_{\substack{\text{stored energy}\\ \text{at time } t}} + \underbrace{\int_0^t \mathscr{R}(z,c,\theta;\dot u,\dot z,\mu)\,\mathrm{d}t}_{\substack{\text{energy dissipated}\\ \text{during } [0,t]}}$$
$$= \underbrace{\mathscr{T}(v_0)+\mathscr{E}(u_0,z_0,c_0)}_{\substack{\text{kinetic and stored energy}\\ \text{at time } t=0}} + \underbrace{\int_0^t \big\langle \mathscr{F}(t),(\dot u,\mu)\big\rangle\,\mathrm{d}t}_{\substack{\text{work done by chemo-}\\ \text{-mechanical load}}}, \tag{4}$$

with the separately (component-wise) quadratic stored energy $\mathscr{E}$, the dissipation rate $\mathscr{R}$, the kinetic energy $\mathscr{T}$, the power of the chemo-mechanical loading $\mathscr{F}$, and the total heat energy $\mathscr{C}$ and the external heat power $\mathscr{H}$ which will be used in (6), defined as

$$\mathscr{E}(u,z,c) := \int_\Omega \varphi(e(u),z,c,\nabla z,\nabla c)\,\mathrm{d}x$$
$$\text{with}\ \ \varphi(e,z,c,\nabla z,\nabla c) = \frac{\varepsilon^2{+}z^2}{2}\mathbb{C}e{:}e + \frac12 M(\beta\mathrm{tr}\,e{-}c)^2$$
$$+ \frac{a_0}{4\varepsilon}(1{-}z)^2 + \frac{\kappa}{2c_{\rm E}}(c{-}c_{\rm E})^2 + \varepsilon a_0|\nabla z|^2 + \frac{\varkappa}{2}|\nabla c|^2, \tag{5a}$$

$$\mathscr{R}(z,c,\theta;v,\dot z,\mu) := \int_\Omega r(z,c,\theta;e(v),\dot z,\nabla\mu)\,\mathrm{d}x \qquad \text{with}\ \ r\ \ \text{from (1d)}, \tag{5b}$$

$$\mathscr{T}(v) := \int_\Omega \frac{\varrho}{2}|v|^2\,\mathrm{d}x, \tag{5c}$$

$$\big\langle \mathscr{F}(t),(v,\mu)\big\rangle := \int_\Omega g(t,\cdot)\cdot v\,\mathrm{d}x + \int_\Gamma f(t,\cdot)\cdot v + j_{\rm B}(t,\cdot)\mu\,\mathrm{d}S, \tag{5d}$$

$$\mathscr{C}(\theta) := \int_\Omega \vartheta\,\mathrm{d}x \qquad \text{with} \qquad \vartheta = C_{\rm v}(\theta) = \int_0^1 c_{\rm v}(s\theta)\,\mathrm{d}s, \tag{5e}$$

$$\mathscr{H}(t) := \int_\Gamma h_{\rm B}(t,x)\,\mathrm{d}S. \tag{5f}$$

In (5a), $\varepsilon > 0$ is a fixed regularization parameter. However, we will not have any ambitions to investigate the limit for $\varepsilon \to 0$; serious difficulties arise even in particular cases as seen in the literature cited in Remark 1 below.

The *total-energy* conservation is then obtained by testing (1d) by 1 and summing it with (4). This yields

$$\underbrace{\mathscr{T}(\dot u(t))}_{\substack{\text{kinetic energy}\\ \text{at time } t}} + \underbrace{\mathscr{E}(u(t),z(t),c(t))}_{\substack{\text{stored energy}\\ \text{at time } t}} + \underbrace{\mathscr{C}(\theta(t))}_{\substack{\text{heat energy}\\ \text{at time } t}}$$
$$= \underbrace{\mathscr{T}(v_0)+\mathscr{E}(u_0,z_0,c_0)+\mathscr{C}(\theta_0)}_{\substack{\text{kinetic and stored and heat energy}\\ \text{at time } t=0}} + \underbrace{\int_0^t \mathscr{H}(t) + \big\langle \mathscr{F}(t),(\dot u,\mu)\big\rangle\,\mathrm{d}t}_{\substack{\text{work done by thermo-}\\ \text{-chemo-mechanical load}}}. \tag{6}$$

The standard thermodynamics behind this model is based on the free energy which separates chemo-mechanical and thermal variables, namely

$$\psi(e,z,c,\nabla z,\nabla c,\theta) = \varphi(e,z,c,\nabla z,\nabla c) + \phi(\theta) \tag{7}$$

with ϕ denoting the thermal part of the *free energy* determined by the heat capacity $c_{\rm v}$ used in (1d) by $\phi''_{\theta\theta} = -c_{\rm v}(\theta)/\theta$. The mentioned "separability" in (7) causes that $c_{\rm v}$ depends only on θ. Adiabatic effects are suppressed, which simplifies thus the model and its analysis, cf. Remark 7. Note that $\sigma = \psi'_e = \varphi'_e$

while $\mu=\psi_c'=\varphi_c'-\mathrm{div}\,\varphi_{\nabla c}'(\nabla c)$. The *entropy* is standardly defined as $\mathfrak{s}=-\psi_\theta'=-\phi_\theta'$ and then the *internal energy* is

$$\mathfrak{u}=\psi+\mathfrak{s}\theta=\varphi+\phi-\theta\phi_\theta'=\varphi(e,z,c,\nabla z,\nabla c)+\vartheta$$

with the heat energy $\vartheta=C_{\rm V}(\theta)$ from (5e).

Remark 1 (*Fracture approximation*)**.** The motivation of (5a) is in particular seen if the diffusion is suppressed by putting $M=0$, $\kappa=0$, and $\varkappa=0$. Then (5a) results in the *Ambrosio-Tortorelli functional*

$$\mathscr{E}(u,z):=\int_\Omega\frac{\varepsilon^2+z^2}{2}\mathbb{C}e(u){:}e(u)+\frac{a_0}{4\varepsilon}(1-z)^2+\varepsilon a_0|\nabla z|^2\,\mathrm{d}x \tag{8}$$

imitating the philosophy that *fracture* is in fact a bulk damage which is eventually complete but localized on very small volumes along evolving surfaces where the fracture propagates. In the static case, this approximation was proposed in [1,2] in fact for the Mumford-Shah functional [42] and the asymptotic analysis for $\varepsilon\to0$ was rigorously executed, inspired by a now classical example in phase transition [41]. Later, the approximate phase-field-type model was extended to the evolutionary case, namely for a rate-independent cohesive damage, in [19], see also also [11,31,32,37] where also inertial forces are sometimes considered, although its limit to the real fracture is still an open problem. The complete damage was combined with diffusion in some other works [24,25]. For various numerical studies on the base of (8) see e.g. [3,9,12]. The important fact here is that $z\ge0$ is automatically granted during the evolution if $z_0\ge0$ in (3), so that we do not need the constraint $z\ge0$ to be explicitly imposed, which would otherwise violate the energy conservation in the scheme in Section 3 below. Avoiding this constraint is possible because $\varphi_z'(e,z,\nabla z)=0$ for $z=0$ so that this contribution to the driving force vanishes when $z\searrow0$ while the contribution $-\mathrm{div}\,\varphi_{\nabla z}'(\nabla z)$ drives z away from negative values.

Remark 2 (*Component-wise quadratic ansatz*)**.** Standardly, the last term in φ from (5a) is rather $\kappa c(\ln(c/c_{\rm E})-1)$. This modification ensures $c>0$ because this terms blows up to ∞ if $c\searrow0$. It yields the chemical potential $\mu=\varphi_c'=M(c-\beta\mathrm{tr}\,e(u))+\kappa\ln(c/c_{\rm E})$ instead of $\mu=M(c-\beta\mathrm{tr}\,e(u))+\kappa(c/c_{\rm E}-1)$ in (1c). Setting $\mathbb{M}(c)=c\mathbb{M}_0$, the flux $j=-\mathbb{M}(c)\nabla\mu$ is then

$$j=-c\mathbb{M}_0\nabla p-\kappa\mathbb{M}_0\nabla c\qquad\text{with the pressure }\ p=M(c-\beta\mathrm{tr}\,e(u)), \tag{9}$$

showing the Darcy and the Fick contributions, respectively. This standard term $\kappa c(\ln(c/c_{\rm E})-1)$ attains its minimum at $c=c_{\rm E}$ while its second-order derivative is κ/c so that the second-order Taylor's expansion of this term around $c=c_{\rm E}$ is, up to a constant, $\frac{\kappa}{2}(c-c_{\rm E})^2/c_{\rm E}$. Keeping the (component-wise) quadratic structure of $\mathscr{E}$, the desired constraint $c\ge0$ can be ensured indirectly by setting $\mathbb{M}(c)=0$ for $c<0$. Hence the diffusant is "frozen" when its concentration would try to fall below zero, which eventually prevents such a fall when relying on the absence of sources on the right-hand side of the diffusion equation (1c) and on the qualification of the initial condition $c_0\ge0$. If we choose $\mathbb{M}(c)=\mathbb{M}_0$ for $c\ge0$, the flux $\mathbb{M}(c)\nabla\mu$ is then

$$j=-\mathbb{M}_0\nabla p-\kappa\mathbb{M}_0\nabla c \tag{10}$$

with p again from (9). It now reveals how our term $\frac{\kappa}{2}(c-c_{\rm E})^2/c_{\rm E}$ in φ from (5a) arises as the Taylor expansion around equilibrium concentration. It also reveals that, by a suitable choice of $\mathbb{M}(c)$, it may yield the same Fick flux as the mentioned standard choice $\kappa c(\ln(c/c_{\rm E})-1)$ while only the Darcy flux is modified. Actually, $\mathbb{M}(c)=\mathbb{M}_0$ for $c\ge0$ together with $\mathbb{M}(c)=0$ for $c<0$ obviously needs $\mathbb{M}(\cdot)$ discontinuous at $c=0$, which would bring analytical difficulties. On the other hand, continuous $\mathbb{M}(\cdot)$ with the degeneracy $\mathbb{M}(c)=0$ for $c<0$ well approximate the desired model and are standardly used in numerical simulations and even are amenable for analysis [15,43].

Remark 3 (*Generalizations: plasticity or Maxwell rheologies*)**.** A combination of damage with plasticity makes a substantial enrichment of the models. A minimal scenario (without extra internal hardening-type variables) uses another internal variable π with values in the set of symmetric deviatoric-free matrices $\mathbb{R}^{d\times d}_{\rm dev}$. Then e in (5a) is to be substituted by $e-\pi$ and a hardening or a gradient terms like $\frac12\kappa_1|\pi|^2$ or $\frac12\kappa_2|\nabla\pi|^2$ are to be added to φ. This substitution is to be applied also to the system (1) which is to be augmented by an additional evolution inclusion governing the evolution of π, namely

$$\sigma_{\rm Y}\mathrm{Dir}(\dot\pi)+\chi_{\rm R}\dot\pi+\kappa_1\pi-\kappa_2\Delta\pi\ni\mathrm{dev}\,\sigma=:\sigma-\frac1d\mathrm{tr}\,\sigma, \tag{11}$$

where $\sigma_{\rm Y}\ge0$ is the yield stress, $\chi_{\rm R}\ge0$ a relaxation time, and $\mathrm{Dir}:\mathbb{R}^{d\times d}_{\rm dev}\rightrightarrows\mathbb{R}^{d\times d}_{\rm dev}$ is the set-valued subdifferential of the Euclidean norm on the set on $\mathbb{R}^{d\times d}_{\rm dev}$. Moreover, a convex term $\sigma_{\rm Y}|\dot\pi|$ or $\sigma_{\rm Y}|\dot\pi|+\chi_{\rm R}|\dot\pi|^2$ is then to be added to the dissipation rate (5b) in order to keep the total-energy balance. The component-wise quadratic structure of $\mathscr{E}$ is kept, so that the discretisation in Section 3 can easily be modified for this situation, too. For a model neglecting heat and diffusant transfer with fractional-step discretisation but using the backward Euler instead of the Crank-Nicolson energy we refer to [29]. If $\sigma_{\rm Y}=0$, we obtain the Maxwell (or, in combination with our Kelvin-Voigt, the so-called Jeffrey) rheology, describing phenomena such as creep or (in geophysical applications, assuming $\chi_{\rm R}$ in (11) large) aseismic slip. If $\chi_{\rm R}=0$, we obtain rate-independent plasticity (built into the context of other rate-dependent phenomena in the whole model, of course) and it should be emphasized that a combination of two rate-independent processes (here damage and plasticity) leading to a nonconvex energy would rise an important issue about the concept of solution; our fractional-step scheme than would yield rather a stress-driven-type solution and holding the energy conservation in the limit would be troublesome, requiring rather the vanishing-viscosity approach $\chi_{\rm R}\to 0$ giving rise to a so-called defect measure, cf. [48] or also [37, Sect. 3.8.3].

Remark 4 (*Further generalizations - constraints*)**.** Certain applications include unilateral constraints on state variables involved in $\mathscr{E}$. Here, it would however corrupt the (component-wise) quadratic structure of $\mathscr{E}$ exploited later in Section 3. For this reason, such constraints can (at least approximately) handled in the dissipation potential. For example, some applications use (up to a constant) the constraint $|\pi|\le 1$ on the plastic strain (called then a transformation strain) in Remark 3. This constraint can approximately be realized by augmenting the yield stress $\sigma_{\rm Y}$ to $\sigma_{\rm Y}+(|\pi|{-}1)^+(\pi{:}\dot\pi)^+/\varepsilon$ in (11) and then $\frac{1}{\varepsilon}((|\pi|{-}1)^+(\pi{:}\dot\pi)^+)|\dot\pi|$ is to be added into the dissipation rate r in (1d). For small $\varepsilon>0$, it ensures that π cannot move too far away from the unit ball in $\mathbb{R}^{d\times d}_{\rm dev}$ while its evolution is again according to (11) if π is inside this ball or is on (or near) its surface but moves in the tangential direction. Another example is an approximate realization of the constraint $0\le z\le 1$, which can be enforced by adding $(-z)^+(-\dot z)^+/\varepsilon+(z{-}1)^+\dot z^+/\varepsilon$ to (1b); in fact, the evolution of z should instead be bi-directional, i.e. the unidirectional constraint $\dot z\le 0$ in (1b) is then to be replaced by Sign $\dot z$ with "Sign" denoting the a set-valued sudifferential of $|\cdot|$. Altogether, $\frac{1}{\varepsilon}(-z)^+((-\dot z)^+)^2+\frac{1}{\varepsilon}(z{-}1)^+(\dot z^+)^2+|\dot z|$ is to be added into the dissipation rate r in (1d). The example of a componentwise quadratic stored energy used in such sort of models is $\varphi(e,z,\nabla z)=\frac12\mathbb{C}(e{-}z\pi){:}(e{-}z\pi)+\varepsilon|\nabla z|^2$. Cf. the models for polycrystalline *shape-memory alloys* undergoing martensitic transformation (i.e. a re-orientation of martensite combined with austenite-martensite phase transformation) in [18, 55], possibly also in combination with plasticity like already used in (11), cf. [4, 53]. Then z has the interpretation of the volume fraction austenite/martensite while π is the transformation strain of martensite; in fact, this part of energy is often strongly dependent on temperature. A combination with diffusion of a fluidic ingredient might be motivated by a metal-hydrid phase transformation where hydrogen causes substantial swelling when diffuses into the polycrystalline metals, cf. e.g. [50, 51]. The swelling with e.g. 30% volume changes during such transformation can easily cause rupture accompanied by emitting vibrations.

Remark 5 (*Biot's model [5]*)**.** Another motivation of (5a) is a popular model of a saturated flow in poroelastic media by M. Biot. The adjective "saturated" is to be reflected by $c\ge\zeta$ with ζ denoting here a *porosity*. In Biot's model, this is not considered as a constraint but is only involved in a "soft" way in the free energy through the so-called Biot term $\frac12 M(\beta{\rm tr}\,e{-}c{+}\zeta)^2$. To keep our (componentwise) quadratic ansatz which allows for energy-conserving discretisation, the Biot modulus M as well as the Biot coefficient β are here considered independent of z and c as often used in applications, cf. e.g. [22, 33]. The porosity ζ in our model is considered fixed (namely 0 for notational simplicity) but in some applications the evolution of porosity is a vital part of the model, the flow rule being coupled with the flow rule for damage (1b) also by the dissipative cross-effects, cf. again e.g. [22, 33]. It needs the constraint $\zeta\ge 0$ which is to be treated approximately as in Remark 4, however.

Remark 6 (*A generalization: healing in damage*)**.** Most engineering applications well comply with the unidirectional damage evolution as considered in (1b) by involving the constraint $\dot z\le 0$, but some other applications (specifically in geophysics [22, 33, 34]) ultimately need to allow for healing, i.e. a bi-directional evolution of z, cf. also [37, 52]. It needs the constraint $z\le 1$ which is to be involved and, in order to keep the componentwise quadratic structure of $\mathscr{E}$, is to be again treated only approximately as in Remark 4.

3. **Time discretisation and its energy-conservation.** We consider a bounded (connected) domain $\Omega\subset\mathbb{R}^d$ with a Lipschitz boundary $\Gamma=\partial\Omega$. Beside the standard notation for the Lebesgue L^p-spaces and $W^{k,p}$ for Sobolev spaces whose k-th distributional derivatives are in L^p-spaces, we will use the abbreviation $H^k=W^{k,2}$. Moreover, we use the standard notation $p'=p/(p{-}1)$, and p^* for the Sobolev exponent $p^*=pd/(d{-}p)$ for $p<d$ while $p^*<\infty$ for $p=d$ and $p^*=\infty$ for $p>d$, and the "trace exponent" $p^\sharp$ defined as $p^\sharp=(pd{-}p)/(d{-}p)$ for $p<d$ while $p^\sharp<\infty$ for $p=d$ and $p^\sharp=\infty$ for $p>d$.

Thus, e.g., $W^{1,p}(\Omega)\subset L^{p^*}(\Omega)$ or $L^{p^{*\prime}}(\Omega)\subset W^{1,p}(\Omega)^*=$ the dual to $W^{1,p}(\Omega)$. In the vectorial case, we will write $L^p(\Omega;\mathbb{R}^n)\cong L^p(\Omega)^n$ and $W^{1,p}(\Omega;\mathbb{R}^n)\cong W^{1,p}(\Omega)^n$.

We consider a fixed time interval $I=[0,T]$ and we denote by $L^p(I;X)$ the standard Bochner space of Bochner-measurable mappings $I\to X$ with X a Banach space. Also, $W^{k,p}(I;X)$ denotes the Banach space of mappings from $L^p(I;X)$ whose k-th distributional derivative in time is also in $L^p(I;X)$. Moreover, we denote by $\mathrm{BV}(I;X)$ the Banach space of the mappings $I\to X$ that have bounded variation on I. By $\mathrm{Meas}(I;X)$ we denote the space of X-valued measures on I. Finally, in what follows, C denotes a positive, possibly large constant.

We first rewrite the 2nd-order equation (1a) as a 1st-order system and also use the heat-transfer equation (1d) slightly rewritten as follows:

$$\dot u = v, \tag{12a}$$

$$\varrho\dot v-\mathrm{div}\,\sigma=0\quad\text{with}\quad \sigma=(\varepsilon^2{+}z^2)(\mathbb{D}e(v){+}\mathbb{C}e(u))+\beta M(\beta\mathrm{tr}\,e(u){-}c)\mathbb{I}, \tag{12b}$$

$$N_{\{\dot z\le0\}}(\dot z)+\frac{a_0z}{2\varepsilon}+z\mathbb{C}e(u){:}e(u)-2a_0\varepsilon\Delta z\ni\frac{a}{2\varepsilon}, \tag{12c}$$

$$\dot c=\mathrm{div}\big(\mathbb{M}(z,c,\theta)\nabla\mu\big)\quad\text{ with }\quad \mu=\Big(M{+}\frac{\kappa}{c_{\scriptscriptstyle\rm E}}\Big)c-\beta M\mathrm{tr}\,e(u)-\kappa-\varkappa\Delta c, \tag{12d}$$

$$\dot\vartheta-\mathrm{div}(\mathbb{K}(z,c,\theta)\nabla\theta)=r(z,c,\theta;e(\dot u),\dot z,\nabla\mu)\qquad\text{with }\ \vartheta=C_{\rm v}(\theta)\ \text{ and}$$
$$\text{with }\ r(z,c,\theta;\dot e,\dot z,\nabla\mu)=(\varepsilon^2{+}z^2)\mathbb{D}\dot e{:}\dot e-\frac{a_1}{\varepsilon}\dot z+\mathbb{M}(z,c,\theta)\nabla\mu{\cdot}\nabla\mu. \tag{12e}$$

Rather for notational simplicity, we consider a time step $\tau>0$ which does not vary within particular time levels and such that T/τ is integer, leading to an equidistant partition of the considered time interval. Let us emphasize, however, that a varying time-step and non-equidistant partitions can be easily implemented because we will always consider only first-order time differences and one-step formulas. In fact, such a varying time-step can be advantageously used for a certain adaptivity to optimize computational costs.

The fractional-step discretisation similar to (13b,c) below has been devised already in [11,32,37] but with $v_\tau^k=(u_\tau^k{-}u_\tau^{k-1})/\tau$ so that the resulting scheme exhibited a strong artificial attenuation instead of energy conservation. In [10], a fully implicit formula for (13b,c) with $\varrho=0$ has been used, implementing an iterative alternating minimization algorithm combined with a backtracking strategy to cope with a global minimization of a nonconvex functional. The global minimization of nonconvex functionals and related difficulties are completely avoided by our fractional-step scheme, however.

Here we will use the numerical approximation by the fractional-step-type time-discretisation combined with the *Crank-Nicolson formula* [14]. The Crank-Nicolson scheme was originally devised for the heat equation and later used for 2nd-order problems in the form (1a), see e.g. [20, Ch.6, Sect.9]. It is different if applied to the dynamical equations transformed into the form (12a,b); then it can be understood as a particular case of the celebrated Hilber-Hughes-Taylor formula [28] and it is sometimes called just a central-difference scheme or a Simo's scheme, cf. e.g. [58, Sect. 12.2] or [56, Sect. 1.6], respectively.

This can be achieved by decoupling the time-discretised system suitably, namely "componentwise". This allows us to qualify $\mathscr{E}$ only "componentwise" and works successfully if the dissipation potentials $\mathscr{R}$'s are separated, as is indeed the case with our system (1). It is called a fractional-step method or sometimes also a Lie-Trotter (or sequential) splitting, and there is an extensive literature about it, cf. [35, 59]. Sometimes, this componentwise-split Crank-Nicolson method is also called the 2nd-order Yanenko method [16]. Here we apply it even iteratively, leading to a 3-step scheme.

This results in the following system of five equations for the five-tuple $(u_\tau^k,v_\tau^k,z_\tau^k,c_\tau^k,\theta_\tau^k)$:

$$\frac{u_\tau^k{-}u_\tau^{k-1}}{\tau}=v_\tau^{k-1/2}, \tag{13a}$$

$$\varrho\frac{v_\tau^k{-}v_\tau^{k-1}}{\tau}-\mathrm{div}\,\widetilde\sigma_\tau^k=g_\tau^k\quad\text{with}\quad\widetilde\sigma_\tau^k=(\varepsilon^2{+}(z_\tau^{k-1})^2)\big(\mathbb{D}e(v_\tau^{k-1/2})+$$
$$+\,\mathbb{C}e(u_\tau^{k-1/2})\big)+\beta M(\beta\mathrm{tr}\,e(u_\tau^{k-1/2}){-}c_\tau^{k-1/2})\mathbb{I}, \tag{13b}$$

$$N_{\{\dot z\le0\}}\Big(\frac{z_\tau^k-z_\tau^{k-1}}{\tau}\Big)+\frac{a_0}{2\varepsilon}z_\tau^{k-1/2}+z_\tau^{k-1/2}\mathbb{C}e(u_\tau^k){:}e(u_\tau^k)-2a_0\varepsilon\Delta z_\tau^{k-1/2}\ni\frac{a}{2\varepsilon}, \tag{13c}$$

$$\frac{c_\tau^k{-}c_\tau^{k-1}}{\tau}=\mathrm{div}\big(\mathbb{M}(z_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1})\nabla\mu_\tau^{k-1/2}\big)$$
$$\text{with}\quad\mu_\tau^{k-1/2}=\Big(M{+}\frac{\kappa}{c_{\scriptscriptstyle\rm E}}\Big)c_\tau^{k-1/2}-\beta M\mathrm{tr}\,e(u_\tau^{k-1/2})-\kappa-\varkappa\Delta c_\tau^{k-1/2}, \tag{13d}$$

$$\frac{\vartheta_\tau^k-\vartheta_\tau^{k-1}}{\tau}-\mathrm{div}(\mathbb{K}(z_\tau^k,c_\tau^k,\theta_\tau^{k-1})\nabla\theta_\tau^k)=\widetilde{r}_\tau^k \quad \text{with} \quad \vartheta_\tau^k=C_\mathrm{v}(\theta_\tau^k) \ \text{ and}$$
$$\text{with} \quad \widetilde{r}_\tau^k=r\Big(z_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1};e(v_\tau^{k-1/2}),\frac{z_\tau^k-z_\tau^{k-1}}{\tau},\nabla\mu_\tau^{k-1/2}\Big) \tag{13e}$$

with the abbreviation

$$u_\tau^{k-1/2}:=\frac{u_\tau^k+u_\tau^{k-1}}{2},\quad v_\tau^{k-1/2}:=\frac{v_\tau^k+v_\tau^{k-1}}{2},\quad z_\tau^{k-1/2}:=\frac{z_\tau^k+z_\tau^{k-1}}{2},\quad c_\tau^{k-1/2}:=\frac{1}{2}(c_\tau^k+c_\tau^{k-1}). \tag{14}$$

In (13b), g_τ^k is an approximation of g at $t=k\tau$, e.g. $g_\tau^k:=\tau^{-1}\int_{(k-1)\tau}^{k\tau}g(t)\,\mathrm{d}t$. This system is accompanied with corresponding boundary conditions

$$\widetilde{\sigma}_\tau^k\nu=f_\tau^k:=\frac{1}{\tau}\int_{(k-1)\tau}^{k\tau}f(t)\,\mathrm{d}t,\qquad \frac{\partial z_\tau^k}{\partial\nu}=0,\qquad \frac{\partial c_\tau^k}{\partial\nu}=0, \tag{15a}$$
$$\mathbb{M}(z_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1})\nabla\mu_\tau^{k-1/2}\cdot\nu=j_{\mathrm{B},\tau}^k:=\frac{1}{\tau}\int_{(k-1)\tau}^{k\tau}j_{\mathrm{B}}(t)\,\mathrm{d}t, \tag{15b}$$
$$\mathbb{K}(z_\tau^k,c_\tau^k,\theta_\tau^{k-1})\nabla\theta_\tau^k\cdot\nu=h_{\mathrm{B},\tau}^k:=\frac{1}{\tau}\int_{(k-1)\tau}^{k\tau}h_{\mathrm{B}}(t)\,\mathrm{d}t, \tag{15c}$$

is to be executed recursively for $k=1,2,...,T/\tau$, starting with $k=1$ by using

$$u_\tau^0=u_0,\qquad v_\tau^0=v_0,\qquad z_\tau^0=z_0,\qquad c_\tau^0=c_0,\qquad \theta_\tau^0=\theta_0. \tag{16}$$

Note that z_τ^k is not used in (13b,d) and thus the system (13) is indeed decoupled. First, one is to solve (13a,b,d) to obtain $(u_\tau^k,v_\tau^k,c_\tau^k)$, then (13c) to obtain z_τ^k, and eventually (13e) to obtain θ_τ^k. This splitting corresponds to the structure of $\mathscr{E}$ which is separately quadratic in (u,c) and in z and of the dissipation rate $\mathscr{R}(z,c,\theta;\cdot,\cdot,\cdot)$ which is additively split in terms of these sets of variables; note that $\mu_\tau^{k-1/2}$ in (13d) couples u_τ^k and c_τ^k but it is still within the set of the (u,v,c)-variables.

An important attribute is also that all three boundary-value subproblems have potentials. Note that (13a,b) is "optically" not symmetric but eliminating v_τ^k by substituting $v_\tau^k=\frac{2}{\tau}(u_\tau^k-u_\tau^{k-1})-v_\tau^{k-1}$ into (13b) one again obtains a potential problem for the couple (u_τ^k,c_τ^k), cf. also [49]. Moreover, in the cases of (13a,b,d) and (13e), these potentials are quadratic while (13c) has a quadratic potential with the linear constraint $z\le z_\tau^{k-1}$. A peculiarity is the structure of the Cahn-Hilliard equation (1c) with the boundary condition in (2). More specifically, let us denote by $\Delta_\mathbb{M}$ the linear operator $\mu\mapsto\mathrm{div}(\mathbb{M}\nabla\mu)$ with the boundary condition $\mathbb{M}\nabla\mu\cdot\nu=0$ on Γ formulated weakly as an operator $H^1_\equiv(\Omega)\to H^1_\equiv(\Omega)^*$ with $H^1_\equiv(\Omega)$ denoting the Sobolev space $H^1_\equiv(\Omega)$ modulo functions which are constant (on each connected component of Ω). Assuming $\mathbb{M}$ symmetric, the linear operator $\Delta_\mathbb{M}$ has a convex quadratic potential $R_\mathbb{M}:\mu\mapsto\int_\Omega\frac{1}{2}\mathbb{M}\nabla\mu\cdot\nabla\mu\,\mathrm{d}x$. Its convex conjugate $R_\mathbb{M}^*:H^1_\equiv(\Omega)^*\to\mathbb{R}$ is again quadratic and it is a potential to the inverse $\Delta_\mathbb{M}^{-1}$. We denote still $\mathfrak{j}_\mathrm{B}(t)\in H^1_\equiv(\Omega)^*$ the linear functional $\mu\mapsto\int_\Gamma j_\mathrm{B}(t,\cdot)\mu\,\mathrm{d}S$. This allows for elimination of the chemical potential μ when realizing that it is equal to $\mathscr{E}_c'$. The evolution (1c) with the boundary condition $(\mathbb{M}\nabla\mu)\cdot\nu=j_\mathrm{B}$ in (2) takes the abstract structure

$$[R^*_{\mathbb{M}(z,c,\theta)}]'(\dot{c})+\mathscr{E}_c'(u,c)=[R^*_{\mathbb{M}(z,c,\theta)}]'\mathfrak{j}_\mathrm{B}(t)$$

where, in particular, μ has been eliminated. This structure can also be identified in our discretization scheme (13d), namely

$$[R^*_{\mathbb{M}(z_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1})}]'\Big(\frac{c_\tau^k-c_\tau^{k-1}}{\tau}\Big)+\mathscr{E}_c'(u_\tau^{k-1/2},c_\tau^{k-1/2})=[R^*_{\mathbb{M}(z_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1})}]'\mathfrak{j}_{\mathrm{B},\tau}^k$$

where $\mathfrak{j}_{\mathrm{B},\tau}^k\in H^1_\equiv(\Omega)^*$ is determined by $j_{\mathrm{B},\tau}^k$ from (15b). Realizing the specific form $R_\mathbb{M}^*:\dot{c}\mapsto\int_\Omega\frac{1}{2}|\mathbb{M}^{-1/2}\nabla\Delta_\mathbb{M}^{-1}\dot{c}|^2\,\mathrm{d}x$, cf. also [37, Formula (5.2.67)], the potential governing the system (13a,b,d) with v_τ^k and μ_τ^k eliminated as described above and with the corresponding boundary conditions (15) reads as

$$(u,c)\mapsto\int_\Omega 2\tau\varrho\Big|\frac{u-\tau v_\tau^{k-1}-u_\tau^{k-1}}{\tau^2}\Big|^2+\frac{\varepsilon^2{+}(z_\tau^{k-1})^2}{\tau}\mathbb{C}e\Big(\frac{u{+}u_\tau^{k-1}}{2}\Big){:}e\Big(\frac{u{-}u_\tau^{k-1}}{2}\Big)$$
$$+\frac{M}{\tau}\Big(\beta\mathrm{tr}e\Big(\frac{u{+}u_\tau^{k-1}}{2}\Big)-\frac{c+c_\tau^{k-1}}{2}\Big)^2+\frac{\kappa}{c_E\tau}\Big(\frac{c+c_\tau^{k-1}}{2}-c_E\Big)^2$$
$$+\frac{\varkappa}{\tau}\Big|\frac{\nabla c{+}\nabla c_\tau^{k-1}}{2}\Big|^2+\frac{\varepsilon^2{+}(z_\tau^{k-1})^2}{2}\mathbb{D}e\Big(\frac{u{-}u_\tau^{k-1}}{\tau}\Big){:}e\Big(\frac{u{-}u_\tau^{k-1}}{\tau}\Big)$$
$$+\frac12\Big|\mathbb{M}^{-1/2}(z_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1})\nabla\Delta^{-1}_{\mathbb{M}(z_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1})}\frac{c{-}c_\tau^{k-1}}{\tau}\Big|^2\,\mathrm{d}x$$
$$-\frac1\tau\int_\Gamma f_\tau^k{\cdot}u\,\mathrm{d}S,-\frac1\tau\Big\langle j_{\mathrm{B},\tau}^k,\Delta^{-1}_{\mathbb{M}(z_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1})}c\Big\rangle \tag{17a}$$

where $\langle\cdot,\cdot\rangle$ in the last expression denotes the duality between $H^1_{\equiv}(\Omega)^*$ and $H^1_{\equiv}(\Omega)$. The potential governing (13c) with the corresponding boundary conditions (15) reads as

$$z\mapsto\int_\Omega\Big(\frac{a_0\varepsilon}{8}+\frac14\mathbb{C}e(u_\tau^k){:}e(u_\tau^k)\Big)z^2+\frac{a_0\varepsilon}{2}|\nabla z|^2+\delta_{\{z\le0\}}(z{-}z_\tau^{k-1})$$
$$-\Big(\frac{a_0}{4\varepsilon}z_\tau^{k-1}{+}\frac12 z_\tau^{k-1}\mathbb{C}e(u_\tau^k){:}e(u_\tau^k)+\frac{a}{2\varepsilon}\Big)z-a_0\varepsilon\nabla z_\tau^{k-1}{\cdot}\nabla z\,\mathrm{d}x, \tag{17b}$$

with $\delta_{\{z\le0\}}(\cdot)$ the indicator function of the set $\{z\le0\}$, and eventually the potentials governing (13e) with the corresponding boundary conditions (15) can be formally written as

$$\theta\mapsto\int_\Omega\frac12\mathbb{K}(z_\tau^k,c_\tau^k,\theta_\tau^{k-1})\nabla\theta{\cdot}\nabla\theta+\frac1\tau\widehat{C}_{\mathrm{v}}(\theta)-\Big(\widetilde{r}_\tau^k{+}\frac{\vartheta_\tau^{k-1}}{\tau}\Big)\theta\,\mathrm{d}x-\int_\Gamma h_{\mathrm{B},\tau}^k\theta\,\mathrm{d}S \tag{17c}$$

with $\widehat{C}_{\mathrm{v}}$ a primitive function of $\widehat{C}_{\mathrm{v}}$. Alternatively, the potential (17a) can be constructed by a linear operator $(\dot c,j)\mapsto\mu$ with $\mu\in H^1_{\equiv}(\Omega)$ the (unique) weak solution of the boundary-value problem $-\mathrm{div}(\mathbb{M}\nabla\mu)=\dot c$ on Ω and $\mathbb{M}\nabla\mu{\cdot}\nu=j$ on Γ acting on a linear subspace satisfying $\int_\Omega\dot c\,\mathrm{d}x=\int_\Gamma j\,\mathrm{d}S$ in the sense of distributions.

After an additional spatial discretisation, it leads to linear algebraic systems or a quadratic-programming problem with box constraints, so the devised scheme is presumably very easy to implement and allows for relatively fine space/time discretisation. On the other hand, (13e) has its right-hand side in $L^1(\Omega)$ which prevents a simple usage of the direct method of the calculus of variations and (17c) is to be understood indeed only formally on our space-continuous level because the infimum of (17c) is $-\infty$ whenever $\widetilde{r}_\tau^k\in L^1(\Omega)\setminus H^1(\Omega)^*$, cf. e.g. [47, Exercise 3.42].

Let us summarize the assumptions needed for all the results below, although the following two propositions hold under slightly weaker assumptions too:

$$\mathbb{C},\mathbb{D}\in\mathbb{R}^{d\times d\times d\times d}\text{ positive definite},\quad\varrho>0,\quad a_0>0,\quad\varkappa>0, \tag{18a}$$
$$\mathbb{M},\mathbb{K}:\mathbb{R}^3\to\mathbb{R}^{d\times d}\text{ uniformly positive definite, bounded, and continuous}, \tag{18b}$$
$$\kappa\ge0,\quad M\ge0,\quad\kappa M>0,\quad\beta\in\mathbb{R},\quad a_1:\mathbb{R}\to\mathbb{R}\text{ bounded and continuous}, \tag{18c}$$
$$c_{\mathrm{v}}:\mathbb{R}\to\mathbb{R}\text{ bounded, continuous, and uniformly positive, i.e. }\inf c_{\mathrm{v}}(\cdot)>0, \tag{18d}$$
$$g\in L^2(I;L^{2^{*\prime}}(\Omega;\mathbb{R}^d)),\qquad f\in L^2(I;L^{2^{\sharp\prime}}(\Gamma;\mathbb{R}^d)), \tag{18e}$$
$$j_{\mathrm{B}}\in L^2(I;L^{2^{\sharp\prime}}(\Gamma)),\qquad h_{\mathrm{B}}\in L^1(I{\times}\Gamma), \tag{18f}$$
$$u_0\in H^1(\Omega;\mathbb{R}^d),\quad v_0\in L^2(\Omega;\mathbb{R}^d),\quad c_0\in H^1(\Omega),$$
$$z_0\in H^1(\Omega),\quad 0\le z_0\le1,\quad\theta_0\in L^1(\Omega),\quad\theta_0\ge0. \tag{18g}$$

Let us comment that the qualification of (18d) is simplified in contrast to e.g. [46,47,50,51], because we do not consider here any adiabatic heat sources or the dependence of c_{v} also on non-thermal variables, which would then need sophisticated interpolation estimates and a certain growth of c_{v}.

Proposition 1 (Existence of a solution to (13)–(15))**.** *Let (18) hold. For any $k=1,...,T/\tau$, the partly decoupled boundary-value problem (13)–(15) possesses a unique weak (or distributional) solution $u_\tau^k,v_\tau^k\in H^1(\Omega;\mathbb{R}^d)$, $z_\tau^k,c_\tau^k\in H^1(\Omega)$, and $\theta_\tau^k\in W^{1,p}(\Omega)$ with any $1\le p<d'=d/(d{-}1)$. Moreover,*

$$-1\le z_\tau^k(x)\le1\quad\text{and}\quad\theta_\tau^k(x)\ge0\qquad\text{for a.a. }x\in\Omega. \tag{19}$$

Let us comment that the negative lower bound on z_τ^k in (19) is quite unexpected and it would not occur if the backward Euler method would be used. It indicates that there is a price to be paid for having energy conservation and thus possible spurious time-oscillations created by the Crank-Nicolson scheme. Anyhow, the mid-point values $z_\tau^{k-1/2}$ still satisfy the expected constraint, namely $z_\tau^{k-1/2}\ge 0$.

Let us also emphasize that, quite naturally and expectedly, the uniqueness of the discrete solution will not be inherited by the limiting continuous solution where selection of various converging subsequences for $\tau\to 0$ may give different solutions and, on top of it, there might be solutions (1)-(2)-(3) not attainable by our discrete scheme. Anyhow, the uniqueness of the discrete solution as far as temperature will play a certain role in the proof of the a-priori estimate (28f) below.

Sketch of the proof of Proposition 1. The conventional weak solution $(u_\tau^k,v_\tau^k,c_\tau^k)$ to the boundary-value problem (13a,b,d)–(15a,b) is by the direct method when realizing that these problems have a single (quadratic strictly convex convex) potential (17a).

Also the variational inequality arising from the boundary-value problem for the inclusion (13c) with the boundary condition from (15a) possesses an underlying potential $\mathscr{E}(u_\tau^k,\cdot,c_\tau^k)$ which is strictly convex and quadratic, and coercive on $H^1(\Omega)$ with the convex constraint coming from the dissipation, cf. (17b). We further use the qualification $z_0\ge 0$ in (18g) and the unidirectional evolution together with the maximum principle. Then, from (13c) for $k=1$, we obtain both $z_\tau^1\le z_\tau^0=z_0\le 1$ and also $z_\tau^{1/2}:=\frac12 z_\tau^1+\frac12 z_\tau^0\ge 0$, i.e. $z_\tau^1\ge -z_\tau^0\ge -1$. For $k=2$, we then obtain similarly $z_\tau^2\le z_\tau^1\le 1$ and $z_\tau^{3/2}:=\frac12 z_\tau^2+\frac12 z_\tau^1\ge 0$, i.e. $z_\tau^2\ge -z_\tau^1\ge -1$. We can then proceed recursively for $k=3,...,T/\tau$, obtaining the bound of z_τ^k in (19). Note that, in particular, the term $(z_\tau^{k-1/2})^2\mathbb{C}e(u_\tau){:}e(u_\tau)$ is integrable. Note also that for the lower bound on z_τ^k, we have counted on the fact that the driving force for damage evolution vanishes when $z_\tau^{k-1/2}\searrow 0$.

As for a distributional solution to (13e)–(15c), we use the L^1-theory for the heat equation; let us emphasize that one cannot use the standard theory of weak solutions because $\widetilde r_\tau^k\in L^1(\Omega)$ does not belong to $H^1(\Omega)^*$ in general. If $c_{\rm v}$ is constant, by the classical Stampacchia [57] transposition method, this linear boundary-value problem has a unique variational solution θ which belongs to $W^{1,p}(\Omega)$ with any $1\le p<d'$. In the general case when $c_{\rm v}$ depends on θ, one can modify it for the semi-linear equation by using the compact embedding in the term $C_{\rm v}(\cdot)$ and its growth restriction; here $C_{\rm v}$ has at most linear growth due to (18d) but even a slower than $d/(d{-}2)$-polynomial growth would suffice, cf. also [47, Prop. 3.31]. We refer to [6,7] which even allows for measure-valued data, although here on the discrete level all right-hand sides are even absolutely continuous. The bound of θ_τ^k in (19) follows from the maximum principle recursively from $\theta_0\ge 0$ assumed in (18g). □

Proposition 2 (Energy conservation)**.** *Let (18) hold. For any $1\le l\le T/\tau$, the following discrete analog of the chemo-mechanical energy balance (4) holds:*

$$\mathscr{T}(v_\tau^l)+\mathscr{E}(u_\tau^l,z_\tau^l,c_\tau^l)+\tau\sum_{k=1}^{l}\mathscr{R}\Big(z_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1};v_\tau^{k-1/2},\frac{z_\tau^k-z_\tau^{k-1}}{\tau},\mu_\tau^{k-1/2}\Big)$$
$$=\mathscr{T}(v_0)+\mathscr{E}(u_0,z_0,c_0)+\tau\sum_{k=1}^{l}\big\langle\mathscr{F}_\tau^k,\big(v_\tau^{k-1/2},\mu_\tau^{k-1/2}\big)\big\rangle \tag{20}$$

with $\mathscr{F}_\tau^k=\tau^{-1}\int_{(k-1)\tau}^{k\tau}\mathscr{F}(t)\,{\rm d}t$. Moreover, denoting $\mathscr{H}_\tau^k=\tau^{-1}\int_{(k-1)\tau}^{k\tau}\mathscr{H}(t)\,{\rm d}t$, also the discrete analog of the total energy conservation (6) holds:

$$\mathscr{T}(v_\tau^l)+\mathscr{E}(u_\tau^l,z_\tau^l,c_\tau^l)+\mathscr{C}(\theta_\tau^l)=\mathscr{T}(v_0)+\mathscr{E}(u_0,z_0,c_0)$$
$$+\mathscr{C}(\theta_0)+\tau\sum_{k=1}^{l}\Big(\mathscr{H}_\tau^k+\big\langle\mathscr{F}_\tau^k,\big(v_\tau^{k-1/2},\mu_\tau^{k-1/2}\big)\big\rangle\Big). \tag{21}$$

Proof. First, we test (13b) by $v_\tau^{k-1/2}$ and at suitable places substitute also $v_\tau^{k-1/2}=\frac1\tau(u_\tau^k{-}u_\tau^{k-1})$ due to (13a) and further test (13d) by $\mu_\tau^{k-1/2}$. After using Green's formula together with the boundary conditions and summation, we obtain the equality

$$\frac{\mathscr{T}(v_\tau^k)-\mathscr{T}(v_\tau^{k-1})}{\tau}+\frac{\mathscr{E}(u_\tau^k,z_\tau^{k-1},c_\tau^k)-\mathscr{E}(u_\tau^{k-1},z_\tau^{k-1},c_\tau^{k-1})}{\tau}$$
$$+\int_\Omega(\varepsilon^2{+}(z_\tau^{k-1})^2)\mathbb{D}e(v_\tau^{k-1/2}){:}e(v_\tau^{k-1/2})$$
$$+\mathbb{M}(z_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1})\nabla\mu_\tau^{k-1/2}{\cdot}\nabla\mu_\tau^{k-1/2}\,{\rm d}x=\big\langle\mathscr{F}_\tau^k,\big(v_\tau^{k-1/2},\mu_\tau^{k-1/2}\big)\big\rangle \tag{22}$$

where we used the structural assumption that both $\mathscr{T}$ and $\mathscr{E}(\cdot,z,\cdot)$ are quadratic. More specifically, for (22), we used the following five bi-nomial formulas:

$$\frac{v_\tau^k-v_\tau^{k-1}}{\tau}\cdot v_\tau^{k-1/2}=\frac{v_\tau^k-v_\tau^{k-1}}{\tau}\cdot\frac{v_\tau^k+v_\tau^{k-1}}{2}=\frac{1}{\tau}\Big(\frac{1}{2}|v_\tau^k|^2-\frac{1}{2}|v_\tau^{k-1}|^2\Big), \tag{23a}$$

$$\begin{aligned}(\varepsilon^2{+}(z_\tau^{k-1})^2)\mathbb{C}e(u_\tau^{k-1/2}){:}e(v_\tau^{k-1/2})&=(\varepsilon^2{+}(z_\tau^{k-1})^2)\mathbb{C}e\Big(\frac{u_\tau^k{+}u_\tau^{k-1}}{2}\Big){:}e\Big(\frac{u_\tau^k{-}u_\tau^{k-1}}{\tau}\Big)\\&=\frac{1}{\tau}\Big(\frac{\varepsilon^2{+}(z_\tau^{k-1})^2}{2}\mathbb{C}e(u_\tau^k){:}e(u_\tau^k)-\frac{\varepsilon^2{+}(z_\tau^{k-1})^2}{2}\mathbb{C}e(u_\tau^{k-1}){:}e(u_\tau^{k-1})\Big),\end{aligned} \tag{23b}$$

$$\begin{aligned}\frac{c_\tau^k{-}c_\tau^{k-1}}{\tau}\kappa\Big(\frac{c_\tau^{k-1/2}}{c_{\rm E}}-1\Big)&=\frac{c_\tau^k{-}c_\tau^{k-1}}{\tau}\kappa\Big(\frac{c_\tau^k{+}c_\tau^{k-1}}{2c_{\rm E}}-1\Big)\\&=\frac{\kappa}{\tau}\Big(\frac{(c_\tau^k)^2}{2c_{\rm E}}-\frac{(c_\tau^{k-1})^2}{2c_{\rm E}}-c_\tau^k+c_\tau^{k-1}\Big)\\&=\frac{1}{\tau}\Big(\frac{\kappa}{2c_{\rm E}}(c_\tau^k{-}c_{\rm E})^2-\frac{\kappa}{2c_{\rm E}}(c_\tau^{k-1}{-}c_{\rm E})^2\Big),\end{aligned} \tag{23c}$$

$$\begin{aligned}&\beta M(\beta{\rm tr}\,e(u_\tau^{k-1/2}){-}c_\tau^{k-1/2}){\rm tr}\,e(v_\tau^{k-1/2})+\frac{c_\tau^k{-}c_\tau^{k-1}}{\tau}\big(Mc_\tau^{k-1/2}-\beta M{\rm tr}\,e(u_\tau^{k-1/2})\big)\\&\quad=\beta M\Big(\beta{\rm tr}\,e\Big(\frac{u_\tau^k{+}u_\tau^{k-1}}{2}\Big)-\frac{c_\tau^k{+}c_\tau^{k-1}}{2}\Big){\rm tr}\,e\Big(\frac{u_\tau^k{-}u_\tau^{k-1}}{\tau}\Big)\\&\qquad+\frac{c_\tau^k{-}c_\tau^{k-1}}{\tau}\Big(M\frac{c_\tau^k{+}c_\tau^{k-1}}{2}-\beta M{\rm tr}\,e\Big(\frac{u_\tau^k{+}u_\tau^{k-1}}{2}\Big)\Big)\\&\quad=\frac{1}{\tau}\Big(\frac{M}{2}\big(\beta{\rm tr}\,e(u_\tau^k)-c_\tau^k\big)^2-\frac{M}{2}\big(\beta{\rm tr}\,e(u_\tau^{k-1})-c_\tau^{k-1}\big)^2\Big),\end{aligned} \tag{23d}$$

$$\varkappa\nabla c_\tau^{k-1/2}{\cdot}\nabla\frac{c_\tau^k{-}c_\tau^{k-1}}{\tau}=\varkappa\nabla\frac{c_\tau^k{+}c_\tau^{k-1}}{2}{\cdot}\nabla\frac{c_\tau^k{-}c_\tau^{k-1}}{\tau}=\frac{1}{\tau}\Big(\frac{\varkappa}{2}|\nabla c_\tau^k|^2-\frac{\varkappa}{2}|\nabla c_\tau^{k-1}|^2\Big). \tag{23e}$$

Then we test (13c) by $\frac{1}{\tau}(z_\tau^k{-}z_\tau^{k-1})$. After using the following two binomial formulas

$$\begin{aligned}z_\tau^{k-1/2}\Big(\frac{a_0}{2\varepsilon}+\mathbb{C}e(u_\tau^k){:}e(u_\tau^k)\Big)\frac{z_\tau^k{-}z_\tau^{k-1}}{\tau}&=\frac{z_\tau^k{+}z_\tau^{k-1}}{2}\Big(\frac{a_0}{2\varepsilon}+\mathbb{C}e(u_\tau^k){:}e(u_\tau^k)\Big)\frac{z_\tau^k{-}z_\tau^{k-1}}{\tau}\\&=\frac{1}{\tau}\Big(\frac{a_0}{2\varepsilon}+\mathbb{C}e(u_\tau^k){:}e(u_\tau^k)\Big)\Big(\frac{1}{2}(z_\tau^k)^2-\frac{1}{2}(z_\tau^{k-1})^2\Big),\end{aligned} \tag{24a}$$

$$\begin{aligned}2a_0\varepsilon\nabla z_\tau^{k-1/2}{\cdot}\nabla\frac{z_\tau^k{-}z_\tau^{k-1}}{\tau}&=2a_0\varepsilon\nabla\frac{z_\tau^k{+}z_\tau^{k-1}}{2}\cdot\nabla\frac{z_\tau^k{-}z_\tau^{k-1}}{\tau}\\&=\frac{1}{\tau}\big(a_0\varepsilon|\nabla z_\tau^k|^2-a_0\varepsilon|\nabla z_\tau^{k-1}|^2\big),\end{aligned} \tag{24b}$$

we obtain

$$\frac{\mathscr{E}(u_\tau^k,z_\tau^k,c_\tau^k)-\mathscr{E}(u_\tau^k,z_\tau^{k-1},c_\tau^k)}{\tau}-\int_\Omega\frac{a(\theta_\tau^{k-1})}{2\varepsilon}\,\frac{z_\tau^k{-}z_\tau^{k-1}}{\tau}\,{\rm d}x=0. \tag{25}$$

In fact, the difference $\mathscr{E}(u_\tau^k,z_\tau^k,c_\tau^k)-\mathscr{E}(u_\tau^k,z_\tau^{k-1},c_\tau^k)$ does not even depend on c_τ^k at all. Summing (22) and (25), we can exploit the cancellation of the terms $\pm\mathscr{E}(u_\tau^k,z_\tau^{k-1},c_\tau^k)$ and, after summing it from $k=1,...,l\le T/\tau$, we obtain (20). When testing (13e) by 1, we obtain

$$\mathscr{C}(\theta_\tau^k)=\mathscr{C}(\theta_\tau^{k-1})+\mathscr{R}\Big(z_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1};v_\tau^{k-1/2},\frac{z_\tau^k{-}z_\tau^{k-1}}{\tau},\mu_\tau^{k-1/2}\Big)+\mathscr{H}_\tau^k.$$

Adding it to (20), the $\mathscr{R}$-terms cancel and we eventually obtain also (21). □

Considering $\{u_\tau^k\}_{k=0,...,K}$ with $K=T/\tau$, we introduce a notation for the piecewise-constant and the piecewise affine interpolants defined respectively by

$$\overline{u}_\tau(t)=u_\tau^k,\qquad \underline{u}_\tau(t)=u_\tau^{k-1},\qquad \overline{\underline{u}}_\tau(t)=u_\tau^{k-1/2},\qquad\text{and} \tag{26a}$$

$$u_\tau(t)=\frac{t-(k{-}1)\tau}{\tau}u_\tau^k+\frac{k\tau-t}{\tau}u_\tau^{k-1}\qquad\text{for }(k{-}1)\tau<t\le k\tau. \tag{26b}$$

The symbols v_τ, $\overline{v}_\tau$, $\underline{v}_\tau$, c_τ, etc., have analogous meanings. In this notation, we can write (13) in a "compact" form closer to (1):

$$\dot{u}_\tau = \underline{\overline{v}}_\tau, \tag{27a}$$

$$\varrho\dot{v}_\tau - \operatorname{div}\widetilde{\sigma}_\tau = \overline{g}_\tau \quad \text{with} \quad \widetilde{\sigma}_\tau = (\varepsilon^2{+}\underline{z}_\tau^2)\big(\mathbb{D}e(\underline{\overline{v}}_\tau) + \mathbb{C}e(\underline{\overline{u}}_\tau)\big) + \beta M(\beta\operatorname{tr} e(\underline{\overline{u}}_\tau){-}\underline{\overline{c}}_\tau)\mathbb{I}, \tag{27b}$$

$$N_{\{\dot{z}\le 0\}}(\dot{z}_\tau) + \frac{a_0}{2\varepsilon}\underline{\overline{z}}_\tau + \underline{\overline{z}}_\tau\mathbb{C}e(\overline{u}_\tau){:}e(\overline{u}_\tau) - 2a_0\varepsilon\Delta\underline{\overline{z}}_\tau \ni \frac{a}{2\varepsilon}, \tag{27c}$$

$$\dot{c}_\tau = \operatorname{div}\big(\mathbb{M}(\underline{z}_\tau, \underline{c}_\tau, \underline{\theta}_\tau)\nabla\underline{\overline{\mu}}_\tau\big) \quad \text{with } \underline{\overline{\mu}}_\tau = \Big(M{+}\frac{\kappa}{c_{\rm E}}\Big)\underline{\overline{c}}_\tau - \beta M\operatorname{tr} e(\underline{\overline{u}}_\tau) - \kappa - \varkappa\Delta\underline{\overline{c}}_\tau, \tag{27d}$$

$$\dot{\vartheta}_\tau - \operatorname{div}\big(\mathbb{K}(\overline{z}_\tau, \overline{c}_\tau, \underline{\theta}_\tau)\nabla\overline{\theta}_\tau\big) = \widetilde{r}_\tau \quad \text{with } \overline{\vartheta}_\tau = C_{\rm v}(\overline{\theta}_\tau) \text{ and with } \widetilde{r}_\tau = r\big(\underline{z}_\tau, \underline{c}_\tau, \underline{\theta}_\tau; e(\underline{\overline{v}}_\tau), \dot{z}_\tau, \nabla\underline{\overline{\mu}}_\tau\big), \tag{27e}$$

where ϑ_τ is the piecewise affine interpolant corresponding to $\overline{\vartheta}_\tau$. Of course, (27) is to be supplemented by the boundary conditions (15) written analogously "compactly", involving $\overline{f}_\tau$, $\overline{j}_{{\rm B},\tau}$, and $\overline{h}_{{\rm B},\tau}$.

4. **Numerical stability and convergence.** Besides existence of discrete solutions and energy conservation proved in Propositions 1–2, another important attribute of the discretisation scheme is its numerical stability in the sense that it complies with certain a-priori estimates:

Proposition 3 (A-priori estimates)**.** *Let again (18) hold. Then the following estimates hold with C and C_p independent of τ:*

$$\|u_\tau\|_{H^1(I;H^1(\Omega;\mathbb{R}^d))} \le C \quad \textit{and} \quad \|\dot{u}_\tau\|_{{\rm BV}(I;H^1(\Omega;\mathbb{R}^d)^*)} \le C, \tag{28a}$$

$$\|v_\tau\|_{L^\infty(I;L^2(\Omega;\mathbb{R}^d))\,\cap\, L^2(I;H^1(\Omega;\mathbb{R}^d))\,\cap\, H^1(I;H^1(\Omega;\mathbb{R}^d)^*)} \le C, \tag{28b}$$

$$\|z_\tau\|_{L^\infty(I;H^1(\Omega))\,\cap\, L^\infty(I\times\Omega)\,\cap\, W^{1,1}(I;L^1(\Omega))} \le C, \tag{28c}$$

$$\|c_\tau\|_{L^\infty(I;H^1(\Omega))\,\cap\, H^1(I;H^1(\Omega)^*)} \le C \quad \textit{and} \quad \|\Delta c_\tau\|_{L^\infty(I;L^2(\Omega))} \le C, \tag{28d}$$

$$\|\mu_\tau\|_{L^\infty(I;L^2(\Omega))\,\cap\, L^2(I;H^1(\Omega))} \le C, \tag{28e}$$

$$\|\theta_\tau\|_{L^\infty(I;L^1(\Omega))} \le C \quad \textit{and} \quad \|\nabla\theta_\tau\|_{L^r(I\times\Omega;\mathbb{R}^d)} \le C_p \quad \textit{for any} \quad r < \frac{d{+}2}{d{+}1}, \tag{28f}$$

$$\|\vartheta_\tau\|_{L^\infty(I;L^1(\Omega))\,\cap\, W^{1,1}(I;H^{(d+3)/2}(\Omega)^*)} \le C. \tag{28g}$$

Sketch of the proof. First, we use the discrete chemo-mechanical energy balance (20) to obtain the first $L^\infty(I)$-estimates in (28b-d) from the uniform bound on the stored energy $\mathscr{E}$ and further the $L^2(I)$-estimate in (28b) and also the estimate of $\nabla\mu_\tau$ in $L^2(I{\times}\Omega;\mathbb{R}^d)$ from the overall dissipated-energy bound. The right-hand side of (20) is to be treated by Young's inequality with the help of the assumptions (18e,f) on g, f, and $j_{\rm B}$ and the uniform quadratic coercivity of $\mathscr{R}(z,c,\theta;\cdot,\cdot,\cdot)$, as well as the Young inequality for estimation of

$$\int_\Gamma j_{{\rm B},\tau}^k\mu_\tau^{k-1/2}\,{\rm d}S \le \|j_{{\rm B},\tau}^k\|_{L^2(\Gamma)}^2/\varepsilon + \varepsilon\|\mu_\tau^{k-1/2}\|_{L^2(\Gamma)}^2 \le \|j_{{\rm B},\tau}^k\|_{L^2(\Gamma)}^2/\varepsilon + \varepsilon N_\Gamma\|\mu_\tau^{k-1/2}\|_{L^2(\Omega)}^2 + \varepsilon N_\Gamma\|\nabla\mu_\tau^{k-1/2}\|_{L^2(\Omega;\mathbb{R}^d)}^2$$

with N_Γ the norm of the trace operator $H^1(\Omega)\to L^2(\Gamma)$; note that the last term can be absorbed by the dissipation potential when choosing $\varepsilon>0$ small while $\|\mu_\tau^{k-1/2}\|_{L^2(\Omega)}^2$ can be estimated by $\|c_\tau^{k-1/2}\|_{L^2(\Omega)}^2+\|\operatorname{tr} e(u_\tau^{k-1/2})\|_{L^2(\Omega)}^2$ and then handled by a discrete Gronwall inequality. Eventually, we thus get also the L^∞-estimate in (28e). Combining it with the mentioned $\nabla\mu_\tau$-estimate, we obtain the second estimate in (28e), too. Then, from the L^∞-estimates (28a,d,e) and from knowing that $\varkappa\Delta\underline{\overline{c}}_\tau = (M{+}\kappa/c_{\rm E})\underline{\overline{c}}_\tau - \beta M\operatorname{tr} e(\underline{\overline{u}}_\tau) - \kappa - \varkappa\Delta\underline{\overline{c}}_\tau - \underline{\overline{\mu}}_\tau$, we deduce the last estimate in (28d).

We now know the bound of $\widetilde{\sigma}_\tau$ from (27b) in $L^2(I;L^2(\Omega;\mathbb{R}^{d\times d}))$ and thus, by comparison, from (27b) we obtain $\varrho\dot{v}_\tau$ bounded in $L^2(I;H^1(\Omega;\mathbb{R}^d)^*)$, i.e. the last estimate in (28b). This yields immediately the bound of $\dot{v}_\tau$ in $L^1(I;H^1(\Omega;\mathbb{R}^d)^*)$ and, using (27a), $\ddot{u}_\tau$ is bounded as a measure in ${\rm Meas}(I;H^1(\Omega;\mathbb{R}^d)^*)$. Thus the second estimate in (28a) is achieved. By comparison, we also obtain the H^1-estimate in (28d).

The $L^\infty(I{\times}\Omega)$-estimate in (28c) follows from the already proved bound (19). The $W^{1,1}$-estimate in (28c) is then a simple consequence of the constraint $\dot{z}_\tau\le 0$ together with the mentioned bound (19).

Then, using also (21), we obtain the $L^\infty(I)$-estimates in (28e,f); in particular, the estimate of $\overline{\theta}_\tau$ in $L^\infty(I;L^1(\Omega))$ is to be shown for executing the test of (27e) by 1 by exploiting also the nonnegativity of

$\overline{\theta}_\tau$ proved already in (19). Furthermore, the L^r-estimate in (28f) needs a sophisticated non-linear test of the heat equation together with a function-space interpolation by the Gagliardo-Nirenberg inequality. More specifically, knowing already that $\overline{\theta}_\tau \in L^\infty(I;L^1(\Omega))$, we test (27e) by $\chi(\overline{\theta}_\tau)$ with an increasing nonlinear function $\chi:[0,+\infty)\to[0,1]$ defined as $\chi(w):=1-(1{+}w)^{-\epsilon}$ with $\epsilon>0$; this test was essentially proposed by E. Feireisl and J. Málek [17], simplifying the original idea of L. Boccardo and T. Gallouët [6]. First, take $1\le r<2$ and estimate the L^r-norm by Hölder's inequality as

$$\begin{aligned}\int_{I\times\Omega}|\nabla\overline{\theta}_\tau|^r\,\mathrm{d}x\mathrm{d}t&=\int_{I\times\Omega}(1+\overline{\theta}_\tau)^{(1+\epsilon)r/2}\frac{|\nabla\overline{\theta}_\tau|^r}{(1+\overline{\theta}_\tau)^{(1+\epsilon)r/2}}\,\mathrm{d}x\mathrm{d}t\\&\le\bigg(\int_{I\times\Omega}(1{+}\overline{\theta}_\tau)^{(1+\epsilon)r/(2-r)}\,\mathrm{d}x\mathrm{d}t\bigg)^{1-r/2}\bigg(\int_{I\times\Omega}\frac{|\nabla\overline{\theta}_\tau|^2}{(1{+}\overline{\theta}_\tau)^{1+\epsilon}}\,\mathrm{d}x\mathrm{d}t\bigg)^{r/2}\\&=C_{\epsilon,r,T}\bigg(\int_0^T\big\|1+\overline{\theta}_\tau(t,\cdot)\big\|_{L^{(1+\epsilon)r/(2-r)}(\Omega)}^{(1+\epsilon)r/(2-r)}\,\mathrm{d}t\bigg)^{1-r/2}L_\epsilon(\overline{\theta}_\tau)^{r/2}\end{aligned}\tag{29}$$

with a constant $C_{\epsilon,r,T}$ dependent on ϵ, r, and T, and with the shorthand notation $L_\epsilon(\theta):=\int_{I\times\Omega}|\nabla\theta|^2/(1{+}\theta)^{1+\epsilon}\,\mathrm{d}x\mathrm{d}t$. Then, with the Gagliardo-Nirenberg inequality, we interpolate the Lebesgue space $L^{(1+\epsilon)r/(2-r)}(\Omega)$ between the spaces $W^{1,r}(\Omega)$ and $L^1(\Omega)$ and in order to exploit the already obtained estimate in $L^\infty(I;L^1(\Omega))$. More in detail, we estimate

$$\big\|1{+}\overline{\theta}_\tau(t,\cdot)\big\|_{L^{(1+\epsilon)r/(2-r)}(\Omega)}\le C_\lambda C_0^{1-\lambda}\Big(C_0+\big\|\nabla\overline{\theta}_\tau(t,\cdot)\big\|_{L^r(\Omega;\mathbb{R}^d)}\Big)^\lambda\tag{30}$$

with $C_0=\mathrm{meas}_d(\Omega){+}C$ with C from the former estimate in (28f) and C_λ from the mentioned Gagliardo-Nirenberg inequality with the weight $0<\lambda<1$; here we choose an optimal weight $\lambda:=(2-r)/(1+\epsilon)$ which leads to the highest possible restriction on r as stated in (28f). Then we can continue in the estimation of (29) as follows:

$$\begin{aligned}&\int_0^T\big\|1+\overline{\theta}_\tau(t,\cdot)\big\|_{L^{(1+\epsilon)r/(2-r)}(\Omega)}^{(1+\epsilon)r/(2-r)}\,\mathrm{d}t\\&\quad\le\int_0^T C_\lambda^{(1+\epsilon)r/(2-r)}C_0^{(1-\lambda)(1+\epsilon)r/(2-r)}\Big(C_0{+}\big\|\nabla\overline{\theta}_\tau(t,\cdot)\big\|_{L^r(\Omega;\mathbb{R}^d)}\Big)^{\lambda(1+\epsilon)r/(2-r)}\mathrm{d}t\\&\quad\le\int_0^T C_\lambda^{(1+\epsilon)r/(2-r)}C_0^{(1-\lambda)(1+\epsilon)r/(2-r)}\Big(C_0{+}\big\|\nabla\overline{\theta}_\tau(t,\cdot)\big\|_{L^r(\Omega;\mathbb{R}^d)}\Big)^r\,\mathrm{d}t\\&\quad=C_1+C_2\int_{I\times\Omega}\big|\nabla\overline{\theta}_\tau\big|^r\,\mathrm{d}x\mathrm{d}t.\end{aligned}\tag{31}$$

Furthermore, we estimate $L_\epsilon(\overline{\theta}_\tau)$ in (29). Let us denote by X the primitive function of $\chi\circ C_\mathrm{v}^{-1}$ with the mentioned nonlinearity $\chi(w):=1-(1{+}w)^{-\epsilon}$ such that $X(0)=0$. Realizing that $\chi'(w)=\epsilon/(1{+}w)^{1+\epsilon}$ and denoting $\kappa_0:=\inf\min_{g\in\mathbb{R}^d}\mathbb{K}(\cdot,\cdot,\cdot)g{\cdot}g>0$, we get

$$\begin{aligned}L_\epsilon(\overline{\theta}_\tau)&=\int_{I\times\Omega}\frac{\chi'(\overline{\theta}_\tau)|\nabla\overline{\theta}_\tau|^2}{\epsilon}\,\mathrm{d}x\mathrm{d}t\le\int_{I\times\Omega}\frac{\chi'(\overline{\theta}_\tau)\mathbb{K}(\overline{z}_\tau,\overline{c}_\tau,\underline{\theta}_\tau)\nabla\overline{\theta}_\tau{\cdot}\nabla\overline{\theta}_\tau}{\kappa_0\epsilon}\,\mathrm{d}x\mathrm{d}t\\&=\int_{I\times\Omega}\frac{\mathbb{K}(\overline{z}_\tau,\overline{c}_\tau,\underline{\theta}_\tau)\nabla\overline{\theta}_\tau{\cdot}\nabla\chi(\overline{\theta}_\tau)}{\kappa_0\epsilon}\,\mathrm{d}x\mathrm{d}t\\&\le\frac{1}{\kappa_0\epsilon}\bigg(\int_{I\times\Omega}\mathbb{K}(\overline{z}_\tau,\overline{c}_\tau,\underline{\theta}_\tau)\nabla\overline{\theta}_\tau\cdot\nabla\chi(\overline{\theta}_\tau)\,\mathrm{d}x\mathrm{d}t+\int_\Omega X(\overline{\theta}_\tau(T,\cdot))\,\mathrm{d}x\bigg)\\&\le\frac{1}{\kappa_0\epsilon}\bigg(\int_\Omega X(\theta_0)\,\mathrm{d}x+\int_{I\times\Gamma}\overline{h}_{\mathrm{B},\tau}\chi(\overline{\theta}_\tau)\,\mathrm{d}S\mathrm{d}t+\int_{I\times\Omega}\widetilde{r}_\tau\chi(\overline{\theta}_\tau)\,\mathrm{d}x\mathrm{d}t\bigg)\\&\le\frac{1}{\kappa_0\epsilon}\Big(\big\|C_\mathrm{v}(\theta_0)\big\|_{L^1(\Omega)}+\big\|\overline{h}_{\mathrm{B},\tau}\big\|_{L^1(I\times\Gamma)}+\big\|\widetilde{r}_\tau\big\|_{L^1(I\times\Omega)}\Big)\,.\end{aligned}\tag{32}$$

The equation (27e) tested by $\chi(\overline{\theta}_\tau)$ has been used for the penultimate inequality, exploiting also that X is convex because both χ and C_v^{-1} are increasing. Joining (29) with (32) and with (31) gives the estimate of the type $\|\nabla\bar{\theta}_\tau\|_{L^r(Q;\mathbb{R}^d)}^r/(1{+}\|\nabla\bar{\theta}_\tau\|_{L^r(Q;\mathbb{R}^d)}^{r(1-r/2)})\le C(1{+}\|\xi(\bar{\theta}_\tau)\|_{L^1(Q)})^{r/2}$, which gives the second estimate in (28f). Cf. e.g. [47, Sect. 12.1] for some more details. However, it should be emphasized that here the procedure (29)–(32) was only formal because we did not have granted $\overline{\theta}_\tau(t)\in H^1(\Omega)$ so that also $\chi(\overline{\theta}_\tau(t))$ does not need to live in $H^1(\Omega)$ and may not be a legitimate test function. This is because we did not regularize the heat equation in order to preserve the discrete energy conservation (21). Yet, the resulting estimate (28f) is correct. Hence, in addition to the standard argumentation, we should still make a regularization: only for this step, considering z_τ, c_τ, $\widetilde{r}_\tau$, $\overline{h}_{\mathrm{B},\tau}$, and θ_0 fixed, we regularize (27e) with corresponding boundary condition by considering $\widetilde{r}_\tau/(1{+}\varepsilon\widetilde{r}_\tau)$, $\overline{h}_{\mathrm{B},\tau}/(1{+}\varepsilon\overline{h}_{\mathrm{B},\tau})$, and $\theta_0/(1{+}\varepsilon\theta_0)$ with some $\varepsilon>0$ in place of by $\widetilde{r}_\tau$, $\overline{h}_{\mathrm{B},\tau}$, and θ_0, respectively. The corresponding solution $\theta_{\tau\varepsilon}$ is then valued in $H^1(\Omega)$ and all the estimates (29)–(32) are legitimate. Arriving thus to the estimate (28f) for $\overline{\theta}_{\tau\varepsilon}$ uniform with respect to ε, we can pass $\varepsilon\to 0$. The limit in $\overline{\vartheta}_{\tau\varepsilon}=C_{\rm v}(\overline{\theta}_{\tau\varepsilon})$ is to be done as in the proof of Proposition 4 but with τ fixed here. Notably, this limit solves the recursive semilinear equation (13e) and is therefore unique, so that this procedure is indeed legitimate for θ_τ considered in the desired estimate (28f).

Eventually, the estimate $\dot{\vartheta}_\tau\in L^1(I;H^{(d+3)/2}(\Omega)^*)$ in (28g) can be obtained by comparison, using that $H^{(d+3)/2}(\Omega)\subset W^{1,\infty}(\Omega)$. $\square$

Let us remark that, in contrast to [51], we have not used a regularization of the right-hand side r in (13e) to make it bounded in a better space than $L^1(I{\times}\Omega)$ which would here violate the energy conservation in the discrete scheme.

A final justification of the model is certainly the convergence as $\tau\to 0$ to a suitably defined weak solution to the continuous initial-boundary-value problem (12) with (2)–(3). This is a fairly nontrivial task. In the literature, such an analysis has been performed for such type of thermally coupled damage-diffusion models in [27] (where the chemical potential was augmented by the time derivative of c) and in [51] (where a regularization by an auxiliary phase field was adopted). The key point is a suitable definition of a weak solution, using the concept of energetic solution by A. Mielke et al. [36, 37, 39] for the rate-independent damage subsystem which is governed by the energy $\mathscr{E}(u,\cdot,c)$ which is convex and therefore this concept is reliable, efficient, and essentially equivalent to the conventional weak solution. In fact, the mentioned energetic-solution concept applies to purely rate-independent systems and its combination with rate-dependent phenomena has been devised in [45, 46], cf. also [37, Chap. 5].

Definition 1 (Weak solution to (1)-(2)-(3))**.** The quadruple (u,z,c,θ) is called a weak solution to the initial-boundary-value problem (1)-(2)-(3) if $u\in H^1(I;H^1(\Omega;\mathbb{R}^d))\cap C_{\rm weak}(I;L^2(\Omega;\mathbb{R}^d))$, $z\in L^\infty(I;H^1(\Omega))\cap \mathrm{BV}(I;L^1(\Omega))$, $c\in C_{\rm weak}(I;H^1(\Omega))$, $\theta\in C_{\rm weak}(I;L^{q_1}(\Omega))\cap L^p(I;W^{1,r}(\Omega))$ with r as in (28f), with μ from (1c) belonging to $L^2(I{\times}\Omega)$, with the measure $\dot{z}\in\mathrm{Meas}(I{\times}\overline{\Omega})$ the distributional time derivative of z, and with $\vartheta=C_{\rm v}(\theta)\in L^1(I{\times}\Omega)$, and:

$$\forall\,\tilde u\in H^1(I{\times}\Omega;\mathbb{R}^d)),\ \tilde u(T)=0:\quad \int_0^T\!\!\int_\Omega \sigma{:}e(\tilde u)-\varrho\dot u{\cdot}\dot{\tilde u}-g{\cdot}\tilde u\,\mathrm{d}x\mathrm{d}t$$
$$=\int_0^T\!\!\int_\Gamma f{\cdot}\tilde u\,\mathrm{d}S\mathrm{d}t+\int_\Omega\varrho v_0{\cdot}\tilde u(0)\,\mathrm{d}x,\qquad\text{with }\sigma\text{ from (1a)},\tag{33a}$$

$$\forall_{\rm a.a.}t\in I\ \forall\,\tilde z\in H^1(\Omega)\cap L^\infty(\Omega),\ \tilde z\le z(t)\text{ on }\Omega:$$
$$\int_\Omega z(t)^2\mathbb{C}e(u(t)){:}e(u(t))+\frac{a_0}{4\varepsilon}(1{-}z(t))^2+\varepsilon a_0|\nabla z(t)|^2\,\mathrm{d}x$$
$$\le\int_\Omega \tilde z^2\mathbb{C}e(u(t)){:}e(u(t))+\frac{a_0}{4\varepsilon}(1{-}\tilde z)^2+\varepsilon a_0|\nabla\tilde z|^2-\frac{a_1}{\varepsilon}(\tilde z{-}z(t))\,\mathrm{d}x,\tag{33b}$$

$$\forall\,\tilde\mu\in H^1(I{\times}\Omega),\ \tilde\mu(T)=0:$$
$$\int_0^T\!\!\int_\Omega\mathbb{M}(z,c,\theta)\nabla\mu{\cdot}\nabla\tilde\mu-c\dot{\tilde\mu}\,\mathrm{d}x\mathrm{d}t=\int_0^T\!\!\int_\Gamma j_{\rm B}\tilde\mu\,\mathrm{d}S\mathrm{d}t+\int_\Omega c_0{\cdot}\tilde\mu(0)\,\mathrm{d}x,\tag{33c}$$

$$\forall\,\tilde c\in L^2(I;H^1(\Omega)):$$
$$\int_0^T\!\!\int_\Omega\varkappa\nabla c{\cdot}\nabla\tilde c+\Big(\Big(M{+}\frac{\kappa}{c_{\rm E}}\Big)c-\beta M\,\mathrm{tr}\,e(u)-\kappa-\mu\Big)\tilde c\,\mathrm{d}x\mathrm{d}t=0,\tag{33d}$$

$$\forall\,\tilde\theta\in W^{1,\infty}(I{\times}\Omega),\ \tilde\theta(T)=0:\ \int_0^T\!\!\int_\Omega\mathbb{K}(z,c,\theta)\nabla\theta{\cdot}\nabla\tilde\theta-\vartheta\dot{\tilde\theta}\,\mathrm{d}x\mathrm{d}t$$
$$=\int_0^T\!\!\int_{\overline\Omega}\tilde\theta\big[r(z,c,\theta;e(\dot u),\dot z,\nabla\mu)\big](\mathrm{d}x\mathrm{d}t)$$
$$+\int_0^T\!\!\int_\Gamma h_{\rm B}\tilde\theta\,\mathrm{d}S\mathrm{d}t+\int_\Omega C_{\rm v}(\theta_0)\tilde\theta(0)\,\mathrm{d}x\tag{33e}$$

with the measure $r\in\mathrm{Meas}(I{\times}\overline{\Omega})$ from (1d), and the energy balance (6) holds for $t=T$ at least as an inequality, i.e.

$$\int_\Omega\frac{\varrho}{2}|\dot u(T)|^2+\varphi(e(u(T)),z(T),c(T),\nabla z(T),\nabla c(T))+C_{\rm v}(\theta(T))\,{\rm d}x$$
$$\le\int_0^T\!\!\int_\Omega g{\cdot}\dot u\,{\rm d}x{\rm d}t+\int_0^T\!\!\int_\Gamma f{\cdot}\dot u+j_{\rm B}\mu+h_{\rm B}\,{\rm d}S{\rm d}t$$
$$+\int_\Omega\frac{\varrho}{2}|v_0|^2+\varphi(e(u_0),z_0,c_0,\nabla z_0,\nabla c_0)+C_{\rm v}(\theta_0)\,{\rm d}x \tag{33f}$$

with φ from (5a), and also with the remaining initial condition $u(0)=u_0$ satisfied.

The inequality (33b) is called a semistability condition and, together with the energy inequality (33f), assembles the definition of the mentioned energetic solution, here built into the context of the other rate-dependent equations. In particular, this semistability replaces the global stability standardly used in energetic solutions. In fact, one can prove that (33f) holds even as an equality and, for smooth solutions, the damage flow rule (1b) holds a.e. on $I{\times}\Omega$.

Proposition 4 (Convergence for $\tau\to0$)**.** *Let (18) hold with $\mathbb{D}=\chi\mathbb{C}$ with some fixed relaxation-time constant $\chi>0$. Then there is a converging subsequence (denoted again by $\{(u_\tau,v_\tau,z_\tau,c_\tau,\theta_\tau)\}_{\tau>0}$ for simplicity) and its limit (u,v,z,c,θ) such that, for the corresponding interpolants $\overline{u}_\tau$, $\overline{v}_\tau$, $\overline{z}_\tau$, and $\underline{z}_\tau$, it holds*

$$u_\tau\to u \quad\text{weakly* in } H^1(I;H^1(\Omega;\mathbb{R}^d))\cap W^{1,\infty}(I;L^2(\Omega;\mathbb{R}^d)), \tag{34a}$$
$$\overline{u}_\tau\to u \quad\text{strongly in } L^2(I;H^1(\Omega;\mathbb{R}^d)), \tag{34b}$$
$$\overline{v}_\tau\to v \quad\text{strongly in } L^2(I;H^1(\Omega;\mathbb{R}^d))\ \text{ and}$$
$$\text{weakly* in } L^2(I;H^1(\Omega;\mathbb{R}^d))\cap L^\infty(I;L^2(\Omega;\mathbb{R}^d)), \tag{34c}$$
$$\overline{z}_\tau(t)\to z(t) \quad\text{weakly* in } H^1(\Omega)\cap L^\infty(\Omega) \text{ for all } t\in I, \tag{34d}$$
$$\underline{z}_\tau(t)\to z(t) \quad\text{weakly* in } H^1(\Omega)\cap L^\infty(\Omega) \text{ for a.a. } t\in I, \tag{34e}$$
$$\dot z_\tau\to\dot z \quad\text{weakly* in } \mathrm{Meas}(I{\times}\overline{\Omega}), \tag{34f}$$
$$c_\tau\to c \quad\text{weakly* in } L^\infty(I;H^1(\Omega)), \tag{34g}$$
$$\nabla\overline{\mu}_\tau\to\nabla\mu \quad\text{strongly in } L^2(I{\times}\Omega;\mathbb{R}^d), \tag{34h}$$
$$\theta_\tau\to\theta \quad\text{weakly in } L^p(I;W^{1,r}(\Omega))\ \text{ with any } r \text{ from (28f)} \tag{34i}$$

for $\tau\to0$, where $\overline{\mu}_\tau$ is from (27d) and μ from (1c). Moreover, $v=\dot u$ and the measure $\dot z$ in (34f) is the distributional time derivative of z, and every (u,z,c,θ) obtained by such a way is a weak solution according Definition 1.

Let us comment that the restriction $\mathbb{D}=\chi\mathbb{C}$ facilitates involving damage not only in the elastic but also in the whole visco-elastic response by using a fine algebraic manipulation. More specifically, introducing the auxiliary variable $w:=\chi v+u$, one can use a parabolic problem for this variable for proving strong convergence which, in turn, is needed for the limit passage in the dissipation energy in the heat-transfer equation.

Sketch of the proof of Proposition 4. We divide the proof into seven steps that are carefully assembled in a specific order.

Step 1: Selection of a convergent subsequence. By the Banach selection principle, we choose a subsequence converging weakly* in the topologies indicated in (28a-f) except the $W^{1,1}$-estimate in (28c) for which we use the Helly's selection principle. More specifically, we can select a subsequence such that (34e,f) holds; in particular (34e) holds for all instants t of continuity of z; recall that functions with bounded variations are continuous with the exception of at most a countable number of time instances. Later, we will also exploit that

$$u_\tau(T)\to u(T) \quad\text{weakly in } H^1(\Omega;\mathbb{R}^d), \tag{35a}$$
$$v_\tau(T)\to v(T) \quad\text{weakly in } L^2(\Omega;\mathbb{R}^d),\ \text{ and} \tag{35b}$$
$$c_\tau(T)\to c(T) \quad\text{weakly in } H^1(\Omega), \tag{35c}$$

which follows from the L^∞-estimates together with the information about the time derivatives (28a,b,d).

Step 2: Convergence in the force equilibrium and diffusion. The limit passage in the semilinear equation (27a,b) towards (12a,b) in the weak formulation (33a) as well as in the semilinear equation (27d) towards (12d) in the weak formulation (33c,d) is easily achievable by using the weak convergence from Step 1 together with the Aubin-Lions compactness theorem for the strong convergence $\mathbb{M}(\underline{z}_\tau,\underline{c}_\tau,\underline{\theta}_\tau)\to\mathbb{M}(z,c,\theta)$. More in detail, since we do not have any direct information about $\dot\theta_\tau$, we can first apply the Aubin-Lions theorem to ϑ_τ where we have time-derivative controlled, cf. (28g). To this goal, let us realize that $\nabla\vartheta_\tau=C_{\rm v}'(\theta_\tau)\nabla\theta_\tau=c_{\rm v}(\theta_\tau)\nabla\theta_\tau$ is estimated in $L^p(I\times\Omega;\mathbb{R}^d)$ through (28f) because we have assumed $c_{\rm v}(\cdot)$ bounded, cf. (18d). Then the strong convergence of $\vartheta_\tau\to\vartheta$ in $L^q(I\times\Omega)$ with any $1\le q<1+2/d$ follows by the interpolation with the estimate (28g). The same convergence applies also for the needed piecewise constant interpolant, i.e. $\underline{\vartheta}_\tau\to\vartheta$, and, by the continuity of the Nemytskiĭ (or here just superposition) mapping induced by the continuous mapping with at most linear growth $C_{\rm v}^{-1}$, also $\underline{\theta}_\tau=C_{\rm v}^{-1}(\underline{\vartheta}_\tau)\to C_{\rm v}^{-1}(\vartheta)=\theta$ in $L^q(I\times\Omega)$. The last equality uses also the weak convergence $\underline{\theta}_\tau\to\theta$ and, in particular, we thus proved $\vartheta=C_{\rm v}(\theta)$, which is a part of Definition 1. Then $\mathbb{M}(\underline{z}_\tau,\underline{c}_\tau,\underline{\theta}_\tau)\to\mathbb{M}(z,c,\theta)$ in any $L^s(I\times\Omega;\mathbb{R}^{d\times d})$ with any $1\le s<\infty$ follows by the continuity of the Nemytskiĭ (or here just superposition) mappings; here (18c) has been used. Thus we can also see that $\mathbb{M}(\underline{z}_\tau,\underline{c}_\tau,\underline{\theta}_\tau)\nabla\overline{\mu}_\tau\to\mathbb{M}(z,c,\theta)\nabla\mu$ weakly in $L^2(I\times\Omega;\mathbb{R}^d)$.

Step 3: Strong convergence of $e(\overline{u}_\tau)$ and of $e(\overline{v}_\tau)$. We use the technique from [37, Step.2 of the proof of Thm. 5.1.2] modified here for our Crank-Nicolson scheme. We write (27b) for $\mathbb{D}=\chi\mathbb{C}$ and use the substitution $\overline{w}_\tau:=\chi\overline{v}_\tau+\overline{u}_\tau$, i.e.

$$\varrho\dot v_\tau-{\rm div}\big((\varepsilon^2{+}\underline{z}_\tau^2)\mathbb{C}e(\overline{w}_\tau)+\beta M(\beta{\rm tr}\,e(\overline{u}_\tau){-}\overline{c}_\tau)\mathbb{I}\big)=\overline{g}_\tau\,. \tag{36}$$

We further add $\varrho\dot u_\tau/\chi$ and use the analogous substitution $w_\tau=\chi v_\tau+u_\tau$, so that (36) reads as

$$\frac{\varrho}{\chi}\dot w_\tau-{\rm div}\big((\varepsilon^2{+}\underline{z}_\tau^2)\mathbb{C}e(\overline{w}_\tau)+\beta M(\beta{\rm tr}\,e(\overline{u}_\tau){-}\overline{c}_\tau)\mathbb{I}\big)=\overline{g}_\tau+\frac{\varrho}{\chi}\dot u_\tau\,. \tag{37}$$

Similarly, we rewrite (12b) proved already in Step 2 by adding $\varrho\dot u/\chi$ and by using the substitution $w:=\chi v+u$ in the form

$$\frac{\varrho}{\chi}\dot w-{\rm div}\big((\varepsilon^2{+}z^2)\mathbb{C}e(w)+\beta M(\beta{\rm tr}\,e(u){-}c)\mathbb{I}\big)=g+\frac{\varrho}{\chi}\dot u\,. \tag{38}$$

We further test the difference (37) and (38) by $\overline{w}_\tau-w$ to obtain

$$\begin{aligned}\int_\Omega\frac{\varrho}{\chi}(\dot w_\tau{-}\dot w)\cdot(\overline{w}_\tau{-}w)+(\varepsilon^2{+}\underline{z}_\tau^2)\mathbb{C}e(\overline{w}_\tau{-}w){:}e(\overline{w}_\tau{-}w)+\beta^2M{\rm tr}\,e(\overline{u}_\tau{-}u)\,{\rm tr}\,e(\overline{w}_\tau{-}w)\,{\rm d}x\\=\int_\Omega\beta M(\overline{c}_\tau{-}c){\rm tr}\,e(\overline{w}_\tau{-}w)+(z^2{-}\underline{z}_\tau^2)\mathbb{C}e(w){:}e(\overline{w}_\tau{-}w)+(\overline{g}_\tau{-}g)\cdot(\overline{w}_\tau{-}w)\\+\frac{\varrho}{\chi}(\dot u_\tau{-}\dot u)\cdot(\overline{w}_\tau{-}w)\,{\rm d}x+\int_\Gamma(\overline{f}_\tau{-}f)\cdot(\overline{w}_\tau{-}w)\,{\rm d}S\end{aligned} \tag{39}$$

holding at a.e. time instant $t\in I$. We integrate (39) over I. We then use that

$$\int_0^T(\dot w_\tau{-}\dot w)\cdot(\overline{w}_\tau{-}w)\,{\rm d}t=\frac12|w_\tau(T){-}w(T)|^2-\frac12|w_\tau(0){-}w(0)|^2 \tag{40}$$

a.e. on Ω, which can be seen by the binomial formula if w is piecewise affine on the partition with the time step τ and then, by arbitrarily refining it, by a general w too; actually, we exploit only the "$\ge$" inequality in (40). Further, using (27a), we can see the estimate

$$\begin{aligned}{\rm tr}\,e(\overline{u}_\tau{-}u)\,{\rm tr}\,e(\overline{w}_\tau{-}w)&={\rm tr}\,e(\overline{u}_\tau{-}u)\,{\rm tr}\,e(\overline{u}_\tau{-}u)+\chi{\rm tr}\,e(\overline{u}_\tau{-}u)\,{\rm tr}\,e(\overline{v}_\tau{-}v)\\&\ge\chi{\rm tr}\,e(\overline{u}_\tau{-}u)\,{\rm tr}\,e(\overline{v}_\tau{-}v)=\chi{\rm tr}\,e(\overline{u}_\tau{-}u)\,{\rm tr}\,e(\dot u_\tau{-}\dot u)\end{aligned}$$

and then, by similar argumentation as used for (40), we can see that

$$\int_0^T{\rm tr}\,e(\overline{u}_\tau{-}u)\,{\rm tr}\,e(\overline{w}_\tau{-}w)\,{\rm d}t\ge\frac{\chi}{2}|{\rm tr}\,e(u_\tau(T){-}u(T))|^2-\frac{\chi}{2}|{\rm tr}\,e(u_\tau(0){-}u(0))|^2 \tag{41}$$

a.e. on Ω. Therefore, exploiting $u_\tau(0)=u_0=u(0)$ and also $w_\tau(0)=\chi v_0+u_0=w(0)$, from (39) we obtain the estimate

$$\begin{aligned}&\varepsilon^2\int_0^T\!\!\int_\Omega\mathbb{C}e(\overline{w}_\tau{-}w){:}e(\overline{w}_\tau{-}w)\,{\rm d}x{\rm d}t\\&\le\int_\Omega\frac{\varrho}{2\chi}|w_\tau(T){-}w(T)|^2\,{\rm d}x+\varepsilon^2\int_0^T\!\!\int_\Omega\mathbb{C}e(\overline{w}_\tau{-}w){:}e(\overline{w}_\tau{-}w)\,{\rm d}x{\rm d}t+\int_\Omega\beta^2M\frac{\chi}{2}|{\rm tr}\,e(u_\tau(T){-}u(T))|^2{\rm d}x\end{aligned}$$

$$\le \int_0^T\!\!\int_\Omega \frac{\varrho}{\chi}(\dot{w}_\tau{-}\dot{w})\cdot(\overline{w}_\tau{-}w) + (\varepsilon^2{+}\underline{z}_\tau^2)\mathbb{C}e(\overline{w}_\tau{-}w){:}e(\overline{w}_\tau{-}w) + \beta^2 M \mathrm{tr}\, e(\underline{u}_\tau{-}u)\,\mathrm{tr}\, e(\overline{w}_\tau{-}w)\,\mathrm{d}x\mathrm{d}t$$
$$= \int_0^T\!\!\int_\Omega \beta M(\overline{c}_\tau{-}c)\,\mathrm{tr}\, e(\overline{w}_\tau{-}w) + (z^2{-}\underline{z}_\tau^2)\mathbb{C}e(w){:}e(\overline{w}_\tau{-}w) + \frac{\varrho}{\chi}(\dot{u}_\tau{-}\dot{u})\cdot(\overline{w}_\tau{-}w)$$
$$+ (\overline{g}_\tau{-}g)\cdot(\overline{w}_\tau{-}w)\,\mathrm{d}x\mathrm{d}t + \int_0^T\!\!\int_\Gamma (\overline{f}_\tau{-}f)\cdot(\overline{w}_\tau{-}w)\,\mathrm{d}S \to 0. \tag{42}$$

The convergence of the right-hand side term of (42) to zero has used $\overline{c}_\tau \to c$ and $(\underline{z}_\tau^2{-}z)\mathbb{C}e(w) \to 0$ in $L^2(I{\times}\Omega;\mathbb{R}^{d\times d})$. Moreover, it also has used that

$$\int_0^T\!\!\int_\Omega (\dot{u}_\tau{-}\dot{u})\cdot(\overline{w}_\tau{-}w)\,\mathrm{d}x\mathrm{d}t \to 0$$

because $\overline{w}_\tau{-}w$ is certainly bounded in $L^2(I{\times}\Omega;\mathbb{R}^d)$ while $\dot{u}_\tau \to \dot{u}$ strongly in $L^2(I{\times}\Omega;\mathbb{R}^d)$ due to the bounds (28a) and the generalized Aubin-Lions theorem for functions whose distributional derivatives are measures, cf. [47, Cor. 7.9].

Then, by using also the Korn inequality, from (42) we obtain $\overline{w}_\tau \to w$ in $L^2(I;H^1(\Omega;\mathbb{R}^d))$. Since $\chi\dot{u}_\tau + u_\tau = \chi\overline{v}_\tau + \overline{u}_\tau + (u_\tau{-}\overline{u}_\tau) = \overline{w}_\tau + (u_\tau{-}\overline{u}_\tau) \to w = \chi v + u = \chi\dot{u} + u$ in $L^2(I;H^1(\Omega;\mathbb{R}^d))$, we can see that $u_\tau \to u$ in $L^2(I;H^1(\Omega;\mathbb{R}^d))$ and then also $\overline{v}_\tau = \dot{u}_\tau \to \dot{u}$ in $L^2(I;H^1(\Omega;\mathbb{R}^d))$, i.e. the strong convergence in (34c). Then also the strong convergence (34b) of $\underline{u}_\tau$ follows.

Step 4: Convergence in the semistability. From (13c) we can see that z_τ^k minimizes the functional $z \mapsto \mathscr{R}(z{-}z_\tau^{k-1}) + 2\mathscr{E}(u_\tau^k, \frac12 z + \frac12 z_\tau^{k-1})$ where the c-variable involved in $\mathscr{E}$ in (5a) is irrelevant here (hence omitted) and similarly $\mathscr{R} = \mathscr{R}(\dot{z})$ also ignores all variables which are irrelevant for minimization in z only. Using the 1-homogeneity of $\mathscr{R}$, we obtain $2\mathscr{E}(u_\tau^k, \frac12 z{+}\frac12 z_\tau^{k-1}) \le 2\mathscr{E}(u_\tau^k, \frac12\tilde{z}{+}\frac12 z_\tau^{k-1}) {+} \mathscr{R}(\tilde{z}{-}z_\tau^k)$ for any $\tilde{z}$. This gives the following discrete (and modified) semi-stability

$$\int_\Omega (\underline{z}_\tau)^2\mathbb{C}e(\overline{u}_\tau){:}e(\overline{u}_\tau) + \frac{a_0}{4\varepsilon}(1{-}\underline{z}_\tau)^2 + \varepsilon a_0|\nabla\underline{z}_\tau|^2\,\mathrm{d}x \le \int_\Omega \Big(\frac{\tilde{z}{-}\underline{z}_\tau}{2}\Big)^2\mathbb{C}e(\overline{u}_\tau){:}e(\overline{u}_\tau)$$
$$+ \frac{a_0}{4\varepsilon}\Big(1{-}\frac{\tilde{z}{-}\underline{z}_\tau}{2}\Big)^2 {+}\, \varepsilon a_0\Big|\nabla\frac{\tilde{z}{-}\underline{z}_\tau}{2}\Big|^2 {-}\, \frac{a_1}{\varepsilon}(\tilde{z} - \overline{z}_\tau)\,\mathrm{d}x \tag{43}$$

holding for a.a. $t \in I$ and for any $\tilde{z} \in H^1(\Omega)\cap L^\infty(\Omega)$ such that $\tilde{z} \le \overline{z}_\tau(t)$.

We now take t fixed such that (34e,f) hold. For the linear/quadratic functional $z \mapsto \mathscr{E}(u,z)$, again now by ignoring the irrelevant constant and the dependence of $\mathscr{E}$ on c, we further denote by $\langle\cdot,\cdot\rangle_{\mathscr{E},u} : Z \times Z \to \mathbb{R}$ the underlying linear/bilinear form defined by

$$\langle z,\tilde{z}\rangle_{\mathscr{E},u} := \big\langle \partial_z\mathscr{E}(u)z,\tilde{z}\big\rangle = \int_\Omega \Big(\mathbb{C}e(u){:}e(u) + \frac{a_0}{4\varepsilon}\Big)z\tilde{z} + \varepsilon a_0\nabla z\cdot\nabla\tilde{z} - \frac{a_0}{2\varepsilon}\tilde{z}\,\mathrm{d}x.$$

Choosing $\tilde{z}$ arbitrary, we use the binomial trick with the so-called mutual recovery sequence $\tilde{z}_\tau = \overline{z}_\tau(t) + \tilde{z} - z(t)$. More specifically, any sequence $\{\tilde{z}_k\}_{k\in\mathbb{N}}$ is called a mutual recovery one with respect to a sequence $\{(u_k,z_k)\}_{k\in\mathbb{N}}$ if

$$\limsup_{k\to\infty}\Big(\mathscr{E}(u_k,\tilde{z}_k) - \mathscr{E}(u_k,z_k) + \mathscr{R}(\tilde{z}_k{-}z_k)\Big) \le \mathscr{E}(u,\tilde{z}) - \mathscr{E}(u,z) + \mathscr{R}(\tilde{z}{-}z). \tag{44}$$

In contrast to the original variant invented in [38] which recovers also u-variable to obtain a full stability, we here have formulated (44) in the (weaker) variant which will lead to semistability as introduced in [45]. The main motivation of the mentioned choice is to make $\mathscr{R}(\tilde{z}_\tau{-}\overline{z}_\tau(t)) = \mathscr{R}(\tilde{z}{-}z(t))$ simply constant while $\tilde{z}_\tau \to \tilde{z}$ weakly*, which makes the limit passage through the nonlinearities in (43) possible, cf. [37] for details about this technique for the backward Euler formula. Here we will still modify the construction (44), designed for the backward-Euler formula, for our Crank-Nicholson scheme. More specifically, we will exploit the following joint continuity

$$\forall\,\tilde{z} \in H^1(\Omega)\cap L^\infty(\Omega): \quad (u,z) \mapsto \big\langle z,\tilde{z}\big\rangle_{\mathscr{E},u} \;\text{ is (strong}{\times}\text{weak)-continuous} \tag{45}$$

and, using elementary algebra and the above mentioned choice of the mutual recovery sequence, obtain the convergence of the $\mathscr{E}$-terms to be used in the modified version of (44):

$$\mathscr{E}(\overline{u}_\tau(t),\underline{z}_\tau) - \mathscr{E}\Big(\overline{u}_\tau(t),\frac{\tilde{z}_\tau{+}\underline{z}_\tau(t)}{2}\Big) = \mathscr{E}\Big(\overline{u}_\tau(t),\frac{\overline{z}_\tau(t){+}\underline{z}_\tau(t)}{2}\Big) - \mathscr{E}\Big(\overline{u}_\tau(t),\frac{\tilde{z}_\tau{+}\underline{z}_\tau(t)}{2}\Big)$$
$$= \mathscr{E}\Big(\overline{u}_\tau(t),\frac{\overline{z}_\tau(t)}{2}\Big) + \frac14\big\langle\overline{z}_\tau(t),\underline{z}_\tau(t)\big\rangle_{\mathscr{E},\overline{u}_\tau(t)} - \mathscr{E}\Big(\overline{u}_\tau(t),\frac{\tilde{z}_\tau}{2}\Big) - \frac14\big\langle\tilde{z}_\tau,\underline{z}_\tau(t)\big\rangle_{\mathscr{E},\overline{u}_\tau(t)}$$
$$= \frac18\big\langle\overline{z}_\tau(t){+}\tilde{z}_\tau,\overline{z}_\tau(t){-}\tilde{z}_\tau\big\rangle_{\mathscr{E},\overline{u}_\tau(t)} + \frac14\big\langle\overline{z}_\tau(t){-}\tilde{z}_\tau,\underline{z}_\tau(t)\big\rangle_{\mathscr{E},\overline{u}_\tau(t)}$$

$$
= \frac{1}{8}\big\langle \overline{z}_\tau(t){+}\tilde z_\tau, z(t){-}\tilde z\big\rangle_{\mathscr{E},\overline{u}_\tau(t)} + \frac{1}{4}\big\langle z(t){-}\tilde z, \underline{z}_\tau(t)\big\rangle_{\mathscr{E},\overline{u}_\tau(t)}
$$

$$
\to \frac{1}{8}\big\langle z(t){+}\tilde z, z(t){-}\tilde z\big\rangle_{\mathscr{E},u(t)} + \frac{1}{4}\big\langle z(t){-}\tilde z, z(t)\big\rangle_{\mathscr{E},u(t)} = \mathscr{E}(u(t),z(t)) - \mathscr{E}\Big(u(t),\frac{\tilde z{+}z(t)}{2}\Big). \tag{46}
$$

For the convergence, we used (45) relying on the fact that, by the previous Step 3, we know that $(\underline{\overline{z}}_\tau)^2\mathbb{C}e(\overline{u}_\tau){:}e(\overline{u}_\tau) \to z^2\mathbb{C}e(u){:}e(u)$ in $L^1(I{\times}\Omega)$ and, having it bounded in $L^\infty(I;L^1(\Omega))$, also $(\underline{\overline{z}}_\tau(t))^2\mathbb{C}e(\overline{u}_\tau(t)){:}e(\overline{u}_\tau(t)) \to z(t)^2\mathbb{C}e(u(t)){:}e(u(t))$ in $L^1(\Omega)$ for a.a. in Ω (possibly under another selection of a subsequence, if needed); here, also (34d) and (34e) have been used proving that $\underline{\overline{z}}_\tau(t) = \frac12\underline{z}_\tau(t) + \frac12\overline{z}_\tau(t) \to \frac12 z(t) + \frac12 z(t) = z(t)$ for a.a. $t \in I$. Then we can easily perform the limit passage in (43), obtaining

$$
\forall \tilde z \in H^1(\Omega)\cap L^\infty(\Omega): \quad \mathscr{E}(u(t),z(t)) \le \mathscr{E}\Big(u(t),\frac{\tilde z{+}z(t)}{2}\Big) + \mathscr{R}\Big(\frac{\tilde z{-}z(t)}{2}\Big). \tag{47}
$$

Now substituting $\tilde z = 2\hat z - z(t)$ so that $\frac{\tilde z+z(t)}{2} = \hat z$ and $\frac{\tilde z-z(t)}{2} = \hat z - z(t)$, we obtain the desired semistability (33b) only with $\hat z$ instead of $\tilde z$.

Step 5: Strong convergence of $\nabla\overline{\underline{\mu}}_\tau$. For a.a. $x \in \Omega$, using again the binomial formula, it holds

$$
\frac12 M\big(\beta\mathrm{tr}\,e(u_\tau(T)) - c_\tau(T)\big)^2 - \frac12 M\big(\beta\mathrm{tr}\,e(u_\tau(0)) - c_\tau(0)\big)^2
= \int_0^T \beta M(\beta\mathrm{tr}\,e(\underline{\overline{u}}_\tau){-}\underline{\overline{c}}_\tau)\mathrm{tr}\,e(\dot u_\tau) + M(\underline{\overline{c}}_\tau{-}\beta\mathrm{tr}\,e(\underline{\overline{u}}_\tau))\dot c_\tau\,\mathrm{d}t. \tag{48}
$$

Testing (36) by $\dot u_\tau$ gives

$$
\int_0^T\!\!\int_\Omega \varrho\dot v_\tau{\cdot}\dot u_\tau + \big((\varepsilon^2{+}\underline{z}_\tau^2)\mathbb{C}e(\underline{\overline{w}}_\tau){:}e(\dot u_\tau) + \beta M(\beta\mathrm{tr}\,e(\underline{\overline{u}}_\tau){-}\underline{\overline{c}}_\tau)\mathrm{tr}\,e(\dot u_\tau)\,\mathrm{d}x\mathrm{d}t
= \int_0^T\!\!\int_\Omega \overline{g}_\tau\dot u_\tau\,\mathrm{d}x\mathrm{d}t + \int_0^T\!\!\int_\Gamma \overline{f}_\tau{\cdot}\dot u_\tau\,\mathrm{d}S\mathrm{d}t. \tag{49}
$$

Using (27a) and again the binomial formula (23a), we can see that $\int_0^T \varrho\dot v_\tau{\cdot}\dot u_\tau\,\mathrm{d}t = \int_0^T \varrho\dot v_\tau{\cdot}\underline{\overline{v}}_\tau\,\mathrm{d}t = \frac{\varrho}{2}|v_\tau(T)|^2 - \frac{\varrho}{2}|v_\tau(0)|^2$ on Ω and merging (49) with (48), we obtain

$$
\int_0^T\!\!\int_\Omega M(\underline{\overline{c}}_\tau{-}\beta\mathrm{tr}\,e(\underline{\overline{u}}_\tau))\dot c_\tau\,\mathrm{d}x\mathrm{d}t
$$

$$
= \int_\Omega \frac{M}{2}\big(\beta\mathrm{tr}\,e(u_\tau(T)){-}c_\tau(T)\big)^2 - \frac{M}{2}\big(\beta\mathrm{tr}\,e(u_\tau(0)){-}c_\tau(0)\big)^2\,\mathrm{d}x - \int_0^T\!\!\int_\Omega \beta M(\beta\mathrm{tr}\,e(\underline{\overline{u}}_\tau){-}\underline{\overline{c}}_\tau)\mathrm{tr}\,e(\dot u_\tau)\,\mathrm{d}x\mathrm{d}t
$$

$$
= \int_\Omega \frac{\varrho}{2}|v_\tau(T)|^2 + \frac12 M\big(\beta\mathrm{tr}\,e(u_\tau(T)) - c_\tau(T)\big)^2 - \frac{\varrho}{2}|v_\tau(0)|^2 - \frac12 M\big(\beta\mathrm{tr}\,e(u_\tau(0)) - c_\tau(0)\big)^2\,\mathrm{d}x
$$

$$
- \int_0^T\!\!\int_\Gamma \overline{f}_\tau{\cdot}\dot u_\tau\,\mathrm{d}S\mathrm{d}t + \int_0^T\!\!\int_\Omega (\varepsilon^2{+}\underline{z}_\tau^2)\mathbb{C}e(\underline{\overline{w}}_\tau){:}e(\dot u_\tau) - \beta M(\beta\mathrm{tr}\,e(\underline{\overline{u}}_\tau){-}\underline{\overline{c}}_\tau)\mathrm{tr}\,e(\dot u_\tau) - \overline{g}_\tau{\cdot}\dot u_\tau\,\mathrm{d}x\mathrm{d}t.
$$

Then, exploiting also the strong convergence $\underline{\overline{w}}_\tau \to w$ proved already in Step 3 as well as (35), we can estimate

$$
\liminf_{\tau\to0}\int_0^T\!\!\int_\Omega M(\underline{\overline{c}}_\tau{-}\beta\mathrm{tr}\,e(\underline{\overline{u}}_\tau))\dot c_\tau\,\mathrm{d}x\mathrm{d}t \ge \int_\Omega \frac{\varrho}{2}|v(T)|^2 + \frac12 M\big(\beta\mathrm{tr}\,e(u(T)) - c(T)\big)^2
- \frac{\varrho}{2}|v(0)|^2 - \frac12 M\big(\beta\mathrm{tr}\,e(u(0)) - c(0)\big)^2\,\mathrm{d}x - \int_0^T\!\!\int_\Gamma f{\cdot}\dot u\,\mathrm{d}S\mathrm{d}t
+ \int_0^T\!\!\int_\Omega (\varepsilon^2{+}z^2)\mathbb{C}e(w){:}e(\dot u) - \beta M(\beta\mathrm{tr}\,e(u){-}c)\mathrm{tr}\,e(\dot u) - g{\cdot}\dot u\,\mathrm{d}x\mathrm{d}t. \tag{50}
$$

Now we can perform the desired estimate:

$$
\int_0^T\!\!\int_\Omega \mathbb{M}(z,c,\theta)\nabla\mu{\cdot}\nabla\mu\,\mathrm{d}x\mathrm{d}t \le \liminf_{\tau\to0}\int_0^T\!\!\int_\Omega \mathbb{M}(\underline{z}_\tau,\underline{c}_\tau,\underline{\theta}_\tau)\nabla\overline{\underline{\mu}}_\tau{\cdot}\nabla\overline{\underline{\mu}}_\tau\,\mathrm{d}x\mathrm{d}t
$$

$$
\le \limsup_{\tau\to0}\int_0^T\!\!\int_\Omega \mathbb{M}(\underline{z}_\tau,\underline{c}_\tau,\underline{\theta}_\tau)\nabla\overline{\underline{\mu}}_\tau{\cdot}\nabla\overline{\underline{\mu}}_\tau\,\mathrm{d}x\mathrm{d}t
$$

$$
= \limsup_{\tau\to0}\Big(\int_0^T\!\!\int_\Gamma \bar{j}_{\mathrm{E},\tau}{\cdot}\overline{\underline{\mu}}_\tau\,\mathrm{d}S\mathrm{d}t - \int_0^T\!\!\int_\Omega \dot c_\tau\overline{\underline{\mu}}_\tau\,\mathrm{d}x\mathrm{d}t\Big)
$$

$$
\begin{aligned}
&= \limsup_{\tau\to0}\bigg(\int_0^T\!\!\int_\Gamma \bar{j}_{\mathrm{E},\tau}{\cdot}\underline{\mu}_\tau\,\mathrm{d}S\mathrm{d}t + \int_0^T\!\!\int_\Omega \Big(\beta M\mathrm{tr}\,e(\overline{u}_\tau) - \Big(M{+}\frac{\kappa}{c_{\scriptscriptstyle\rm E}}\Big)\overline{c}_\tau + \kappa\Big)\dot{c}_\tau - \varkappa\nabla\overline{c}_\tau{\cdot}\nabla\dot{c}_\tau\,\mathrm{d}x\mathrm{d}t\bigg)\\
&= \limsup_{\tau\to0}\bigg(\int_0^T\!\!\int_\Gamma \bar{j}_{\mathrm{E},\tau}{\cdot}\underline{\mu}_\tau\,\mathrm{d}S\mathrm{d}t + \int_0^T\!\!\int_\Omega \big(M(\beta\mathrm{tr}\,e(\overline{u}_\tau){-}\overline{c}_\tau\big)\dot{c}_\tau\,\mathrm{d}x\mathrm{d}t\\
&\qquad + \int_\Omega \frac{\kappa}{2c_{\scriptscriptstyle\rm E}}c_0^2 + \frac{\varkappa}{2}|\nabla c_0|^2 + \kappa c_0 - \frac{\kappa}{2c_{\scriptscriptstyle\rm E}}c_\tau(T)^2 - \frac{\varkappa}{2}|\nabla c_\tau(T)|^2 - \kappa c_\tau(T)\,\mathrm{d}x\bigg)\\
&\le \int_\Omega \frac{\kappa}{2c_{\scriptscriptstyle\rm E}}c_0^2 + \frac{\varkappa}{2}|\nabla c_0|^2 + \kappa c_0 + \frac{\varrho}{2}|v_0|^2 + \frac{1}{2}M\big(\beta\mathrm{tr}\,e(u+0){-}c_0\big)^2 - \frac{\kappa}{2c_{\scriptscriptstyle\rm E}}c(T)^2\\
&\qquad - \frac{\varkappa}{2}|\nabla c(T)|^2 - \kappa c(T) - \frac{\varrho}{2}|v(T)|^2 - \frac{1}{2}M\big(\beta\mathrm{tr}\,e(u(T)) - c(T)\big)^2\,\mathrm{d}x\\
&\qquad + \int_0^T\!\!\int_\Omega \beta M(\beta\mathrm{tr}\,e(u){-}c)\mathrm{tr}\,e(\dot{u}) - \big((\varepsilon^2{+}z^2)\mathbb{C}e(w){:}e(\dot{u}) + g{\cdot}\dot{u}\,\mathrm{d}x\mathrm{d}t\\
&\qquad + \int_0^T\!\!\int_\Gamma f{\cdot}\dot{u} + j_{\scriptscriptstyle\rm B}{\cdot}\mu\,\mathrm{d}S\mathrm{d}t = \int_0^T\bigg(\int_\Gamma j_{\scriptscriptstyle\rm B}{\cdot}\mu\,\mathrm{d}S - {}_{H^1(\Omega)^*}\big\langle\dot{c},\mu\big\rangle_{H^1(\Omega)}\bigg)\,\mathrm{d}t\\
&= \int_0^T\!\!\int_\Omega \mathbb{M}(z,c,\theta)\nabla\mu{\cdot}\nabla\mu\,\mathrm{d}x\mathrm{d}t,
\end{aligned}
\tag{51}
$$

where we used the identities $\int_0^T\overline{c}_\tau{\cdot}\dot{c}_\tau\,\mathrm{d}t = \frac{1}{2}c_\tau^2(T) - \frac{1}{2}c_\tau^2(0)$ and $\int_0^T\nabla\overline{c}_\tau{\cdot}\nabla\dot{c}_\tau\,\mathrm{d}t = \frac{1}{2}|\nabla c_\tau(T)|^2 - \frac{1}{2}|\nabla c_\tau(0)|^2$ on Ω. We also used that c and μ are already proved to solve (1c) in the weak sense. Note that we cannot rely on an estimate of $\dot{c}$ in a Lebesgue space so that we have to use a duality between $\dot{c}$ and μ relying on the $H^1(I;H^1(\Omega)^*)$-estimate (28d). The last equation can be obtained by testing the boundary-value problem for c by a spatial mollification of μ and then making a limit passage. Altogether, (51) yields $\lim_{\tau\to0}\int_0^T\int_\Omega\mathbb{M}(\underline{z}_\tau,\underline{c}_\tau,\underline{\theta}_\tau)\nabla\underline{\mu}_\tau{\cdot}\nabla\underline{\mu}_\tau\,\mathrm{d}x\mathrm{d}t = \int_0^T\int_\Omega\mathbb{M}(z,c,\theta)\nabla\mu{\cdot}\nabla\mu\,\mathrm{d}x\mathrm{d}t$. From this, we can see that

$$
\begin{aligned}
\big\|\nabla\underline{\mu}_\tau{-}\nabla\mu\big\|^2_{L^2(I\times\Omega;\mathbb{R}^d)} &\le \int_0^T\!\!\int_\Omega \frac{\mathbb{M}(\underline{z}_\tau,\underline{c}_\tau,\underline{\theta}_\tau)}{\inf\mathbb{M}(\mathbb{R}^3)}\nabla(\underline{\mu}_\tau{-}\mu){\cdot}\nabla(\underline{\mu}_\tau{-}\mu)\,\mathrm{d}x\mathrm{d}t\\
&= \int_0^T\!\!\int_\Omega \frac{\mathbb{M}(\underline{z}_\tau,\underline{c}_\tau,\underline{\theta}_\tau)}{\inf\mathbb{M}(\mathbb{R}^3)}\nabla\underline{\mu}_\tau{\cdot}\nabla\underline{\mu}_\tau\,\mathrm{d}x\mathrm{d}t + \int_0^T\!\!\int_\Omega \frac{\mathbb{M}(\underline{z}_\tau,\underline{c}_\tau,\underline{\theta}_\tau)}{\inf\mathbb{M}(\mathbb{R}^3)}\nabla(\mu{-}2\underline{\mu}_\tau){\cdot}\nabla\mu\,\mathrm{d}x\mathrm{d}t\\
&\to \int_0^T\!\!\int_\Omega \frac{\mathbb{M}(z,c,\theta)}{\inf\mathbb{M}(\mathbb{R}^3)}\nabla\mu{\cdot}\nabla\mu\,\mathrm{d}x\mathrm{d}t + \int_0^T\!\!\int_\Omega \frac{\mathbb{M}(z,c,\theta)}{\inf\mathbb{M}(\mathbb{R}^3)}\nabla(\mu{-}2\mu){\cdot}\nabla\mu\,\mathrm{d}x\mathrm{d}t = 0,
\end{aligned}
$$

which proves (34h).

Step 6: Convergence in the heat-transfer equation. From the convergence proved in Steps 3 and 5, specifically (34c,f,h), we know that $\tilde{r}_\tau \to r$ weak* in $\mathrm{Meas}(I{\times}\overline{\Omega})$ and thus the convergence of the distributional solution to the semi-linear equation (27e) towards (12e) is easy.

Step 7: Convergence in the energy balance. Eventually, we obtain the inequality (33f) by weak lower semicontinuity from the discrete energy balance (21) written for $l = T/\tau$. □

Remark 7 (*Another generalization: concentration-dependent heat capacity*)**.** The heat capacity can naturally be affected by the content of the fluid c, i.e. $c_{\rm v} = c_{\rm v}(c,\theta)$. This can be modelled by modifying the free energy (7) as

$$
\psi(e,z,c,\nabla z,\nabla c,\theta) = \varphi(e,z,c,\nabla z,\nabla c) + \phi(c,\theta). \tag{52}
$$

The entropy $\mathfrak{s} = -\phi'_\theta(c,\theta)$ now becomes c-dependent and substituting it into the so-called entropy equation, i.e. $\theta\dot{\mathfrak{s}} + \mathrm{div}\,j = r =$ heat production rate, gives

$$
c_{\rm v}(c,\theta)\dot{\theta} + \mathrm{div}\,j = r + \theta\phi''_{c\theta}(c,\theta)\dot{c} \qquad \text{with}\ \ c_{\rm v}(c,\theta) = -\theta\phi''_{\theta\theta}(c,\theta).
$$

This reveals that the heat capacity $c_{\rm v}$ becomes temperature-dependent and the right-hand side of the heat-transfer equation is augmented by the adiabatic-like term $\theta\phi''_{c\theta}(c,\theta)\dot{c}$. The internal energy $\mathfrak{u} = \psi{+}\mathfrak{s}\theta$ equals to $\varphi(e,z,c,\nabla z,\nabla c){+}\phi(c,\theta){-}\theta\phi'_\theta(c,\theta)$. The chemical potential then becomes temperature-dependent as it is augmented to $\mu = \varphi'_c(e,z,c,\nabla z,\nabla c) + \phi'_c(c,\theta) - \mathrm{div}\,\varphi'_{\nabla c}(\nabla c)$. Testing (1c) by μ gives, in addition, the term $\phi'_c(c,\theta)\dot{c}$. In the overall energy balance, this term balances the rate of the thermal part of the internal energy by obvious calculations, cancelling the terms $\pm\phi'_\theta(c,\theta)\dot{\theta}$, yields

$$
\frac{\partial}{\partial t}(\phi(c,\theta) - \theta\phi'_\theta(c,\theta)) = \phi'_c(c,\theta)\dot{c} - \theta\phi''_{\theta\theta}(c,\theta)\dot{\theta} - \theta\phi''_{c\theta}(c,\theta)\dot{c}.
$$

Estimation of the mentioned adiabatic term $\theta\phi''_{c\theta}(c,\theta)\dot{c}$ needs some "viscosity" that would control $\dot{c}$. Following Gurtin's ideas [21], this is achieved by considering a so-called viscous Cahn-Hilliard equation with the chemical potential

$$\mu = \varphi'_c(e,z,c,\nabla z,\nabla c) + \phi'_c(c,\theta) - \operatorname{div}\varphi'_{\nabla c}(\nabla c) + \alpha\dot{c} \quad \text{ with } \alpha > 0\,;$$

cf. e.g. also [15,27,40,43,44]. The heat-production rate r is then augmented by $\alpha|\dot{c}|^2$ and Step 5 in the above proof considerably simplifies.

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REFERENCES

[1] L. Ambrosio and V. M. Tortorelli. Approximation of functional depending on jumps via by elliptic functionals via Γ-convergence. *Comm. Pure Appl. Math.*, 43:999–1036, 1990.

[2] L. Ambrosio and V. M. Tortorelli. On the approximation of free discontinuity problems. *Bollettino Unione Mat. Italiana*, 7:105–123, 1992.

[3] M. Artina, M. Fornasier, S. Micheletti, and S. Perotto. Anisotropic mesh adaptation for crack detection in brittle materials. *SIAM J. Sci. Comput.*, 37:B633–B659, 2015.

[4] F. Auricchio, A. Reali, and U. Stefanelli. A three-dimensional model describing stress-induced solid phase transformation with permanent inelasticity. *Int. J. Plasticity*, 23:207–226, 2007.

[5] M. A. Biot. General theory of three-dimensional consolidation. *J. Appl. Phys.*, 12:155–164, 1941.

[6] L. Boccardo and T. Gallouët. Non-linear elliptic and parabolic equations involving measure data. *J. Funct. Anal.*, 87:149–169, 1989.

[7] L. Boccardo and T. Gallouët. Nonlinear elliptic equations with right hand side measures. *Comm. Partial Differential Equations*, 17:641–655, 1992.

[8] E. Bonetti, C. Heinemann, C. Kraus, and A. Segatti. Modeling and analysis of a phase field system for damage and phase separation processes in solids. *Preprint arXiv 1312.1623v2.*

[9] B. Bourdin, G. A. Francfort, and J.-J. Marigo. Numerical experiments in revisited brittle fracture. *J. Mech. Phys. Solids*, 48:797–826, 2000.

[10] B. Bourdin, G. A. Francfort, and J.-J. Marigo. The variational approach to fracture. *J. Elasticity*, 91:5–148, 2008.

[11] B. Bourdin, C. J. Larsen, and C. L. Richardson. A time-discrete model for dynamic fracture based on crack regularization. *Int. J. of Fracture*, 10:133–143, 2011.

[12] S. Burke, C. Ortner, and E. Süli. An adaptive finite element approximation of a generalised Ambrosio-Tortorelli functional. *Math. Meth. Models Appl. Sci.*, 23:1663–1697, 2013.

[13] J. W. Cahn and J. E. Hilliard. Free energy of a uniform system I. Interfacial free energy. *J. Chem. Phys.*, 28:258–267, 1958.

[14] J. Crank and P. Nicolson. A practical method for numerical evaluation of solutions of partial differential equations of the heat conduction type. *Proc. Camb. Phil. Soc.*, 43:50–67, 1947.

[15] C. M. Elliott and H. Garcke. On the Cahn-Hilliard equation with degenerate mobility. *SIAM J. Math. Anal.*, 27:404–423, 1996.

[16] I. Faragó. Splitting methods and their application to the abstract Cauchy problems. Lect. Notes Comp.Sci. 3401, pages 35–45. Springer, Berlin, 2005.

[17] E. Feireisl and J. Málek. On the Navier-Stokes equations with temperature-dependent transport coefficients. *Diff. Equations Nonlin. Mech.*, pages 14pp.(electronic), Art.ID 90616, 2006.

[18] M. Frost, B. Benešová, and P. Sedlák. A microscopically motivated constitutive model for shape memory alloys: formulation, analysis and computations. *Math. Mech. of Solids*, 2014. doi:10.1177/1081286514522474.

[19] A. Giacomini. Ambrosio-Tortorelli approximation of quasi-static evolution of brittle fractures. *Calc. Var. Partial Diff. Eqs.*, 22:129–172, 2005.

[20] R. Glowinski, J.-L. Lions, and R. Trémolières. *Numerical analysis of variational inequalities.* North-Holland, Amsterdam, 1981. (French original Dunod, Paris, 1976).

[21] M. E. Gurtin. Generalized Ginzburg-Landau and Cahn-Hilliard equations based on a microforce balance. *Physica D*, 92:178–192, 1996.

[22] Y. Hamiel, V. Lyakhovsky, and A. Agnon. Coupled evolution of damage and porosity in poroelastic media: theory and applications to deformation of porous rocks. *Geophys. J. Int.*, 156:701–713, 2004.

[23] C. Heinemann and C. Kraus. Existence of weak solutions for Cahn-Hilliard systems coupled with elasticity and damage. *Adv. Math. Sci. Appl.*, 21:321359, 2011.

[24] C. Heinemann and C. Kraus. Degenerating Cahn-Hilliard systems coupled with mechanical effects and complete damage processes. *Mathematica Bohemica*, 139:315–331, 2014.

[25] C. Heinemann and C. Kraus. *Phase Separation Coupled with Damage Processes – Analysis of Phase Field Models in Elastic Media*. Springer Fachmedien, Wiesbaden, 2014.

[26] C. Heinemann and C. Kraus. Existence of weak solutions for a PDE system describing phase separation and damage processes including inertial effects. *Preprint arXiv 1502.05861v1*, 2015.

[27] C. Heinemann, C. Kraus, E. Rocca, and R. Rossi. A temperature-dependent phase-field model for phase separation and damage. *Preprint arXiv 1510.03755v1*, 2015.

[28] H. M. Hilber, T. J. R. Hughes, and R. L. Taylor. Improved numerical dissipation for time integration algorithms in structural dynamics. *Earthquake Eng. Struct. Dyn.*, 5:283–292, 1977.
[29] L. Jakabčin. A visco-elasto-plastic evolution model with regularized fracture. *ESAIM Control, Optim., Calc. Var.*, 22:148–168, 2016.
[30] J. Kruis, T. Koudelka, and T. Krejčí. Multi-physics analyses of selected civil engineering concrete structure. *Commun. Comput. Phys.*, 12:885–918, 2012.
[31] C. J. Larsen. Models for dynamic fracture based on griffith's criterion. In K. Hackl, editor, *IUTAM Symp. on Variational Concepts with Appl. to the Mech. of Mater.*, pages 131–140. Springer, 2010.
[32] C. J. Larsen, C. Ortner, and E. Süli. Existence of solution to a regularized model of dynamic fracture. *Math. Models Meth. Appl. Sci.*, 20:1021–1048, 2010.
[33] V. Lyakhovsky and Y. Hamiel. Damage evolution and fluid flow in poroelastic rock. *Izvestiya, Physics of the Solid Earth*, 43:13–23, 2007.
[34] V. Lyakhovsky, Y. Hamiel, and Y. Ben-Zion. A non-local visco-elastic damage model and dynamic fracturing. *J. Mech. Phys. Solids*, 59:1752–1776, 2011.
[35] G. Marchuk. *Splitting and alternating direction methods*. North Holland, Amsterdam, 1990.
[36] A. Mielke. Evolution in rate-independent systems (Ch. 6). In C. Dafermos and E. Feireisl, editors, *Handbook of Differential Equations, Evolutionary Equations, vol. 2*, pages 461–559. Elsevier B.V., Amsterdam, 2005.
[37] A. Mielke and T. Roubíček. *Rate-Independent Systems – Theory and Application*. Springer, New York, 2015.
[38] A. Mielke, T. Roubíček, and U. Stefanelli. Γ-limits and relaxations for rate-independent evolutionary problems. *Calc. Var. Part. Diff. Eqns.*, 31:387–416, 2008.
[39] A. Mielke and F. Theil. On rate–independent hysteresis models. *Nonl. Diff. Eqns. Appl.*, 11:151–189, 2004.
[40] A. Miranville. A model of Cahn-Hilliard equation based on a microforce balance. *C. R. Acad. Sci. Paris Sér. I Math.*, 328:1247–1252, 1999.
[41] L. Modica and S. Mortola. Il limite nella Γ-convergenza di una famiglia di funzionali ellittici. *Boll. Unione Mat. Italiana A*, 14:526–529, 1977.
[42] D. Mumford and J. Shah. Optimal approximations by piecewise smooth functions and associated variational problems. *Comm. Pure Appl. Math.*, 42:577–685, 1989.
[43] A. Novick-Cohen. The Cahn-Hilliard equation. In C. M. Dafermos and E. Feireisl, editors, *Handbook of Differential Equations – Evolutionary Equations*, chapter 4, pages 201–228. Elsevier, 2008.
[44] R. Rossi. On two classes of generalized viscous Cahn-Hilliard equations. *Comm. Pure Appl. Anal.*, 4:405–430, 2005.
[45] T. Roubíček. Rate independent processes in viscous solids at small strains. *Math. Methods Appl. Sci.*, 32:825–862, 2009. Erratum Vol. 32(16) p. 2176.
[46] T. Roubíček. Thermodynamics of rate independent processes in viscous solids at small strains. *SIAM J. Math. Anal.*, 42:256–297, 2010.
[47] T. Roubíček. *Nonlinear Partial Differential Equations with Applications*. Birkhäuser, Basel, 2nd edition, 2013.
[48] T. Roubíček. Adhesive contact of visco-elastic bodies and defect measures arising by vanishing viscosity. *SIAM J. Math. Anal.*, 45:101–126, 2013.
[49] T. Roubíček and C. G. Panagiotopoulos. Energy-conserving time-discretisation of abstract dynamical problems with applications in continuum mechanics of solids. *(Preprint arXiv no.1605.09762)*.
[50] T. Roubíček and G. Tomassetti. Thermomechanics of hydrogen storage in metallic hydrides: modeling and analysis. *Discr. Cont. Dyn. Syst. B*, 14:2313–2333, 2014.
[51] T. Roubíček and G. Tomassetti. Thermomechanics of damageable materials under diffusion: modeling and analysis. *Zeit. angew. Math. Phys.*, 66:3535–3572, 2015.
[52] T. Roubíček and J. Valdman. Perfect plasticity with damage and healing at small strains, its modelling, analysis, and computer implementation. *SIAM J. Appl. Math.*, 75:314–340, 2016.
[53] A. Sadjadpour and K. Bhattacharya. A micromechanics inspired constitutive model for shape-memory alloys. *Smart Mater. Structures*, 16:1751–1765, 2007.
[54] C. H. Scholz. *The Mechanics of Earthquakes and Faulting*. Cambridge Univ. Press, Cambridge, 2nd edition, 2002.
[55] P. Sedlák, M. Frost, B. Benešová, T. B. Zineb, and P. Šittner. Thermomechanical model for NiTi-based shape memory alloys including R-phase and material anisotropy under multi-axial loadings. *Intl. J. Plasticity*, 39:132–151, 2012.
[56] J. C. Simo and J. R. Hughes. *Computational Inelasticity*. Springer, Berlin, 1998.
[57] G. Stampacchia. Le problème de Dirichlet pour les équations elliptiques du second ordre à coefficients discontinus. *Ann. Inst. Fourier (Grenoble)*, 15:189–258, 1965.
[58] L. Wang. *Foundations of Stress Waves*. Elsevier, Amsterdam, 2007.
[59] N. N. Yanenko. *The Method of Fractional Steps*. Springer, Berlin, 1971.

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