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Approximation in multiscale modelling of microstructure evolution in shape-memory alloys

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Approximation in multiscale modelling of microstructure evolution in shape-memory alloys[1]

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Abstract: Various models of microstructure in deformation gradient and its evolution arising in martensitic mechanically-induced isothermal phase transformation are surveyed and scrutinized, focusing on over-bridging of various scales of the problem and its numerical approximation. In particular, numerically efficient model of a relaxed problem is shown to be approximated by conventional but computationally less efficient model based on standard partial differential inequalities.

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1 Introduction, principles of SMAs

Shape-memory alloys (=SMAs) are representatives of so-called smart materials which enjoy important applications especially in engineering and human medicine. SMAs exhibit specific, *hysteretic* stress/strain response and a so-called *shape-memory effect*. The mechanism behind it is quite simple: atoms tend to be arranged in several crystalographic configurations having different symmetry groups: higher symmetrical one (referred to as the *austenite* phase, typically cubic) has higher heat capacity while lower symmetrical one (called the *martensite* phase, typically tetragonal, orthorhombic, monoclinic, or a rhomboedric R-phase) has lower heat capacity and may exist, by symmetry, in several variants. We refer to [5, 11, 49, 43] for a thorough survey. Coexistence of various phases or phase variants and their (usually) fast reaction on (usually) slowly evolving external loading typically lead to complicated *microstructure* (cf. Figure fig:1(left) below) with very complex *evolution* behaviour, which gives an ultimate time/spatial *multiscale character* to the problem whose modelling thus becomes extremely difficult.

Confining to isothermal models based on *continuum mechanics*, there are several kinds of models depending on how the microstructure is described: here we focus on a "microscopical", or PDE-type model, based on conventional partial differential equations or inequalities in terms of deformation with possibly some order parameter, and on a "mesoscopical" model expressed in terms of displacements combined with special gradient Young measures to reflect better a multiscale character of the problem, cf. [4, 31, 32] or also [55, Chap.6]. Other models may involve further internal variables like volume fractions etc., for a survey see [57].

Particular difficulty is in modelling of evolution of microstructures to hit efficiently the hysteretic response, cf. [51]. To this point, we adopt a concept of *generalized standard materials* whose internal parameters (here volume fractions) are subjected to a *rate-independent* flow rule,

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which presumably result to a quasi-static rate-independent evolution when the loading-rate is infinitesimally slow.

Although models on particular levels are to more or less extent supported by rigorous mathematical and numerical analysis, the bridge between them is mostly missing. Beside surveying and ordering those type of results already available, the main goal of this contribution is in showing that the mentioned *PDE-type rate-independent model* may actually *approximate the mesoscopical model*. This thus gives a certain justification of particular models and clearer insight under what circumstances they apply, as well as a rigorous mathematical support of existing efficient numerical algorithms. Due to the wide of this topic, only the most essential aspects of mathematical proofs are presented.

2 PDE-type models based on conventional variational inequalities

We will build the model by exploiting the concept of a so-called *generalized standard solids* (due to Halphen and Nguyen [19]) combined with a *viscous-like response* in a Kelvin-Voigt-type rheology and inertia at *large strains*. We allow for a so-called *gradient theory* as far as deformation gradient concern and we address an isothermal case only.

2.1 Generalized standard materials, gradient theory, Kelvin-Voigt rheology, and variational principles

We consider $\Omega \subset \mathbb{R}^d$ a bounded smooth domain which we identify with the reference shape of the body (=the stress-free austenite). We denote by $y : \Omega \to \mathbb{R}^d$ the deformation of the body, and we let $F = \nabla y$. Then $u(x) = y(x)-x$ is the displacement of $x \in \Omega$, so that the *deformation gradient* is given by $F = \nabla y = \mathbb{I} + \nabla u$, where $\mathbb{I} \in \mathbb{R}^{d\times d}$ denotes the identity matrix. In order to describe phase transformation, we introduce a vectorial *order parameter* $z : \Omega \to \mathbb{R}^m$. To account for the so-called "interfacial effects", we introduce, in addition to the standard stress $S : \Omega \to \mathbb{R}^{d\times d}$, a *hyper-stress* $H : \Omega \to \mathbb{R}^{d\times d\times d}$ augmenting to S through $-\mathrm{div}\, H$. We further accept the concept of *hyperelastic material* with a specific *stored energy* $\varphi_{\varepsilon,\kappa}(F, G, z)$ (with parameters ε and k to be specified below in (2.11a) and with the tensor G as a placeholder for ∇F, i.e. the mentioned gradient theory) from which S and H can be derived as partial derivatives $[\varphi_{\varepsilon,\kappa}]'_F$ and $[\varphi_{\varepsilon,\kappa}]'_G$, respectively. The overall *stored energy* is thus

$$\Phi_{\varepsilon,\kappa}(y, z) = \int_\Omega \varphi_{\varepsilon,\kappa}(\nabla y, \nabla^2 y, z)\,\mathrm{d}x. \tag{2.1}$$

Moreover, given a mass density $\varrho > 0$, the overall *kinetic energy*

$$T_{\mathrm{kin}}(\dot y) = \frac{\varrho}{2}\int_\Omega |\dot y|^2\,\mathrm{d}x. \tag{2.2}$$

Another ingredient is a specific *dissipation energy* rate $\xi(\dot F, \dot z) := \frac14 \mathbb{D}(\dot F+\dot F^\top):(\dot F+\dot F^\top) + \zeta(\dot z)$. We consider $\zeta : \mathbb{R}^m \to \mathbb{R}$ to be continuous and positively homogeneous, thus non-smooth at zero, which is related with an activated rate-independent character of evolution of z itself, although the overall system will be rate dependent due to inertia given by ϱ in (2.2) and viscosity determined by $\mathbb{D}$. The overall pseudo-potential of dissipative forces Ξ and the dissipation-energy rate R are then

$$\Xi(\dot y, \dot z) = \int_\Omega \frac12 \mathbb{D}e(\dot y){:}e(\dot y) + \zeta(\dot z)\,\mathrm{d}x, \qquad R(\dot y, \dot z) = \int_\Omega \mathbb{D}e(\dot y){:}e(\dot y) + \zeta(\dot z)\,\mathrm{d}x \tag{2.3}$$

with $e(\dot y)=\frac12(\nabla\dot y+\nabla\dot y^\top)$. The last concept consists in adopting the *Kelvin-Voigt rheology* with (only infinitesimally frame-indifferent) viscosity so the the overall stress is $\sigma_{\rm tot}=\mathbb{D}e(\dot y)+S-{\rm div}\,H$. Then Halphen-Nguyen's standard generalized material [19] (see also e.g. [38]) is described by the system of *momentum equilibrium* ${\rm div}\,\sigma_{\rm tot}+f=\varrho\frac{\partial^2}{\partial t^2}y$ and the *flow rule* for the vector of internal parameters, which in our case means respectively

$$\varrho\frac{\partial^2 y}{\partial t^2}-{\rm div}\Big(\mathbb{D}e\big(\frac{\partial y}{\partial t}\big)+[\varphi_{\varepsilon,\kappa}]'_F(\nabla y,\nabla^2 y,z)-{\rm div}\,[\varphi_{\varepsilon,\kappa}]'_G(\nabla y,\nabla^2 y,z)\Big)=f, \tag{2.4a}$$

$$\partial\zeta\big(\frac{\partial z}{\partial t}\big)+[\varphi_{\varepsilon,\kappa}]'_z(\nabla y,\nabla^2 y,z)\ni 0, \tag{2.4b}$$

where $\partial\zeta$ denotes the subdifferential of the convex function ζ and f is an external bulk force. Several variational principles are supporting the system (2.4). The *Hamilton variation principle* adapted for nonconservative systems (cf. also Bedford [8, Section 1.3]) uses the Lagrangean $L(y,z,\dot y):=T_{\rm kin}(\dot y)-V(y,z)$ with the free energy $V(y,z):=\Phi_{\varepsilon,\kappa}(y,z)-\int_\Omega f\cdot y\,{\rm d}x$ and then (2.4) can be derived as the first-order condition (=critical point) for

$$\int_0^T L(y,z,\dot y)-\big\langle F,(u,z)\big\rangle\,{\rm d}t\quad\text{is stationar with a fixed }\ F:=\Xi'(\dot u,\dot z); \tag{2.5}$$

here F is thus in a position of a postulated nonconservative force; of course, here rather $F\in\partial\Xi'(\dot u,\dot z)$, however. Another approach postulates another Lagrangean as

$$\mathscr{L}(y,z,\dot y,\dot z):=\frac{{\rm d}}{{\rm d}t}\Phi_{\varepsilon,\kappa}+\Xi=\big\langle[\Phi_{\varepsilon,\kappa}]'_y(y,z),\dot y\big\rangle+\big\langle[\Phi_{\varepsilon,\kappa}]'_z(y,z),\dot z\big\rangle+\Xi(\dot u,\dot z), \tag{2.6}$$

and then (2.4) can be derived as the first-order condition for

$$(\dot y,\dot z)\mapsto\mathscr{L}(y,z,\dot y,\dot z)-\big\langle\mathscr{F},\dot y\big\rangle\quad\text{is minimal for any time }\ t, \tag{2.7}$$

where $\mathscr{F}$ is in a position of the bulk force, i.e. here $\langle\mathscr{F},v\rangle=\int_\Omega(f-\varrho\frac{\partial^2}{\partial t^2}y)\cdot v\,{\rm d}x$. One refers to (2.7) as a *minimum dissipation-potential principle*, cf. [6, 20, 21]. Degree-1 homogeneity of ζ, and thus of $\Xi(\dot y,\cdot)$ too, still allows for further interpretation of the flow rule (2.4b). Defining the convex "elastic domain" $K:=\partial_{\dot z}\Xi(\dot y,0)\equiv\partial_{\dot z}\Xi(0)$, the inclusion (2.4b) written as $\partial_{\dot z}\Xi(\frac{{\rm d}z}{{\rm d}t})+[\Phi_{\varepsilon,\kappa}]'_z(y,z)\ni 0$ means just $\langle\omega-\sigma_{\rm d},w-\frac{{\rm d}z}{{\rm d}t}\rangle\ge 0$ for any w and any $\omega\in\partial_{\dot z}\Xi(w)$, where we denoted the so-called thermodynamical *driving force* $\sigma_{\rm d}:=-[\Phi_{\varepsilon,\kappa}]'_z(y,z)$. In particular, for $w=0$ one obtains

$$\Big\langle\sigma_{\rm d},\frac{{\rm d}z}{{\rm d}t}\Big\rangle=\max_{\omega\in K}\Big\langle\omega,\frac{{\rm d}z}{{\rm d}t}\Big\rangle, \tag{2.8}$$

where we also used that always $\sigma_{\rm d}\in\partial_{\dot z}\Xi(\frac{{\rm d}z}{{\rm d}t})\subset\partial_{\dot z}\Xi(0)=K$, which employs the degree-1 homogeneity of $\Xi(\dot y,\cdot)$, so that always $\langle\sigma_{\rm d},\frac{{\rm d}z}{{\rm d}t}\rangle\le\max_{\omega\in K}\langle\omega,\frac{dz}{dt}\rangle$. The identity (2.8) says that the dissipation due to the driving force $\sigma_{\rm d}$ is maximal provided that the order-parameter rate $\frac{{\rm d}z}{{\rm d}t}$ is kept fixed while the vector of possible driving stresses ω varies freely over all admissible driving stresses from K. This just resembles so-called Hill's *maximum-dissipation principle* [23]. As the model is so far local in terms of z (cf. Sect. 2.3 for a generalization, however), one can localize (2.8) to obtain

$$\sigma_{\rm d}\cdot\frac{\partial z}{\partial t}=\max_{\omega\in K_0}\ \omega\cdot\frac{\partial z}{\partial t}\qquad\text{a.e. on }\Omega,\quad K_0:=\partial\zeta(0),\quad \sigma_{\rm d}=-[\Phi_{\varepsilon,\kappa}]'_z(y,z). \tag{2.9}$$

Note also that, given $K_0 \subset \mathbb{R}^m$, one can determine ζ as the Legendre-Fenchel conjugate $\delta^*_{K_0}$ to the indicator function δ_{K_0} of this convex set K_0. In terms of K_0, by standard convex-analysis calculus, (2.8) can also be written as

$$\frac{\partial z}{\partial t} \in \big[\partial\delta^*_{K_0}\big]^{-1}\big(\sigma_{\rm d}\big) = \partial\delta_{K_0}\big(\sigma_{\rm d}\big) = N_{K_0}\big(\sigma_{\rm d}\big) \tag{2.10}$$

where $N_{K_0}(\sigma_{\rm d})$ denotes the normal cone to K_0 at $\sigma_{\rm d}$.

2.2 Shape-memory-alloy modelling

We consider $m{-}1$ variants of martensite which are standardly determined, in the stress-free state, by *distortion matrices* U_μ, $\mu = 2, ..., m$, while the cubic austenite corresponds to $U_1 = \mathbb{I}$. Further, inspired by [18, 40, 42], we define a bounded Lipschitz mapping $\mathcal{L} : \mathbb{R}^{3\times3} \to \mathbb{R}^m$ that identifies particular phases of phase variants, namely we assume that $\mathcal{L}$ is frame indifferent, $\mathcal{L}_\mu \geq 0$ and $\mathcal{L}_\mu(F) = 1$ if $F^\top F$ lives near $U_\mu^\top U_\mu$ for all $\mu = 1, ..., m$ and $\sum_{\mu=1}^m \mathcal{L}_\mu = 1$. Then, using the concept of *St.Venant-Kirchhoff material* for each particular phase variant (cf. [49, Sect.6.6] or also [32]), we postulate

$$\varphi_{\varepsilon,\kappa}(F, G, z) := \phi(F) + \frac{\kappa}{2}\big|z - \mathcal{L}(F)\big|^2 + \frac{\varepsilon}{2}\big|G\big|^2, \quad \text{with} \tag{2.11a}$$

$$\phi(F) := \widetilde{\min}\bigg(\Big(\frac{1}{2}\sum_{i,j,k,l=1}^{d} E^\mu_{ij}\mathbb{C}^\mu_{ijkl}E^\mu_{kl}\Big)_{\mu=1,...,m}\bigg) \quad \text{where} \tag{2.11b}$$

$$E^\mu := \frac{R_\mu^\top(U_\mu^\top)^{-1}F^\top F U_\mu^{-1}R_\mu - \mathbb{I}}{2}, \qquad \widetilde{\min} : \mathbb{R}^m \to \mathbb{R}, \tag{2.11c}$$

where $\mathbb{C}^\mu = \{\mathbb{C}^\mu_{ijkl}\}$ is the 4th-order tensor of *elastic moduli* satisfying the usual symmetry relations depending also on symmetry of the specific μ-phase (variant) μ and E^μ is the *Green-Lagrange strain* tensor related to the distortion of μ-phase, and R_μ is a rotation matrix transforming the basis of the austenite to the basis of the martensitic variant μ (in particular $R_1 = \mathbb{I}$). The another vectorial variable z plays a role of an order parameter. As to $\widetilde{\min} : \mathbb{R}^m \to \mathbb{R}$, in the simplest variant, one can consider just $\widetilde{\min}(e_1, ..., e_m) := \min(e_1, ..., e_m)$ which is, however, nonsmooth although it still complies with Definition 2.2. Yet, e.g. Definition 2.1(iv) needs $\widetilde{\min}$ smooth and one can consider e.g. $\widetilde{\min}(e_1, ..., e_m) := -K\ln(\sum_{\mu=1}^m {\rm e}^{-e_\mu/K})$ with some $K > 0$. For a sophisticated construction method of ϕ based on cubic C^2-splines fitted with experimentally measured wells and elastic moduli in specific shape-memory materials we refer to [24]. The constant κ is rather introduced for modelling to allow for mathematical analysis and is assumed to be large so that presumably z is mostly close to $\mathcal{L}(\nabla y)$, cf. also (2.22) below, so that the vectorial order parameter z essentially is mostly of the form $(0, ..., 1, ..., 0)$ on domains occupied by particular pure phase variants. Note that (2.11a) yields $\varphi_{\varepsilon,\kappa}(F, \cdot, \cdot)$ quadratic, from which we can take some benefits later, cf. e.g. (2.18).

Then, putting (2.11) into (2.4) turns it to the system

$$\varrho\frac{\partial^2 y}{\partial t^2} - {\rm div}\,\Big(\mathbb{D}e\big(\frac{\partial y}{\partial t}\big) + \phi'(\nabla y) + \kappa\big(z{-}\mathcal{L}(\nabla y)\big)\mathcal{L}'(\nabla y) - \varepsilon{\rm div}\,\nabla^2 y\Big) = f, \tag{2.12a}$$

$$\partial\zeta\big(\frac{\partial z}{\partial t}\big) + \kappa z \ni \kappa\mathcal{L}(\nabla y). \tag{2.12b}$$

We consider and initial-boundary value problem for (2.12) and complete this system with initial conditions

$$y(0) = y_0, \qquad \frac{\partial y}{\partial t}(0) = \dot{y}_0, \qquad z(0) = z_0. \tag{2.13}$$

We have also to specify boundary conditions for y. Usually a specimen is loaded by (in some idealization) some hard-device on some part of the boundary $\Gamma_0 \subset \Gamma := \partial\Omega$ which on the rest $\Gamma_1 = \Omega \setminus \Gamma_0$ it is free. We consider, for simplicity, time-constant Dirichlet boundary conditions and a load by traction force:

$$y(x) = x \quad \text{for a.a. } x{\in}\Gamma_0, \qquad\qquad \varepsilon\nabla^2 y{:}(\nu{\otimes}\nu) = 0 \quad \text{on } \Gamma, \tag{2.14a}$$

$$\Big(\mathbb{D}e\big(\frac{\partial y}{\partial t}\big) + \phi'(\nabla y) + \kappa\big(z{-}\mathcal{L}(\nabla y)\big)\mathcal{L}'(\nabla y) - \varepsilon\mathrm{div}\,\nabla^2 y\Big)\nu \\ +\ \varepsilon(\mathrm{div}_{\rm s}\nu)\nabla^2 y{:}(\nu{\otimes}\nu) - \varepsilon\mathrm{div}_{\rm s}(\nabla^2 y{\cdot}\nu) = g \quad \text{on } \Gamma_1, \tag{2.14b}$$

where ν denotes the unit outward normal to Γ, and $\mathrm{div}_{\rm s} := \mathrm{Trace}(\nabla_{\rm s})$ denotes the $(d{-}1)$-dimensional "surface divergence" with the the tangential derivative $\nabla_{\rm S}$ defined as $\nabla_{\rm S} v = \nabla v - (\nabla v{\cdot}\nu)\nu$. The right-hand side g in (2.14b) represents the "true" surface force, which is related with the occurence of the $\mathrm{div}_{\rm S}$-terms in (2.14b); this rather technical effect is well known in mechanics of complex (also called nonsimple) continua, and we refer to [17, 50, 64] for details. The generalization for time-varying Dirichlet condition is much more realistic for most experiments and mathematically possible but rather very technical especially if physically relevant multiplicative decomposition is considered; cf. [36] for the case of plasticity at large strains.

Without going into details, a suitable weak-solution concept may rely on positive homogeneity of ζ and combine concept of energetic solution from theory of rate independent processes by Mielke at al. [16, 37, 40, 41] adapted for coupling with viscous/inertial effects [59].

We use the standard notation L^p for Lebesgue spaces, $W^{k,p}$ for Sobolev spaces, and $M(\cdot)$ for spaces of measures, and further we denote $I := [0,T]$ with a fixed time horizon T, $Q := I{\times}\Omega$, $\Sigma_i = I{\times}\Gamma_i$, and $\mathrm{BV}(I;X)$ (resp. $C_{\rm w}(I;X)$) for bounded-variation (resp. weakly continuous) mappings $I \to X$. Let us further denote $W^{k,p}_{\Gamma_0}(\Omega) := \{v \in W^{k,p}_{\Gamma_0}(\Omega);\ v|_{\Gamma_0} = 0\}$. Consistently with "$:$" and "$\cdot$" meaning summation over 2 or 1 indices used already above, by "$\vdots$" we will abbreviate summation over 3 indices.

Definition 2.1 *The pair (y,z) is called an energetic solution to the initial-boundary value problem (2.12)–(2.13)–(2.14) if*
(i) $y \in C_{\rm w}(I;W^{2,2}(\Omega;\mathbb{R}^d))$,
(ii) $\frac{\partial y}{\partial t} \in L^2(Q;\mathbb{R}^d) \cap C_{\rm w}(I;L^2(\Omega;\mathbb{R}^d)) \cap W^{1,2}(I;W^{2,2}_{\Gamma_0}(\Omega;\mathbb{R}^d)^*)$,
(iii) $z \in C_{\rm w}(I;L^2(\Omega;\mathbb{R}^m)) \cap \mathrm{BV}(I;L^1(\Omega;\mathbb{R}^m))$,
(iv) the momentum equation (2.12a) holds in a usual weak sense, i.e.

$$\int_Q \Big(\mathbb{D}e\big(\frac{\partial y}{\partial t}\big) + \phi'(\nabla y) + \kappa\big(z{-}\mathcal{L}(\nabla y)\big)\mathcal{L}'(\nabla y)\Big){:}\nabla v + \varepsilon\nabla^2 y \,\vdots\, \nabla^2 v \\ - \varrho\frac{\partial y}{\partial t}{\cdot}\frac{\partial v}{\partial t}\mathrm{d}x\mathrm{d}t = \int_Q f{\cdot}v\mathrm{d}x\mathrm{d}t + \int_{\Sigma_1} g{\cdot}v\mathrm{d}S\mathrm{d}t + \int_\Omega \varrho\dot{y}_0{\cdot}v\mathrm{d}x \tag{2.15}$$

for any z smooth with $z(T)=0$ and $z|_{\Sigma_0}=0$,

(v) *the following energy balance (as an inequality) holds:*

$$\Phi_{\varepsilon,\kappa}(y(T),z(T))+T_{\rm kin}\Big(\frac{\partial y}{\partial t}(T)\Big)+{\rm Var}_\zeta(z;I)+\int_Q\mathbb{D}e\big(\frac{\partial y}{\partial t}\big){:}e\big(\frac{\partial y}{\partial t}\big)\,{\rm d}x{\rm d}t$$
$$\le\Phi_{\varepsilon,\kappa}(y_0,z_0)+T_{\rm kin}\big(\dot y_0\big)+\int_Q f\cdot\frac{\partial y}{\partial t}\,{\rm d}x{\rm d}t+\int_{\Sigma_1}g\cdot\frac{\partial y}{\partial t}\,{\rm d}S{\rm d}t, \tag{2.16}$$

where ${\rm Var}_\zeta(z;I)=\sup\sum_{i=1}^k\int_\Omega\zeta(z(t_i,x)-z(t_{i-1},x))\,{\rm d}x$ with the supremum taken over all partitions of the type $0{=}t_0{<}t_1{<}...{<}t_k{=}T$, $k{\in}\mathbb{N}$, i.e. the total variation of z over I with respect to ζ,

(vi) *the following so-called "semi-stability" holds for a.a. $t{\in}I$:*

$$\forall\,v{\in}L^2(\Omega;\mathbb{R}^m):\ \Phi_{\varepsilon,\kappa}\big(y(t),z(t)\big)\le\Phi_{\varepsilon,\kappa}\big(y(t),v\big)+\int_\Omega\zeta\big(v{-}z(t)\big)\,{\rm d}x, \tag{2.17}$$

(vii) *the initial conditions $y(0)=y_0$ and $z(0)=z_0$ hold.*

An important fact, shown in [59], is that Definition 2.1 is indeed consistent and selective in the sense that any classical solution to (2.12)–(2.13) is also the energetic one and, conversely, any energetic solution which is also smooth enough is a classical one if $\varphi_{\varepsilon,\kappa}(y,G,\cdot)$ is convex, e.g. in the case (2.11a). Important feature of this definition is also that, under some further mild data qualification, the energy balance (2.16) holds as an equality, as shown in [59, Prop.5.4] by using technique for fully-rate independent processes [16, 37, 38]. Let us also remark that the integral identity (2.15) has been casted from (2.12a) with (2.14) by using twice Green formula on Ω and once a surface Green-type formula $\int_\Gamma w{:}((\nabla_{\rm S}v){\otimes}\nu)\,{\rm d}S=\int_\Gamma({\rm div}_{\rm S}\nu)(w{:}(\nu{\otimes}\nu)v-{\rm div}_{\rm S}(w{\cdot}\nu)v\,{\rm d}S$.

Proposition 2.1 *Let $\varepsilon>0$, $\kappa<\infty$, $\mathbb{D}$ be positive definite, $d\le3$, φ be from (2.11) with $\widetilde{\min}:\mathbb{R}^m\to\mathbb{R}$ smooth and having at most linear growth, $f\in L^2(Q;\mathbb{R}^d)$, $g\in L^2(\Sigma_1;\mathbb{R}^d)$, $y_0\in W^{2,2}(\Omega;\mathbb{R}^d)$, $z\in L^2(\Omega;\mathbb{R}^m)$, and $\dot y_0\in L^2(\Omega;\mathbb{R}^d)$. Then there is an energetic solution to (2.12)–(2.13)–(2.14) in the sense of Definition 2.1.*

Sketch of the proof. First, one makes an implicit discretization in time, showing existence of a discrete solution by a direct method of Calculus of Variations, using that ϕ from (2.11) as at most polynomial growth of order 4 and $W^{2,2}(\Omega)$ is compactly embedded into $W^{1,4}(\Omega)$ as $d\le3$. Then a-priori estimates of the type (i)–(iii) in Definition 2.1 can be proved and convergence can be shown by using linearity of the highest-order terms in (2.12a) and Aubin-Lions' compact-embedding theorem for $\phi'(\nabla y)+\kappa\mathcal{L}'(\nabla y)$, while the limit passage to (2.16) is by weak* lower-semicontinuity and to (2.17) by a weak convergence of z and the quadratic structure of $\varphi_{\varepsilon,\kappa}(F,G,\cdot)$ in (2.11a). This last property allows for writing (2.17) integrated over I in the form

$$\int_0^T\!\!\bigg(\Phi_{\varepsilon,\kappa}\big(y,v\big)-\Phi_{\varepsilon,\kappa}\big(y,z\big)+\int_\Omega\zeta\big(v{-}z\big)\,{\rm d}x\bigg){\rm d}t=\int_Q\frac{\kappa}{2}\big|v{-}\mathcal{L}(\nabla y)\big|^2-\frac{\kappa}{2}\big|z{-}\mathcal{L}(\nabla y)\big|^2+\zeta\big(v{-}z\big)\,{\rm d}x{\rm d}t$$
$$=\int_Q\frac{\kappa}{2}|v|^2-\frac{\kappa}{2}|z|^2-\kappa(v{-}z)\cdot\mathcal{L}(\nabla y)+\zeta\big(v{-}z\big)\,{\rm d}x{\rm d}t$$
$$=\int_Q\kappa(v{-}z)\cdot\Big(\frac{z}{2}{+}\frac{v}{2}{-}\mathcal{L}(\nabla y)\Big)+\zeta\big(v{-}z\big)\,{\rm d}x{\rm d}t, \tag{2.18}$$

where the limit passage is easy even by mere weak convergence of z's when taking a suitable sequence of test functions v's to hold the differences $(v-z)$'s constant (cf. (3.6) below) and when also again using Aubin-Lions' theorem for the term $\mathcal{L}(\nabla y)$; for details see [59]. $\square$

2.3 Nonlocal modifications of stored energy or of dissipation

Modifications of the biharmonic term in (2.12a) that would allow for sharp interfaces between particular phases (i.e. jumps of ∇y across $(d-1)$-dimensional manifolds) are sometimes employed. One option is to make this term nonlinear to admit BV- instead of $W^{1,2}$-structure of ∇y, i.e. the interfacial energy like $\int_\Omega \varepsilon|\nabla y|\mathrm{d}x$ instead of $\int_\Omega \frac{\varepsilon}{2}|\nabla^2 y|^2\mathrm{d}x$ would occur in (2.1) from (2.11a), cf. [34] for a similar idea in terms of z. Alternatively, advocated e.g. by [52, 53, 54], in the linear setting one can replace this interfacial energy by a *nonlocal* form $\frac{\varepsilon}{4}\int_\Omega\int_\Omega \frac{|\nabla y(x)-\nabla y(\tilde x)|^2}{|x-\tilde x|^{d+2\gamma}}\mathrm{d}x\mathrm{d}\tilde x$ with some $0<\gamma<1$, obtaining mathematically the same compactifying effect and, for $\gamma<1/2$, allowing for the mentioned sharp interfaces. Then the stress $\mathrm{div}\nabla^2 y$ is replaced by

$$\big[\sigma_{\rm if}(\nabla y)\big](x) := \int_\Omega \frac{\nabla y(x)-\nabla y(\tilde x)}{|x-\tilde x|^{d+2\gamma}}\mathrm{d}\tilde x, \tag{2.19a}$$

so that (2.12a) takes the form

$$\varrho\frac{\partial^2 y}{\partial t^2} - \mathrm{div}\Big(\mathbb{D}e\big(\frac{\partial y}{\partial t}\big) + \phi'(\nabla y) + \kappa\mathcal{L}'(\nabla y) + \varepsilon\sigma_{\rm if}(\nabla y)\Big) = f + \kappa z. \tag{2.19b}$$

The boundary conditions (2.14) then simplifies by omitting the second condition in (2.14a) and modifying (2.14b) correspondingly. Definition 2.1 then just replaces $W^{2,2}$ with $W^{1+\gamma,2}$ if $\gamma > d/4$ and existence of energetic solutions can be shown by entirely the same way as before, using now compact embedding of the Sobolev-Slobodetskiĭ space $W^{1+\gamma,2}(\Omega)$ into $W^{1,4}(\Omega)$. If $\gamma \le d/4$, we must use $W^{1+\gamma,2}(\Omega)\cap W^{1,4}(\Omega)$ instead of $W^{2,2}(\Omega)$ and a subtle argument for weak lower-semicontinuity of $\Phi_{\varepsilon,\kappa}$ relying on $\phi\ge 0$.

Another useful nonlocal modification of the models (2.12) or (2.19) with (2.12b), advocated by [14, Remark 4.3] or [65, Sect.5] in context of ferromagnetism and in [46, Formulas (2)-(3)] or [47, Formula (4) with (8)] for the case of damage (cf. also an overview and in particular [25, Formulas 26.12-13] in the context of plasticity) and allowing for further up-scaling, consists in modifying (2.3) as

$$R(\dot z) := \int_\Omega \zeta(\mathfrak{S}\dot z)\,\mathrm{d}x \tag{2.20}$$

with $\mathfrak{S} : L^2(\Omega)\to L^2(\Omega)$ a linear continuous injective operator. If $\mathfrak{S}$ is the identity, we get the previous case. If $\mathfrak{S}$ is compact, we get some regularizing effect. Then (2.12b) results to

$$\mathfrak{S}^*\partial\zeta\big(\mathfrak{S}\frac{\partial z}{\partial t}\big) + \kappa z \ni \kappa\mathcal{L}(\nabla y), \tag{2.21}$$

where $\mathfrak{S}^* : L^2(\Omega)\to L^2(\Omega)$ denotes the adjoint mapping to $\mathfrak{S}^*$. Then Definition 2.1 modifies just by taking $\zeta\circ\mathfrak{S}$ in place of ζ both in (2.16) and in (2.17) and (ii) replaces $z\in \mathrm{BV}(I;L^1(\Omega;\mathbb{R}^m))$ by $\mathfrak{S}z\in \mathrm{BV}(I;L^1(\Omega;\mathbb{R}^m))$. If $\mathfrak{S}$ is compact, existence of energetic solutions in this case is even simpler because convergence through (2.17) now may alternatively employ the compactifying property of $\mathfrak{S}$ for direct passage to the limit in $\int_Q \zeta(\mathfrak{S}(v-z))\,\mathrm{d}x\mathrm{d}t$ by continuity. For usage of Aubin-Lions' theorem for a strong convergence in z's, it is important that $\mathfrak{S}$ is assumed injective.

One can think e.g. about $\mathfrak{S} := (\mathrm{I}-\epsilon\Delta)^{-1}$ in the sense that $\tilde{v} = \mathfrak{S}v := (\mathrm{I}-\epsilon\Delta)^{-1}v$ is understood as the unique weak solution of the boundary value problem $\tilde{v} - \epsilon\Delta\tilde{v} = v$ on Ω with the boundary conditions $\frac{\partial}{\partial\nu}\tilde{v} = 0$ on $\partial\Omega$, cf. e.g. [46, Formula (2) with (9)] and [47, Formula (4) with (16)]. The linear mapping $(\mathrm{I}-\epsilon\Delta)^{-1}$ is then obviously a homeomorphism $W^{1,2}(\Omega)^* \to W^{1,2}(\Omega)$ so that altogether we have $(\mathrm{I}-\varepsilon\Delta)^{-1} : L^2(\Omega) \Subset W^{1,2}(\Omega)^* \to W^{1,2}(\Omega) \Subset L^2(\Omega)$ where the first compact embedding is just an adjoint mapping to the compact embedding $W^{1,2}(\Omega) \Subset L^2(\Omega)$. Moreover, for $\epsilon > 0$ small, such $\mathfrak{S}$ is close to the identity I on $L^2(\Omega)$ and also the resulting solutions are expected to be close to those with $\mathfrak{S}$ omitted; cf. Proposition 3(iii) for the quasi-static case.

2.4 The model with $\kappa = \infty$ as a limit for $\kappa \to \infty$

The motivation for implementing the phase-field concept (i.e. introducing the variable z and $\kappa < \infty$) is some sort of a regularization to facilitate some cases of upscaling in Sect. 3 (cf. Proposition 3.1) and augmentation for anisothermal cases (not addressed here, however). Yet, it is of interest to see how the model behaves for $\kappa \to \infty$.

It is not difficult to see that the estimates of the type (i)–(iii) in Definition 2.1 (modified possibly as mentioned above is Sect. 2.3) are uniform with respect to κ and one can ask a question how energetic solutions, let us now denote them by (u_κ, z_κ), behave for $\kappa \to \infty$. An additional estimate

$$\big\|z_\kappa - \mathcal{L}(\nabla y_\kappa)\big\|_{L^\infty(I;L^2(\Omega;\mathbb{R}^m))} \le C\kappa^{-1/2} \to 0 \tag{2.22}$$

indicates that in the limit the phase-field z is merely determined by the deformation gradient $z = \mathcal{L}(\nabla y)$. The term $\frac{1}{2}\kappa|z - \mathcal{L}(F)|^2$ in (2.11a) is replaced by an indicator function of the constraint $z = \mathcal{L}(F)$ and then we denote the resulted function by $\varphi_{\varepsilon,\infty}$ and, referring to (2.1), then also $\Phi_{\varepsilon,\infty}$, i.e.

$$\Phi_{\varepsilon,\infty}(y,z) = \begin{cases} \int_\Omega \phi(\nabla y) + \frac{\varepsilon}{2}\sigma_{\rm if}(\nabla y){:}\nabla y \,\mathrm{d}x & \text{if } z = \mathcal{L}(\nabla y) \text{ a.e. on } \Omega, \\ +\infty & \text{elsewhere.} \end{cases} \tag{2.23}$$

The semi-stability (2.17) then becomes just a trivial identity. In (2.23), either $\sigma_{\rm if}(\nabla y) = -\mathrm{div}\, H = -\mathrm{div}(\nabla^2 y)$ or $\sigma_{\rm if}(\nabla y)$ from (2.19a). Alternatively, z can be eliminated by using the constraint in (2.23) which is explicit in z. Therefore, the limit solution has to be understood differently, namely in a usual week sense. Here, the limit problem is the system

$$\varrho\frac{\partial^2 y}{\partial t^2} - \mathrm{div}\Big(\mathbb{D}e\big(\frac{\partial y}{\partial t}\big) + \phi'(\nabla y) + (\mathfrak{S}^*\omega){\cdot}\mathcal{L}'(\nabla y) + \varepsilon\sigma_{\rm if}(\nabla y)\Big) = f, \tag{2.24a}$$

$$\omega \in \partial\zeta\Big(\mathfrak{S}\big(\mathcal{L}'(\nabla y) : \nabla\frac{\partial y}{\partial t}\big)\Big), \tag{2.24b}$$

with $\omega \in L^\infty(Q;\mathbb{R}^m)$ a vectorial "direction" of phase-transformation processes currently undergoning. By the definition of $\partial\zeta$, the *weak solution* u then standardly means the properties (i)–(ii) from Definition 2.1 together with that

$$\int_Q \zeta(\mathfrak{S}v) + \omega{\cdot}\Big(v - \mathfrak{S}\big(\mathcal{L}'(\nabla y){:}\nabla\frac{\partial y}{\partial t}\big)\Big) - \zeta\Big(\mathfrak{S}\big(\mathcal{L}'(\nabla y){:}\nabla\frac{\partial y}{\partial t}\big)\Big)\mathrm{d}x\mathrm{d}t \ge 0 \tag{2.25}$$

holds for any $v \in L^1(Q;\mathbb{R}^m)$, and (2.24a) holds in a usual weak sense, and also the initial and boundary conditions (2.13)–(2.14) hold, possibly modified for (2.19a). Of course, we must now assume $z_0 = \mathcal{L}(\nabla y_0)$. For $\mathfrak{S}$ not compact (e.g. the identity), (2.25) would not serve well because of the term $\int_Q \omega\cdot\mathfrak{S}(\mathcal{L}'(\nabla y){:}\nabla\frac{\partial y}{\partial t})$. This term must be then substituted from (2.24a) tested by $\frac{\partial y}{\partial t}$, which results to the inequality

$$\int_Q \zeta(\mathfrak{S}v) + \omega\cdot v\,\mathrm{d}x\mathrm{d}t \geq \int_Q \zeta\Big(\mathfrak{S}\big(\mathcal{L}'(\nabla y){:}\nabla\frac{\partial y}{\partial t}\big)\Big) + \mathbb{D}e\big(\frac{\partial y}{\partial t}\big){:}\big(\frac{\partial y}{\partial t}\big)\mathrm{d}x\mathrm{d}t$$
$$+ T_{\rm kin}\Big(\frac{\partial y}{\partial t}(T)\Big) + G_{\varepsilon,\kappa}\big(T, y(T), z(T)\big) - T_{\rm kin}\big(y_0\big) - G_{\varepsilon,\kappa}\big(0, y_0, z_0\big) \tag{2.26a}$$

where $T_{\rm kin}$ is from (2.2) and where we abbreviated

$$G_{\varepsilon,\kappa}(t, y, z) := \Phi_{\varepsilon,\kappa}(y, z) - \int_\Omega f(t)\cdot y\,\mathrm{d}x - \int_{\Gamma_1} g\cdot y\,\mathrm{d}S. \tag{2.26b}$$

The definition of the weak solution (2.24a) with (2.26) works not only for $\kappa = \infty$ but also for $\kappa < \infty$ and existence of a weak solution then follows from Proposition 2.1 because any energetic solution (y_κ, z_κ) induces also a weak one $(y_\kappa, \omega_\kappa)$ by $\omega_\kappa := \kappa\mathfrak{S}^{-1}(\mathcal{L}(\nabla y_\kappa) - z_\kappa)$.

Proposition 2.2 *Let $\varepsilon > 0$, $\mathfrak{S}$ be linear, continuous, injective, and $\mathbb{D}$, f and g be as in Proposition 2.1. Then the energetic solutions (y_κ, z_κ) to (2.12)–(2.13)–(2.14) in the sense of Definition 2.1 converge, after conversion into the weak solutions $(y_\kappa, \omega_\kappa)$, for $\kappa \to \infty$ (in terms of subsequences) to a weak solution (y, ω) to (2.24), i.e. satisfying (2.24a) in a usual weak sense and (2.26) for $\kappa = \infty$. In particular, a weak solution to (2.24) does exist.*

Sketch of the proof: A-priori estimates of y_κ in the spaces from Definition 2.1(i)–(ii) are uniform in κ, and also ω_κ is bounded in $L^\infty(Q;\mathbb{R}^m)$ because $\omega_\kappa \in \partial\zeta(\mathfrak{S}\frac{\partial}{\partial t}z_\kappa)$. All terms in (2.24a) are linear except $(\mathfrak{S}^*\omega)\cdot\mathcal{L}'(\nabla y)$ for which we use weak* convergence (of a subsequence) of ω's and strong convergence of ∇y's by Aubin-Lions' theorem. The limit passage in (2.26a) is then by weak continuity and weak lower-semicontinuity in the left-hand and the right-hand sides, respectively. □

In [48], the existence of a weak solution to (2.24) was proved only with a modification for a higher-order viscosity of the type ${\rm div}^2\nabla^2\frac{\partial y}{\partial t}$.

2.5 Quasi-static evolution

It is generally interesting to study various limits if the rate-dependent effects (i.e. here inertia and viscosity) are suppressed. Vanishing $\mathbb{D}$ has been scrutinized in [51] for (2.24) even for $\mathfrak{S}$ omitted (i.e. $\mathfrak{S}$ identity) but considering still a higher-order interfacial term like ${\rm div}^3\nabla^3 y$, showing convergence to a weak solution to a hyperbolic variational inequality, and similar results apply to (2.12), too. Slowing down the loading rate might be expected, after scaling time to a fixed interval, say $[0, 1]$, to lead to suppression of both the inertial and of the viscous terms. This effect has actually been shown in [59, Prop.6.2] but under assumptions which would here require ϕ and $\mathcal{L}$ quadratic. This is not realistic in our applications and hence this scaling is unfortunately not clear in our case.

Anyhow, one can alternatively study the quasi-static evolution problem itself, i.e. just (2.12) or (2.24) with $\varrho = 0$ and $\mathbb{D}$ together with (2.13), or possibly with the modification (2.19). Namely, (2.12)–(2.13)–(2.14) with (2.19) yields the problem

$$-{\rm div}\,\big(\phi'(\nabla y) + \kappa\mathcal{L}'(\nabla y) + \varepsilon\sigma_{\rm if}(\nabla y)\big) = f + \kappa z, \tag{2.27a}$$

$$\mathfrak{S}^*\partial\zeta\big(\mathfrak{S}\frac{\partial z}{\partial t}\big) + \kappa z \ni \kappa\mathcal{L}(\nabla y), \qquad z(0) = z_0, \tag{2.27b}$$

with $\sigma_{\rm if}(\nabla y)$ again either $-{\rm div}\,\nabla^2 y$ or from (2.19a) and with (2.14) modified possibly as mentioned above. Note that we naturally also forgot the conditions $y(0)=y_0$ and $\frac{\partial y}{\partial t}(0)=\dot y_0$ from (2.13). Similarly, (2.24) reduces to

$$-\,{\rm div}\,\big(\phi'(\nabla y)+(\mathfrak{S}^*\omega)\cdot\mathcal{L}'(\nabla y)+\varepsilon\sigma_{\rm if}(\nabla y)\big)=f,\qquad y(0)=y_0, \tag{2.28a}$$

$$\omega\in\partial\zeta\Big(\mathfrak{S}\big(\mathcal{L}'(\nabla y):\nabla\frac{\partial y}{\partial t}\big)\Big); \tag{2.28b}$$

note that we prescribed y at $t=0$ because z is no longer involved in the problem but, in fact, only $\mathcal{L}(\nabla y(t))=\mathcal{L}(\nabla y_0)$ matters at $t=0$.

As $\frac{\partial y}{\partial t}$ and thus also $f\cdot\frac{\partial y}{\partial t}$ are not controlled in the quasistatic case, we must qualify $f\in W^{1,1}(I;L^2(\Omega;\mathbb{R}^d))$ and $g\in W^{1,1}(I;W^{1/2,2}(\Omega;\mathbb{R}^d))$, and make by-part integration in time. Let ${\rm B}(I;X)$ denote the space of bounded measurable mappings $I\to X$. Definition 2.1 then modifies to:

Definition 2.2 (Mielke & al. [40, 40, 42]) *The pair (u,z) is an energetic solution to (2.27), resp. (2.28), if*
(i) $u\in{\rm B}(I;W^{1+\gamma,2}(\Omega;\mathbb{R}^d))$,
(ii) $z\in{\rm B}(I;L^2(\Omega;\mathbb{R}^m))$ *and* $\mathfrak{S}z\in{\rm BV}(I;L^1(\Omega;\mathbb{R}^m))$,
(iii) employing $G_{\varepsilon,\kappa}$ from (2.26b), the following energy balance (as an inequality) holds:

$$G_{\varepsilon,\kappa}(T,y(T),z(T))+{\rm Var}_{\zeta\circ\mathfrak{S}}(z;I)\le G_{\varepsilon,\kappa}(0,y_0,z_0)+\int_Q\frac{\partial f}{\partial t}\cdot y\,{\rm d}x{\rm d}t+\int_{\Sigma_1}\frac{\partial g}{\partial t}\cdot y\,{\rm d}S{\rm d}t, \tag{2.29}$$

(iv) the so-called stability holds for each $t\in I$, $\tilde y\in W^{1+\gamma,2}(\Omega;\mathbb{R}^d)$, and $\tilde v\in L^2(\Omega;\mathbb{R}^m)$:

$$G_{\varepsilon,\kappa}\big(t,y(t),z(t)\big)\le G_{\varepsilon,\kappa}\big(t,\tilde y,\tilde v\big)+\int_\Omega\zeta\big(\mathfrak{S}(\tilde v-z(t))\big)\,{\rm d}x, \tag{2.30}$$

(v) the initial condition $y(0)=y_0$, resp. $z(0)=z_0=\mathcal{L}(\nabla y_0)$, holds.

Note that Definition 2.2 is completely derivative-free in the sense that neither from $\frac{\partial y}{\partial t}$, $\frac{\partial z}{\partial t}$, ϕ', nor $\mathcal{L}'$ are involved. Note also that in case $\kappa=\infty$, ω from (2.28) does not occur in Definition 2.2 and, assuming $z_0=\mathcal{L}(\nabla y_0)$, (2.29) implies $z=\mathcal{L}(\nabla y)$ a.e. on Q and thus, in fact, even $z\in L^\infty(Q;\mathbb{R}^m)$.

Proposition 2.3 *Let $\varepsilon>0$ be fixed, $\mathfrak{S}$ be linear, continuous, injective, $f\in W^{1,1}(I;L^2(\Omega;\mathbb{R}^d))$, $g\in W^{1,1}(I;W^{1/2,2}(\Omega;\mathbb{R}^d))$, and let $z_0=\mathcal{L}(\nabla y_0)\in L^\infty(\Omega;\mathbb{R}^m)$ be stable. Then:*
(i) for any $\kappa\le\infty$, there exists an energetic solution (y_κ,z_κ) to (2.27), resp. (2.28) in the above sense.
(ii) Moreover, if $\mathfrak{S}$ is compact, then (in terms of selected subsequences) (y_κ,z_κ) converges for $\kappa\to\infty$ to energetic solutions (y,z) to (2.28) in the sense that $\frac{\partial}{\partial t}G_{\varepsilon,\kappa}(t,y_\kappa)\to\frac{\partial}{\partial t}G_{\varepsilon,\infty}(t,y_\infty)$ weakly in $L^1(0,T)$ and that $\mathfrak{S}z_\kappa(t)\to\mathfrak{S}z(t)$ weakly in $L^1(\Omega;\mathbb{R}^m)$, $G_{\varepsilon,\kappa}(t,y_\kappa(t),z_\kappa(t))\to G_{\varepsilon,\infty}(t,y(t),z(t))$, ${\rm Var}_{\zeta\circ\mathfrak{S}}(z_\kappa;[0,t])\to{\rm Var}_{\zeta\circ\mathfrak{S}}(z;[0,t])$, $z_\kappa(t)\to z(t)$ weakly $L^2(\Omega;\mathbb{R}^m)$ for all $t\in I$, and there is another subsequence (depending on t) such that $y_\kappa(t)\to y(t)$ weakly in $W^{1+\gamma,2}(\Omega;\mathbb{R}^d)$.
(iii) If $\kappa<\infty$ is fixed and $\{\mathfrak{S}_k\}_{k\in\mathbb{N}}$ is a sequence of linear, continuous, injective operators converging in $\mathscr{L}(L^2(\Omega),L^2(\Omega))$ to the identity, then the corresponding energetic solutions (y_k,z_k) converge in the above sense to energetic solutions of the problem with $\mathfrak{S}$ omitted, in particular $\mathfrak{S}_kz_k(t)\to z(t)$ weakly in $L^1(\Omega;\mathbb{R}^m)$ and ${\rm Var}_{\zeta\circ\mathfrak{S}_k}(z_k;[0,t])\to{\rm Var}_\zeta(z;[0,t])$.

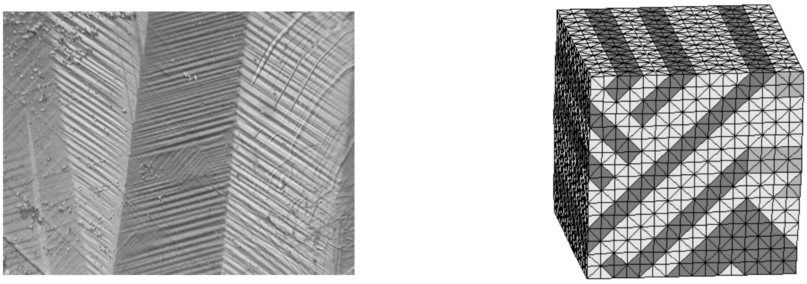

Figure 1:
Left: microstructure in orthorhombic martensite of a CuAlNi single-crystal observed on a specimen surface through an optical microscope; courtesy of Silvia Ignacová (Institute of Physics, Academy of Sciences of the Czech Republic).
Right: Simplectical FEM discretization of a cube and tetragonal martensite tempted to form a 2nd-order-laminated microstructure (with 2 variants active depicted in different gray intensities) in a (1,0,0)-oriented NiMnGa single-crystal loaded in (1,0,0)-direction; courtesy of Marcel Arndt (Rheinische Friedrichs-Wilhelms Univ., Bonn).

Sketch of the proof: Existence for $\kappa < \infty$ as well as for $\kappa = \infty$ follows standardly from theory of rate-independent processes [16, 37, 40, 41]. The convergence (ii) for $\kappa \to \infty$ follows from [39] when realizing continuity of the dissipative potential (for which compactness of $\mathfrak{S}$ is employed) and Γ-convergence of $\Phi_{\varepsilon,\kappa}$ to $\Phi_{\varepsilon,\infty}$ (for which we just realize the penalty-structure of the problem and Γ-convergence of the penalty function technique applied here to the constraint $z = \mathcal{L}(\nabla y)$). Similarly the convergence (iii) of energetic solutions for $\mathfrak{S}_k \to \mathrm{I}$ in $\mathscr{L}(L^2(\Omega), L^2(\Omega))$ follows from [39] when realizing the uniform convergence of the corresponding dissipation potentials while the stored-energy functional is fixed. $\square$

2.6 Numerical approximation by implicit time discretization and FEM

All problems presented above bears implicit discretization in time (which was, in fact, a technique behind the proofs of existence of solutions) combined with conformal finite-element discretization in space by conformal *finite-element method* (FEM). The implicit time discretization results to recursive boundary-value problems that have a variational structure and their solutions can advantageously find by minimization of certain functionals.

As to spatial discretization, considering simplectical triangulations of a polyhedral Ω and Pn-elements, one must choose $n \geq 2$ for y due to the "interfacial" terms if $\gamma \geq 1/2$. As for z, Pn-elements with $n \geq 0$ suffice if $\kappa < \infty$. If $\kappa = \infty$, however, polynomial elements are not compatible with the nonlinear constraint $z = \mathcal{L}(\nabla y)$ in general. Yet, if $\gamma < 1/2$ in (2.19a), one can use P1-elements for y and P0-elements for z, which complies with $z = \mathcal{L}(\nabla y)$.

Convergence for both space and time discretization simultaneously to weak or energetic solutions to the corresponding problems is then rather routine modification of the previous proofs without any spatial discretization.

Rate-independent model with $\kappa = \infty$ and $\mathfrak{S}$ identity and a nonlocal interfacial term (2.19a) with $\gamma = 1/4$ has been implemented by using P1-elements for y and used for specific simulations in [2, 3]. Just one snapshot of a discretization by 24576 tetrahedral elements is depicted for an illustration on Figure 1(right), while some evolution "movie" can be found in [3]. It should be emphasized that the mathematical-programming problems arising after time- and FEM-discretization at each time level are extremely difficult because they posses simultaneously all usual troublesome features, i.e. they are simultaneously nonconvex, multidimensional, and nonsmooth (due to multiwell character of SMA stored energies, ultimately needed fine spatial discretizations, and due to nonsmooth ζ to describe the activate character of phase transformation, respectively). Getting successful numerical simulations is thus rather miraculous, and various sophisticated techniques had to be combined, in particular a like-simulated-annealing algorithm for global optimization and permanent checking energy balance (2.29) during simulation to detect a possible failure in finding a "good" (if not just global) minimizer of the incremental problem at a current time level.

For another 3D simulations but without rate-independent activated dissipation we refer also to [27].

3 "Mesoscopical" models based on Young measures

Microstructure (=fast spatial oscillations of ∇y) in SMAs represents ultimate feature even if "only" single-crystals are of an interest and, as Figure 1(left) clearly indicates, modelling of SMA gets thus ultimately a *spatially multiscale* character. Its effective modelling needs special approaches especially in situations which are "mesoscopically" inhomogeneous and representative-volume-element philosophy (like on Figure 1(right)) hardly can be adopted. One way is presented in this section, justified by limiting the models from Section 2.

3.1 Young measures

The microstructure at a current $x \in \Omega$ (and a current time t considered for a moment fixed) will "mesoscopically" be described, beside the "macroscopical" deformation gradient ∇y, also by a distribution ν_x of the deformation gradient (arising philosophically by spatial oscillations of the deformation gradient "in a neighbourhood" of x and can backward be reconstructed by this philosophy, cf. Figure 2 below). Such (probability) distributions thus parameterized by $x \in \Omega$ are called *Young measures*. Taking into account the p-coercivity of the stored energy ϕ, the so-called L^p-Young measures are defined as

$$\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d}) := \Big\{\nu \in L^\infty_{\rm w}(\Omega;M(\mathbb{R}^{d\times d}))\,;\ \int_\Omega\int_{\mathbb{R}^{d\times d}}|F|^p\nu_x({\rm d}F){\rm d}x < +\infty,\\ \nu_x \text{ is a probability measure on } \mathbb{R}^{d\times d} \text{ for a.a. } x\in\Omega\Big\}, \tag{3.1}$$

where $\nu_x := \nu(x)$. Here, $L^\infty_{\rm w}(\Omega;M(\mathbb{R}^{d\times d})) \cong L^1(\Omega;C_0(\mathbb{R}^{d\times d}))^*$ is the Banach space of weakly measurable functions from Ω to the set of Radon measures $M(\mathbb{R}^{n\times n}) \cong C_0(\mathbb{R}^{d\times d})^*$ on $\mathbb{R}^{d\times d}$. It should be emphasized that, though ν_x is a "probability" measure, the model is purely deterministic. The "product" $\bullet$ is defined as the contraction over the measure on $\mathbb{R}^{d\times d}$ but not over $x \in \Omega$, i.e.

$$\big[h\bullet\nu\big](x) := \int_{\mathbb{R}^{d\times d}} h(x,F)\,\nu_x({\rm d}F). \tag{3.2}$$

We will use this notation even if h depends only on F, like ϕ or $\mathcal{L}$. A trivial L^p-Young measure corresponding to the deformation gradient of $y \in W^{1,p}(\Omega;\mathbb{R}^d)$ is $\{\nu_x\}_{x\in\Omega}$ composed from Dirac measures $\nu_x = \delta_{\nabla y(x)}$; then we write briefly $\nu = \delta_{\nabla y}$. We say that ν is a gradient L^p-Young measure if it is attainable in the sense that, for all $h \in L^1(\Omega;C_0(\mathbb{R}^{d\times d}))$, it holds $\langle\nu,h\rangle := \int_\Omega\int_{\mathbb{R}^{d\times d}} h(x,F)\nu_x({\rm d}F){\rm d}x = \lim_{k\to\infty}\langle\nu,\delta_{\nabla y_k}\rangle$ for some bounded sequence $\{y_k\}_{k\in\mathbb{N}}$ in $W^{1,p}(\Omega;\mathbb{R}^d)$. The set of the gradient L^p-Young measures will be denoted by $\mathscr{G}^p(\Omega;\mathbb{R}^{d\times d})$. If $d > 1$, then $\mathscr{G}^p(\Omega;\mathbb{R}^{d\times d}) \neq \mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d})$.

The space $W^{1,p}(\Omega;\mathbb{R}^d)$ is dense in the set $Q := \{(y,\nu)\in W^{1,p}(\Omega;\mathbb{R}^d)\times\mathscr{G}^p(\Omega;\mathbb{R}^{d\times d});\ \mathrm{Id}\bullet\nu = \nabla y\}$ if embedded by $y\mapsto(y,\delta_{\nabla y})$; here Id: $\Omega\times\mathbb{R}^{d\times d}\to\mathbb{R}^{d\times d}:(x,F)\mapsto F$. If $d>1$, Q is nonconvex in $W^{1,p}(\Omega;\mathbb{R}^d)\times L^\infty_{\rm w}(\Omega;M(\mathbb{R}^{d\times d}))$. A weakly* continuous extension of $\Phi_{0,\kappa}$ to Q is defined by

$$\bar\Phi_\kappa\big(\nu,z\big) = \int_\Omega \phi\bullet\nu + \frac{\kappa}{2}\big|z-\mathcal{L}\bullet\nu\big|^2\mathrm{d}x. \tag{3.3}$$

Likewise, for $\kappa=\infty$, we define

$$\bar\Phi_\infty\big(\nu,z\big) = \begin{cases}\int_\Omega\phi\bullet\nu\,\mathrm{d}x & \text{if } z=\mathcal{L}\bullet\nu \text{ a.e. on }\Omega,\\ +\infty & \text{elsewhere.}\end{cases} \tag{3.4}$$

3.2 Approximation for space scaling: passage $\varepsilon\to0$

When "zooming-out" the PDE-type model, we will suppress the influence of the interfacial energies. It is thus natural to send ε to 0 in (2.12a), (2.24a), (2.27a), or (2.28a). We can see this from the argument that terms like $|\nabla y|^2$ and $\varepsilon|\nabla^2y|^2$ resulting in (2.1) from (2.11a) are physically dimensionless (before multiplied by elastic moduli to get specific energy in J/m^3) so that ε has, in fact, the physical dimension m^2 and thus it scales together with scaling the length unit.

Proposition 3.1 *Let $\kappa<\infty$ be fixed, $\phi\ge0$, $\mathfrak{S}$ linear continuous injective (possibly noncompact), and $(y_\varepsilon,z_\varepsilon)$ be an energetic solution to (2.12a) with (2.13)–(2.14) using $y(0)=y_{0\varepsilon}$ such that $\delta_{\nabla y_{0\varepsilon}}\to\nu^0$ weakly*. Then, a selected subsequence does exist and (y,ν,z) such that $y_\varepsilon\to y$ in $L^\infty(I;W^{1,p}(\Omega;\mathbb{R}^d))\cap W^{1,2}(I;L^2(\Omega;\mathbb{R}^d))\cap W^{2,2}(I;W^{1+\gamma,2}(\Omega;\mathbb{R}^d)^*)$ weakly*, $\delta_{\nabla y_\varepsilon}\to\nu$ weakly* in the sense of L^p-Young measures on Q, $z_\varepsilon\to z$ weakly* in $L^\infty(I;L^2(\Omega;\mathbb{R}^m))$, and $\mathfrak{S}z_\varepsilon\to\mathfrak{S}z$ weakly* in $\mathrm{BV}(I;M(\Omega;\mathbb{R}^m))$, and $\mathfrak{S}z\in\mathrm{BV}(I;L^1(\Omega;\mathbb{R}^m))$, and (y,ν,z) satisfies*

$$\varrho\frac{\partial^2y}{\partial t^2}-\mathrm{div}\Big(\mathbb{D}e\big(\frac{\partial y}{\partial t}\big)+\phi'\bullet\nu+\kappa\mathcal{L}'\bullet\nu\Big)=f+\kappa z, \tag{3.5a}$$

$$\bar\Phi_\kappa(\nu(T),z(T))+T_{\rm kin}\Big(\frac{\partial y}{\partial t}(T)\Big)+\mathrm{Var}_{\zeta\circ\mathfrak{S}}(z;I)$$
$$+\int_Q\mathbb{D}e\big(\frac{\partial y}{\partial t}\big){:}e\big(\frac{\partial y}{\partial t}\big)\,\mathrm{d}x\mathrm{d}t\le\bar\Phi_\kappa(\nu^0,z_0)+T_{\rm kin}(\dot y_0)+\int_Q f\cdot\frac{\partial y}{\partial t}\,\mathrm{d}x\mathrm{d}t, \tag{3.5b}$$

$$\forall\text{(a.a.) }t\in I\ \forall v\in L^2(\Omega;\mathbb{R}^m):\qquad \bar\Phi_\kappa\big(\nu(t),z(t)\big)\le\bar\Phi_\kappa\big(\nu(t),v\big)+\int_\Omega\zeta\big(\mathfrak{S}(v{-}z(t))\big)\,\mathrm{d}x, \tag{3.5c}$$

$$\nabla y=\mathrm{Id}\bullet\nu\ \text{ a.e. on } Q,\quad \nu_{t,\cdot}\in\mathscr{G}(\Omega;\mathbb{R}^{d\times d})\ \text{ for a.a. } t\in I, \tag{3.5d}$$

where (3.5a) is understood in a weak sense and the initial conditions (2.13) hold with $y(0)=y_0$ replaced by $\nu_{0,\cdot}=\nu^0$, while (2.14) holds with $\varepsilon=0$.

Note that, obviously, (3.5a), (3.5b), and (3.5c) correspond to (2.12a), (2.16), and (2.17), respectively. The system (3.5) then serves as a definition of an energetic solution in case $\varepsilon=0$. It should be emphasized, however, that (3.5a) bears only rather limitted information, i.e. has rather low selectivity, cf. [55, Remark 5.3.8] or [60]. Thus (3.5) is to be understood rather as a basic framework for finer investigations.

Sketch of the proof: First, we have the a-priori estimates for $y_\varepsilon \in L^\infty(I;W^{1,p}(\Omega;\mathbb{R}^d)) \cap W^{1,2}(I;L^2(\Omega;\mathbb{R}^d)) \cap W^{2,2}(I;W^{1+\gamma,2}(\Omega;\mathbb{R}^d)^*)$ and z_ε in $L^\infty(I;L^2(\Omega;\mathbb{R}^m))$ and $\mathfrak{S}z_\varepsilon \in \mathrm{BV}(I;L^1(\Omega;\mathbb{R}^m))$ independent of $\varepsilon > 0$. Then one takes a weakly* convergent subsequence and pass to the limit in (2.12a) by weak* continuity to get (3.5a), and in (2.16) by weak* lower semicontinuity to get (3.5b); the lower-semicontinuity concerns both $\liminf_{\varepsilon\to 0}\mathrm{Var}_{\zeta\circ\mathfrak{S}}(z_\varepsilon;I) \geq \mathrm{Var}_{\zeta\circ\mathfrak{S}}(z;I)$ and the stored energy where we rely on $z_\varepsilon - \mathcal{L}(\nabla y_\varepsilon) \to z - \mathcal{L}\bullet\nu$ weakly* in $L^2(\Omega;\mathbb{R}^m)$ and then on the convexity of $|\cdot|^2$ and on the weak convergence $\phi(\nabla y_\varepsilon) \to \phi\bullet\nu$ weakly* in measures on $\bar\Omega$. The passage in (2.17) is by the "binomial trick" (2.18) with $\zeta\circ\mathfrak{S}$ in place of ζ in general, using that now $\mathcal{L}(\nabla y_\varepsilon) \to \mathcal{L}\bullet\nu$ weakly* in $L^\infty(Q;\mathbb{R}^m)$. More in detail, taking a general $\tilde v$ and the test function $v := v_\varepsilon = \tilde v + z_\varepsilon - z$ for (2.18), for $\kappa < \infty$ fixed and $\varepsilon\to 0$ we get

$$
\begin{aligned}
\int_0^T \Big(\Phi_{\varepsilon,\kappa}(y_\varepsilon, v_\varepsilon) - \Phi_{\varepsilon,\kappa}(y_\varepsilon, z_\varepsilon) + \int_\Omega \zeta\big(v_\varepsilon - z_\varepsilon\big)\,\mathrm{d}x\Big)\mathrm{d}t \qquad&\\
= \int_Q \kappa(v_\varepsilon - z_\varepsilon)\cdot\Big(\frac{z_\varepsilon}{2} + \frac{v_\varepsilon}{2} - \mathcal{L}(\nabla y_\varepsilon)\Big) + \zeta\big(v_\varepsilon - z_\varepsilon\big)\,\mathrm{d}x\mathrm{d}t&\\
= \int_Q \kappa(\tilde v - z)\cdot\Big(\frac{z_\varepsilon}{2} + \frac{v_\varepsilon}{2} - \mathcal{L}(\nabla y_\varepsilon)\Big) + \zeta\big(\tilde v - z\big)\,\mathrm{d}x\mathrm{d}t&\\
\to \int_Q \kappa(\tilde v - z)\cdot\Big(\frac{z}{2} + \frac{\tilde v}{2} - \mathcal{L}\bullet\nu\Big) + \zeta\big(\tilde v - z\big)\,\mathrm{d}x\mathrm{d}t&\\
= \int_0^T \Big(\bar\Phi_\kappa(\nu, \tilde v) - \bar\Phi_\kappa(\nu, z) + \int_\Omega \zeta\big(\tilde v - z\big)\,\mathrm{d}x\Big)\mathrm{d}t.& \qquad (3.6)
\end{aligned}
$$

Here, in fact, some technicalities should however be mentioned: due to the L^p-apriori bounds for ∇y_ε, one cannot a-priori exclude concentration effects in $|\nabla y_\varepsilon|^p$ so that one gets rather a so-called generalized Young functional η in the limit which satisfies (3.5). More specifically, $\eta \in H^*$ with H a separable normed linear space of Carathéodory integrands $\Omega\times\mathbb{R}^{d\times d} \to \mathbb{R}$ containing $L^1(\Omega;C_0(\mathbb{R}^{d\times d}))$ and also all nonlinearities occuring in (3.5) and such that η is a weak* cluster point of $\{i_H(\nabla y_\varepsilon)\}_{\varepsilon>0}$ with $i_H : L^p(\Omega;\mathbb{R}^{d\times d}) \to H^*$ the embedding defined by $\langle i_H(v), h\rangle := \int_\Omega h(x, v(x))\,\mathrm{d}x$ for all $h \in H$. Yet its so-called p-nonconcentrating modification, having the L^p-Young-measure representation denoted by ν, satisfies (3.5) too because it has the same effect in (3.5a,d) involving only nonlinearities of the growth less than p and p-nonconcentrating modification of a gradient generalized Young functional is also a gradient generalized Young functional (proved, in fact, in [15, 28]), while (3.5b) cannot be destroyed when replacing η by ν because of $\lim_{|F|\to\infty}\phi(F)/|F|^p \geq 0$ (since $\phi \geq 0$ is assumed), and eventually (3.5c) remains the same because the only p-growth term $\phi\bullet\eta$ (which indeed may possibly change when replaced by $\phi\bullet\nu$) is on both sides of this inequality. For more details about generalized Young functionals and their p-nonconcentrating modification, we refer to [55, Sect.3.4] and [56]. □

Passage $\varepsilon \to 0$ in the case $\kappa = \infty$, i.e. (2.24a), does not seem clear because the quadratic nature in terms of z used for Proposition 3.1 is not at disposal. On the other hand, in the rate-independent cases (2.27a) or (2.28a), such a passage is possible no matter whether κ is finite or not, provided we use the regularization by $\mathfrak{S}$ and then rely on Γ-convergence technique [39]. Thus we have:

Proposition 3.2 *Let κ be fixed (finite or not), $\mathfrak{S}$ linear continuous injective compact, $f\in W^{1,1}(I;L^2(\Omega;\mathbb{R}^d))$, and $z_{0\varepsilon} = \mathcal{L}(\nabla y_{0\varepsilon}) \in L^\infty(\Omega;\mathbb{R}^m)$ be stable for the functionals*

$(G_{\varepsilon,\kappa}(0,\cdot,\cdot),R)$ and $\delta_{\nabla y_{0\varepsilon}} \to \nu^0$, and $(y_\varepsilon,z_\varepsilon)$ be an energetic solution to (2.27a) or (2.28a). Then, a selected subsequence does exist and $(y,\nu,z)\in \mathrm{B}(I;W^{1,p}(\Omega;\mathbb{R}^d))\times \mathrm{B}(I;M(\mathbb{R}^{d\times d})\times C_{\mathrm{w}}(I;L^2(\Omega;\mathbb{R}^m))$ such that $\mathfrak{S}z \in \mathrm{BV}(I;L^1(\Omega))$, the power $\int_\Omega \frac{\partial f}{\partial t}(\cdot,x)\cdot y_\varepsilon(\cdot,x)\,\mathrm{d}x + \int_{\Gamma_1}\frac{\partial g}{\partial t}(\cdot,x)\cdot y_\varepsilon(\cdot,x)\,\mathrm{d}S$ converges to $\int_\Omega \frac{\partial f}{\partial t}(\cdot,x)\cdot y(\cdot,x)\,\mathrm{d}x + \int_{\Gamma_1}\frac{\partial g}{\partial t}(\cdot,x)\cdot y(\cdot,x)\,\mathrm{d}S$ weakly in $L^1(0,T)$ and that, for all $t\in I$, $\mathfrak{S}z_\varepsilon(t)\to\mathfrak{S}z(t)$ weakly in $L^1(\Omega;\mathbb{R}^m)$, $G_{\varepsilon,\kappa}(t,y_\varepsilon(t),z_\varepsilon(t))\to \bar G_\kappa(t,y(t),\nu_{t,\cdot},z(t))$ where we denoted $\bar G_\kappa(t,y,\nu,z):=\bar\Phi_\kappa(\nu,z)-\int_\Omega f(t)\cdot y\,\mathrm{d}x-\int_{\Gamma_1}g(t)\cdot y\,\mathrm{d}S$, further $\mathrm{Var}_{\zeta\circ\mathfrak{S}}(z_e;[0,t])\to\mathrm{Var}_{\zeta\circ\mathfrak{S}}(z;[0,t])$, $z_\varepsilon(t)\to z(t)$ weakly $L^2(\Omega;\mathbb{R}^m)$, and there is another subsequence (depending on t) such that $y_\varepsilon(t)\to y(t)$ weakly in $W^{1,p}(\Omega;\mathbb{R}^d)$ and $\delta_{\nabla y_\varepsilon(t)}\to\nu_{t,\cdot}$ weakly in the sense of Young measures, and (y,ν,z) satisfies (3.5d) and*

$$\bar G_\kappa(T,y(T),\nu_{T,\cdot},z(T))+\mathrm{Var}_{\zeta\circ\mathfrak{S}}(z;I)\le \bar G_\kappa(0,y_0,\nu^0,z_0)+\int_Q\frac{\partial f}{\partial t}\cdot y\,\mathrm{d}x\mathrm{d}t+\int_{\Sigma_1}\frac{\partial g}{\partial t}\cdot y\,\mathrm{d}S\mathrm{d}t, \tag{3.7a}$$

$$\forall\, t\in I\ \ \forall(\tilde y,\tilde\nu,v)\in W^{1,p}(\Omega;\mathbb{R}^m)\times\mathscr{G}(\Omega;\mathbb{R}^{d\times d})\times L^2(\Omega;\mathbb{R}^m),\ \ \nabla\tilde y=\mathrm{Id}\bullet\tilde\nu:$$
$$\bar G_\kappa\big(t,y(t),\nu(t),z(t)\big)\le \bar G_\kappa\big(t,\tilde y,\tilde\nu,v\big)+\int_\Omega\zeta\big(\mathfrak{S}(v-z(t))\big)\,\mathrm{d}x, \tag{3.7b}$$

and the initial conditions (2.13) hold with $y(0)=y_0$ replaced by $\nu_{0,\cdot}=\nu^0$, while (2.14) holds with $\varepsilon=0$.

Obviously, (3.5a), (3.5b), and (3.5c) correspond to (2.12a), (2.16), and (2.17), respectively. The system (3.5) then serves as a definition of an energetic solution in the quasistatic case with $\varepsilon=0$. Moreover, (ν^0,z_0) is stable and (3.7a) is, in fact, an equality.

Sketch of the proof: We use the abstract results [39] based on continuity of the dissipative potential (for which compactness of $\mathfrak{S}$ is employed) and on the Γ-convergence of $\{\bar\Phi_{\varepsilon,\kappa}\}_{\varepsilon>0}$ for $\varepsilon\to0$ to $\bar\Phi_\kappa$, where

$$\bar\Phi_{\varepsilon,\kappa}(\nu,z)=\begin{cases}\Phi_{\varepsilon,\kappa}(y,z) & \text{if } \nu=\delta_{\nabla y},\\ +\infty & \text{otherwise.}\end{cases} \tag{3.8}$$

For this, we just realize that always $\bar\Phi_{\varepsilon,\kappa}\ge\bar\Phi_\kappa$ and that, taking $\{y_\varepsilon\}_{\varepsilon>0}$ such that $\delta_{\nabla y_\varepsilon}\to\nu$ weakly* and simultaneously $\varepsilon\nabla^2y_\varepsilon\to0$ in $L^2(\Omega;\mathbb{R}^{d\times d\times d})$, then $(\nabla y_\varepsilon,z_\varepsilon)$ with $z_\varepsilon=\mathcal{L}(\nabla y_\varepsilon)$ form the recovery sequence in the sense that $\bar\Phi_{\varepsilon,\kappa}(\delta_{\nabla y_\varepsilon},z_\varepsilon)=\Phi_{\varepsilon,\kappa}(\nabla y_\varepsilon,z_\varepsilon)\to\bar\Phi_\kappa(\nu,z)$; it works both for κ finite and for $\kappa=\infty$. Again, like in the proof of Proposition 3.1, some technicalities should be mentioned: due to the L^p-apriori bounds for ∇y_ε, one cannot a-priori exclude concentration effects in $|\nabla y_\varepsilon|^p$ so that, like in the proof of Proposition 3.1, one gets rather a generalized Young functional η in the limit which satisfies (3.7). Yet, now (3.7b) for $v=z(t)$ reveals that (y,η) minimizes a coercive functional $\bar G_\kappa(t,\cdot,\cdot,z(t))$ and thus η itself must be p-nonconcentrating, having the gradient-Young-measure representation denoted by ν, which then satisfies (3.7). Here, in fact, the mimization principle allows us to say that $\{|\nabla y_\varepsilon(t,\cdot)|^p\}_{\varepsilon>0}$ is equi-integrable and thus generated L^p-Young measure bears enough information so that the argumentation via the generalized Young functionals can be avoided. □

3.3 Numerical approximation and implementation of Young measures

Numerical strategies to solve the problems in Section 3.2 is to make a fully implicit discretization in time to get a recursive minimization problems and then somehow discretize the set of admissible pairs

$$\big\{(y,\nu)\in W^{1,p}(\Omega;\mathbb{R}^d)\times\mathscr{G}^p(\Omega;\mathbb{R}^{d\times d});\ \nabla y=\mathrm{Id}\bullet\nu\big\}. \tag{3.9}$$

First approximation is by exploiting finite-elements in space. The simplest way is to triangulate Ω (assumed polygonal for this reason) by a simplectical triangulation $\mathscr{T}_h$, $h>0$ a mesh parameter, and restrict to element-wise affine y and element-wise homogeneous ν; here "homogeneous" means spatially constant. Then some other discretization of ν on particular finite elements is to be done. For general considerations see [35, 55, 58]. Utilization of Young measures for numerical calculations was first implemented in [44] in the 1D-case. In a multidimensional case, $\mathscr{G}^p(\Omega;\mathbb{R}^{d\times d})$ in (3.9) cannot be described explicitly, which is related with lack of a local characterization of quasiconvex functions; cf. [29]. Except very special cases like [12] allowing for explicit calculations of the quasi-convex envelopes, essentially the only efficient option, imitating to some extent what "mother nature" also do, cf. again Figure 1(left), is at least to approximate some Young measures from $\mathscr{G}^p(\Omega;\mathbb{R}^{d\times d})$ by using a concept of *laminates* [45].

An example of a Young measure $\nu\in\mathscr{G}^p(\Omega;\mathbb{R}^{d\times d})$ describing a so-called 1st-order *laminate* with an underlying macroscopic deformation $y\in W^{1,p}(\Omega;\mathbb{R}^d)$ is

$$\nu=\{\nu_x\}_{x\in\Omega},\qquad \nu_x=\xi_0(x)\delta_{F_1(x)}+\big(1-\xi_0(x)\big)\delta_{F_2(x)}, \tag{3.10a}$$

$$\big[\xi_0F_1+(1-\xi_0)F_2\big](x)=\nabla y(x),\qquad F_1(x)-F_2(x)=a_0(x)\otimes n_0(x), \tag{3.10b}$$

$$0\le\xi_0(x)\le1,\qquad a_0(x),n_0(x)\in\mathbb{R}^d, \tag{3.10c}$$

with δ_F again denoting Dirac's measure supported at F. Note that the latter part of (3.10b) is just $\mathrm{Rank}(F_1-F_2)\ge1$, the so-called *Hadamard rank-1 condition* for two affine deformations to be mutually compatible without cracking the material. This process can be re-iterated: a 2nd-order laminate with the macroscopic deformation y as above is $\nu=\{\nu_x\}_{x\in\Omega}$, where

$$\begin{aligned}\nu_x=\ &\xi_0(x)\xi_1(x)\delta_{F_1(x)}+\xi_0(x)\big(1-\xi_1(x)\big)\delta_{F_2(x)}\\ &+\big(1-\xi_0(x)\big)\xi_2(x)\delta_{F_3(x)}+\big(1-\xi_0(x)\big)\big(1-\xi_2(x)\big)\delta_{F_3(x)}\,,\end{aligned} \tag{3.11a}$$

with (dropping for simplicity a dependence on x)

$$F_1-F_2=a_1\otimes n_1,\qquad F_3-F_4=a_2\otimes n_2\,, \tag{3.11b}$$

$$\xi_1F_1+(1-\xi_1)F_2-\xi_2F_3-(1-\xi_2)F_4=a_0\otimes n_0\,, \tag{3.11c}$$

$$\nabla y=\xi_0\xi_1F_1+\xi_0(1-\xi_1)F_2+(1-\xi_0)\xi_2F_3+(1-\xi_0)(1-\xi_2)F_4 \tag{3.11d}$$

and $0\le\xi_i\le1$, $a_i,n_i\in\mathbb{R}^d$, $i\in\{0,1,2\}$. Now, (3.11b) expresses the rank-1 connection of the "lower" laminates the of (F_1,F_2) and of (F_3,F_4), while (3.11c) expresses the rank-1 connection of the average deformation gradient of those "lower" laminates. Analogously, we can get laminates of an arbitrary order which are often called *sequential laminates*. Let us denote this set as

$$\mathscr{G}^{p,\ell}_{\rm lam}(\Omega;\mathbb{R}^{d\times d}):=\Big\{\nu\in\mathscr{G}^p(\Omega;\mathbb{R}^{d\times d});\ \ \nu_x\text{ is a }\ell\text{-order laminate for a.a. }x\in\Omega\Big\}.$$

Unfortunately, not every $\nu\in\mathscr{G}^p(\Omega;\mathbb{R}^{d\times d})$ is of the form of a sequential laminate, or even cannot be attained by sequential laminates, which can be interpreted that microstructures might be much more chaotic; this is connected with the Šverák's celebrated counterexample [63] that rank-one convexity does not imply quasiconvexity (at least if $d\ge3$). In spite of this negative result, we

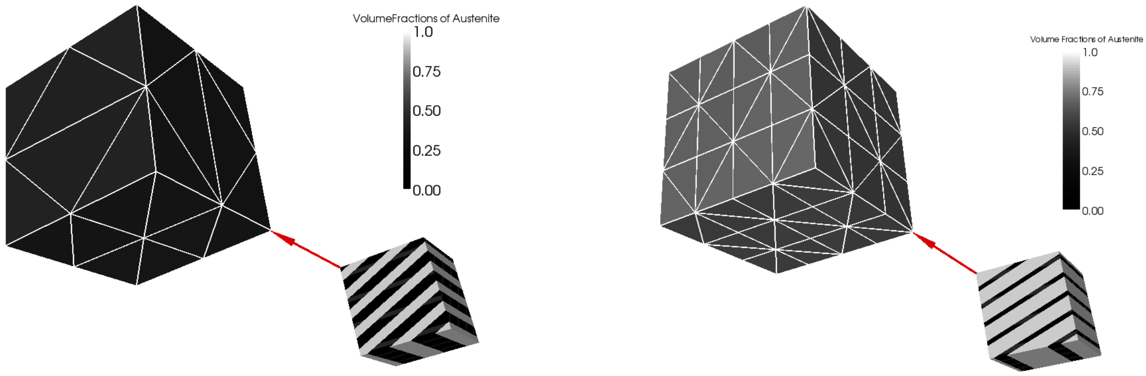

Figure 2: Two different simplectical triangulations of a cubic specimen in a (1,0,0)-oriented NiTi single-crystal loaded inhomogeneously in (1,1,1)-direction and the 2nd-order laminate in rhomboedric martensite reconstructed (and visualized here as 3D small cube at one selected simplectical elements) from the calculated Young measure in R-phase; courtesy of Barbora Benešová, Charles Univ. Prague

can construct a (theoretically convergent) implementable discretization by making implicit time discretization with a time step $\tau > 0$ and restricting the set (3.9) to a finite-dimensional manifold

$$Q_{h,\ell} := \Big\{(y,\nu) \in W^{1,\infty}(\Omega;\mathbb{R}^d) \times \mathscr{G}^{p,\ell}_{\rm lam}(\Omega;\mathbb{R}^{d\times d}); \quad \nabla y = {\rm Id}\bullet\nu,\ \ \nu|_\triangle \text{ homogeneous for any } \triangle{\in}\mathscr{T}_h\Big\}. \tag{3.12}$$

In the quasistatic case one calculates the approximation $(y^k_{\tau,h,\ell}, \nu^k_{\tau,h,\ell}, z^k_{\tau,h,\ell})$ by the recursively minimization of $(y,\nu,z) \mapsto \bar{G}_\kappa(t,y,\nu,z) + \int_\Omega \zeta(z{-}z^{k-1}_{\tau,h,\ell}){\rm d}x$ on $Q_{h,\ell} \times \{\tilde{z}{\in}L^\infty(\Omega;\mathbb{R}^m);\ \tilde{z}|_\triangle$ constant for any $\triangle \in \mathscr{T}_h\}$, while in the dynamical case also the terms $\frac{1}{2}\varrho(y{-}2y^{k-1}_{\tau,h,\ell}{+}y^{k-2}_{\tau,h,\ell})^2/\tau^2 + \frac{1}{2}\mathbb{D}e(y{-}y^{k-1}_{\tau,h,\ell}) : (y{-}y^{k-1}_{\tau,h,\ell})/\tau$ are to be involved; here k refers to the particular time level $t = k\tau$. Fixing $\kappa \le \infty$ and even fixing $\ell{\in}\mathbb{N}{\cup}\{0\}$, one can prove convergence for $(\tau,h) \to (0,0)$ in the lines of Proposition 3.1 or 3.2.

Convergence analysis for the case $\kappa = \infty$ was also performed in [32] but with a regularizing term $|\nabla z|^2$ in the stored energy while admitting $\mathfrak{S}$ to be omitted (i.e. $\mathfrak{S} =$ identity). This, however, ultimately required to use the (now auxiliary) problems with $\kappa < \infty$ to get convergence only conditioned under an implicit stability criterion of the type $h \le H(\kappa)$.

In each case, the convergence holds even for a fixed $\ell \ge 0$, in spite of the mentioned Šverák's counterexample [63]. In fact, in actual simulations in particular problems, if ℓ is chosen too small, an extremely slow convergence can be expected because the oscillations of ∇y must be realized through very fine triangulation of Ω rather than by the laminated Young measure itself.

Usage of (iterated) laminates have been exploited for some evolution of relaxed problems in SMA modelling in [4, 6, 7, 9, 10, 32, 61, 62] or plasticity modelling in [21] or, for the static SMA-case, also [1, 4, 13, 22, 30, 31, 33] and [55, Chap.6]. Even, a more sophisticated and realistic dissipation counting also for rotation of laminates, not only for volume-fraction evolution, was implemented for 2nd-order laminates at small strains in [6] just by fixing such rotations to 0; like also in [26], the dissipation potential thus depends also on the state itself.

Here, on Figure 2, we only illustrate how a (here 2nd-order) laminate can be visualized in 3D-case from a calculated Young measure in the form (3.11).

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