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# Analysis and Numerics for Rate-Independent Processes

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ZUSAMMENFASSUNG. Many inelastic processes such as elastoplasticity, damage, crack propagation, and phase transformations in smart materials can be modeled by rate-independent processes. Because of the inherent nonsmoothness, standard PDE methods do not apply, and specific variational principles must be exploited. During the meeting analytical and numerical approaches

## Introduction by the Organisers

This conference brought together the mathematicians and engineers concerned with the study of rate-independent processes. The topics involved the physical and mechanical modeling, the analytical treatment as well as the development of numerical algorithms and the computational aspects.

Rate-independent processes occur when a system undergoes loadings varying on a time scale much slower than the internal relaxation times of the system. However, the system still stays in metastable states and does not find its thermodynamical equilibrium because of internal frictional processes. There are many well-established macroscopic theories, which show good agreement with experiments, for instance the classical theory of linearized elastoplasticity. This theory has been established a century ago, but its mathematical foundations were only understood 30 years ago using the theory of convex analysis and variational inequalities. Another classical driving theme in this area is the theory of Coulomb friction between rigid or elastic bodies.

Within the last decade similar models have been developed in several areas of mechanics of solids, some of them on a phenomenological basis and others relying on an improved understanding of the microstructures. Such areas include multifunctional or active materials (e.g., shape-memory alloys, ferromagnetism, magneto– and electro-strictivity) and inelastic processes in solids (e.g., elastoplasticity, damage, delamination, fatigue, brittle fracture, crack growth).

Although many of these models are used in engineering, their mathematical understanding is insufficient and efficient numerical algorithms for the computation of approximate solutions are few. The main problem is the inherent nonsmoothness of the modeling because of rate independence.

We discussed a new approach based on an energetic formulation, which provides a broad basis for treating quite general models using topological, geometrical and measure theoretical methods that do not require a Banach space structure. It was shown in various presentations that this approach allows one to go beyond linearized elastoplasticity and to treat fully nonlinear mechanical problems, like crack formation and growth, or elastoplasticity with softening.

Finally, the modeling of the formation and evolution of microstructures was debated in several talks and gave rise to a better understanding of the physical and mathematical underlying principles.

The specific methods discussed were:

- energetic formulation of rate-independent processes
- variational and quasi-variational inequalities
- geometric evolution on metric spaces and its connections to gradient flows for non-convex energies
- techniques from functions of bounded variations and deformations
- regularizations techniques: viscous regularization in time and gradient regularization in space
- justification of rate-independent models from viscous systems with wiggly energies (stochastic potential)
- time-incremental discretizations, discontinuous Galerkin method in time
- space discretizations: conforming and nonconforming finite elements
- regularization of nonsmoothness: phase-field approximations for cracks
- Γ-convergence and relaxation of ill-posed problems
- deriving evolution equations for microstructures and in materials
- Young measure techniques for spatial and temporal oscillations

The specific applications discussed were:

- elastoplasticity with hardening or softening, dislocation plasticity
- damage evolution in solids and structures
- crack propagation in brittle materials
- hysteretic effects in shape-memory alloys (martensitic transformations)

The continuous downpour of Black Forest Rain created a cosy atmosphere that fostered the interaction between the different mathematical and engineering communities.

## Workshop: Analysis and Numerics for Rate-Independent Processes

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# Abstracts

## Threshold-based Quasi-static Brittle Damage Evolution
### Adriana Garroni
### (joint work with C.J. Larsen)

Many interesting phenomena in mechanics, like fracture, plasticity, and damage, have been studied through variational models. These models are often inspired by a threshold criterion. The general idea is that fracture occurs where the strain has a singularity, the plastic behaviour starts if the stress reaches the yield surface, and the material is damaged where the strain exceeds a given threshold.

With this in mind, we attempt to formulate a model for damage evolution based explicitly on a strain threshold, without any reference to an energetic cost for damage. We then compare this with the variational model for damage proposed by Francfort and Marigo, [4]. Here two states, undamaged and damaged, are given by two elastic well-ordered tensors, $A_s$ and $A_w$, and the energy is given by

$$\int_\Omega W(e(u))\,dx - \int_\Omega f\,u\,dx\,,$$

where $e(u) = \frac{\nabla u + \nabla u^T}{2}$ is the symmetrized gradient and

$$W(\varepsilon) = \min\left\{\frac{1}{2}A_s\varepsilon\,\varepsilon\,,\ \frac{1}{2}A_w\varepsilon\,\varepsilon + K\right\}\,.$$

This energy density is not quasi-convex; thus in the minimization procedure we expect microstructure, in other words we expect a relaxation phenomenon. The quasi-convex envelope of $W$ can be represented as follows

$$QW(\varepsilon) = \min_{\theta\in[0,1]}\ \min_{A\in G_\theta(A_s,A_w)}\left\{\frac{1}{2}A_s\varepsilon\,\varepsilon + K\theta\right\}\,,$$

where $G_\theta(A_s, A_w)$ is the $G$-closure of $A_s$ and $A_w$ mixed with volume fractions $1-\theta$ and $\theta$.

Given an external loading $f(t)$ parametrized by time and starting from this formula, a relaxed quasi-static evolution for this model (that also includes irreversibility of damage) was constructed in [3]. There, it was proved that there exists a time parametrized family of elastic tensors $A(t,x)$ (mixture of $A_s$ and $A_w$ with proportion $\Theta(t,x)$) satisfying a monotonicity property (irreversibility of the damage), a minimality condition and an energy balance.

In the case $\Theta(t,x) \in \{0,1\}$, i.e., $\Theta(t,\cdot) = \chi_{D(t)}(\cdot)$, we say that $D(t)$ is a strong solution of this energy bases formulation.

For the threshold problem we restrict our analysis to the scalar (anti-plane deformations) isotropic case ($A_s = \alpha I$ and $A_w = \beta I$) and we have the following definition for $t \mapsto D(t)$ to be a theshold-based quasi-static damage evolution with threshold $\lambda$:

(1) Monotonicity: $t \mapsto D(t)$ is increasing

(2) Threshold: Setting $\sigma_{D(t)}I := \alpha I \chi_{D(t)} + \beta I(1 - \chi_{D(t)})$ and $u(t)$ to be the solution of
$$-\mathrm{div}(\sigma_{D(t)}\nabla u(t)) = f(t),$$
we have $|\nabla u(t)| \leq \lambda$ a.e. in $\Omega \setminus D(t)$

(3) $D(t)$ is necessary: $\forall E \subset D(t)$ with $|E| > 0$, and all $\Delta t$ sufficiently small, $\exists \tau < t$ such that if for each $\Delta t < t - \tau$ we consider the solution $v$ of
$$-\mathrm{div}(\sigma_{D(\tau+\Delta t)\setminus(E\setminus D(\tau))}\nabla v) = f(\tau + \Delta t),$$
we have $|\nabla v(x)| > \lambda$ for some $x \in [D(\tau + \Delta t) \cap E] \setminus D(\tau)$.

In fact, we can show that there is a correspondence between the $K$ in [3] and the threshold $\lambda$ such that if a set-valued function $D$ is a strong solution to the variational formulation in [3], then it is a solution to the above threshold problem.

We then formulate a corresponding "microstructure"-based threshold model, and attempt to show that solutions in [3] are solutions to this threshold model. This is in general false. There is an interesting issue about G-closures that prevents us from concluding that variational solutions are threshold solutions, and so we are led to reformulate and prove existence for a new variational formulation, which we can show are also threshold solutions.

## LITERATUR

[1] Chambolle, A.; Giacomini, A.; Ponsiglione, M. , Crack initiation in brittle materials. *Arch. Rational Mech. Anal.*, to appear.

[2] Dal Maso, G.; Desimone, A.; Mora, M., Quasistatic evolution problems for linearly elastic-perfectly plastic materials. *Arch. Rational Mech. Anal.*, **180** (2006), 237–291.

[3] Francfort, G. A.; Garroni, A., A variational view of brittle damage evolution, *Arch. Rational Mech. Anal.*, **182** (2006), no. 1, 125–152.

[4] Francfort, G. A.; Marigo, J.J., Stable damage evolution brittle continuous medium *Eur. J.Mech. A/Solids*, **12**, no. 2 (1993), 149-189.

[5] Francfort, G. A.; Murat, F. Homogenization and optimal bounds in linear elasticity. *Arch. Rational Mech. Anal.* **94** (1986), no. 4, 307–334.

[6] Garroni, A. ; Larsen, C. J., Threshold-based Quasi-static Brittle Damage Evolution, in preparation.

[7] Milton, G. W. The theory of composites. Cambridge Monographs on Applied and Computational Mathematics, 6. Cambridge University Press, Cambridge, 2002.

# Well-posedness and approximation of problems in gradient plasticity and related models

## B. DAYA REDDY

(joint work with Jules K. Djoko, Francois Ebobisse, Andrew McBride)

The well-established phenomenon of size-dependent behaviour, together with significant developments in manufacture at the mesoscopic level, are two factors that have influenced investigations into various extensions of classical theories of plasticity. A further motivating factor is the absence of a length scale in the classical theories, with the result that computational solutions exhibit pathological mesh-dependent behaviour. These extensions generally have lead to theories that

incorporate non-locality, as opposed to classical flow theories which are of a local nature (see, for example, [5]).

The purpose of this presentation is to focus on one such set of extensions, which are referred to as gradient theories, and which are characterised by the inclusion of terms involving the gradient of plastic strain and other variables associated with plastic deformation. The problem is formulated with specific reference to a model investigated in [7], in which non-locality takes the form of a term invloving the laplacian of the scalar hardening parameter in the yield function.

It is shown that the problem may be formulated as a variational inequality of the form

$$(1) \qquad\qquad a(w, z - \dot{w}) + j(z) - j(\dot{w}) \geq \ell(z - \dot{w})$$

in which $w = (u, p, \gamma)$, where $u$ is displacement, $p$ is plastic strain, and $\gamma$ is the hardening parameter, all defined in approproate Hilbert spaces. Here $z$ is an arbitrary member of the same spaces.

The bilinear form $a(\cdot, \cdot)$ is continuous, symmetric and coercive, the functional $j(\cdot)$ is convex, continuous and positively homogeneous, and $\ell(\cdot)$ is a bounded linear functional. The problem (1) is shown to be well-posed even for the case of softening, provided that the coefficient associated with the gradient term is sufficiently large.

Fully discrete approximations of (1) are considered, in which spatial discretization is achieved using a discontinuous Galerkin (dG) formulation and a backward Euler approximation is used in time. The approximation is shown to be of order $O(\kappa + h^{1/2})$, where $\kappa$ is the time step and $h$ the mesh size. The dG formulation used is a symmteric interior penalty approach, though the method is easily extended to other dG formulations. For problems of classical plasticity it is known [2] that the finite element error estimate can be improved to one of $O(h)$, under assumptions on the regularity of the solution and provided that the material coefficients are piecewise constant. Whether such an extension can be made in the case of a dG formulation for gradient plasticity requires further investigation.

We also investigate the properties of a predictor-corrector algorithm used to solve the fully discrete problem. This algorithm is based on that introduced in [8, 9], and in an equivalent form, better suited to the formulation here, in [1] (see also [6] for extensions of the algorithm). It is shown that the algorithm converges for various choices of predictor, specifically the elastic, secant and tangent predictor, though the tangent predictor requires the introduction of a perturbation to ensure convergence. Finally, some numerical examples serve to illustrate the properties of solutions and of the algorithms introduced.

Further details of the results presented in this talk may be found in [3, 4].

## Literatur

[1] W. W. Bird and J. B. Martin, *A secant approximation for holonomic elastic-plastic incremental analysis with a von Mises yield condition*, Engineering Computations **3** (1986), 192–201.

[2] C. Carstensen, *Numerical analysis of the primal problem of elastoplasticity with hardening*, Numerische Mathematik **82**, 577-597.

[3] J. K. Djoko, F. Ebobisse, A. McBride, and B. D. Reddy, *A Discontinuous Galerkin formulation for classical and gradient plasticity. Part 1: Formulation and analysis*, Computer Methods in Applied Mechanics and Engineering, to appear

[4] J. K. Djoko, F. Ebobisse, A. McBride, and B. D. Reddy, *A Discontinuous Galerkin formulation for classical and gradient plasticity. Part 1: Algorithms and numerical analysis*, In Review.

[5] N. A. Fleck and J. W. Hutchinson. *Strain gradient plasticity*, Advances in Applied Mechanics, **33** (1997), 295–361.

[6] W. Han and B. D. Reddy. *Plasticity: Mathematical Theory and Numerical Analysis*, Springer-Verlag, New York, 1999.

[7] H.-B. Mülhaus and E. C. Aifantis. *A variational principle for gradient plasticity*, International Journal of Solids and Structures, **28** (1991), 845–857.

[8] J. C. Simo and R. L. Taylor, *Consistent tangent operators for rate-independent elastoplasticity*, Computer Methods in Applied Mechanics and Engineering **48** (1985), 101–118.

[9] J. C. Simo and R. L. Taylor, *Return mapping algorithm for plane stress elastoplasticity*, International Journal for Numerical Methods in Engineering **22** (198), 649–670.

# Sharp upper bounds for a variational problem with singular perturbation

### Sergio Conti

### (joint work with Camillo De Lellis)

In the theory of phase transitions one is often faced with singularly perturbed nonconvex variational problems. A by-now classical example, which is appropriate for fluid-fluid phase transitions, is

$$(1) \qquad F_\varepsilon[u, \Omega] \;=\; \int_\Omega \left\{ \frac{(1-u^2)^2}{\varepsilon} + \varepsilon|\nabla u|^2 \right\} dx \; ,$$

where $u : \Omega \subset \mathbb{R}^n \to \mathbb{R}$. In 1977, Modica and Mortola have shown [13] that as $\varepsilon \to 0$ the family of functionals $F_\varepsilon$ converges, in the sense of $\Gamma$-convergence, to

$$(2) \qquad F_0[u, \Omega] = \begin{cases} \frac{8}{3}\mathrm{Per}_\Omega(\{u = 1\}) & \text{if } u \in BV(\Omega; \{1, -1\}) \, , \\ \infty & \text{else.} \end{cases}$$

Solid-solid phase transitions are instead described by functionals of the type

$$(3) \qquad G_\varepsilon[u, \Omega] \;=\; \int_\Omega \left\{ \frac{\mathrm{dist}^2(\nabla u, K)}{\varepsilon} + \varepsilon|\nabla^2 u|^2 \right\} dx \; ,$$

where $u : \Omega \subset \mathbb{R}^n \to \mathbb{R}^n$, and $K = SO(n)\{A, B\} \subset \mathbb{R}^{n \times n}$. For $n = 2$ a $\Gamma$ convergence result to a functional similar to (2) was obtained in [6]; the higher dimensional case is open. The dependence on a gradient field makes (3) substantially more rigid, and the limit functional turns out to be finite only on a special class of piecewise affine functions.

We consider here the Eikonal functional, which arose in the last decades as model for different physical problems, ranging from liquid crystals [2] to blistering in

thin films [14], convection patterns [11] and magnetism in thin films [9]. Precisely,

$$(4) \qquad I_\varepsilon[u,\Omega] \;=\; \int_\Omega \left\{ \frac{(1-|\nabla u|^2)^2}{\varepsilon} + \varepsilon|\nabla^2 u|^2 \right\} dx\,,$$

with $u : \Omega \subset \mathbb{R}^2 \to \mathbb{R}$. This depends, much as (3), on a gradient field; however, the unknown $u$ is a scalar and the null set of the nonconvex potential, namely, $S^1$, is connected. Both facts make (4) considerably softer than (3), and indeed the space on which the limit is defined is much larger.

A straightforward computation shows that the optimal one-dimensional interface approximating the limiting function $t(x) = x_1 \cos\theta + |x_2| \sin\theta$ is

$$(5) \qquad u_\varepsilon(x) = x_1 \cos\theta + \ln\left[ 2\cosh\frac{x_2}{\varepsilon/\sin\theta} \right],$$

and that its energy is $\frac{8}{3}\sin^3\theta$ per unit length of the interface. This motivates the conjecture, first formulated in [2], that the limiting functional can be written as

$$(6) \qquad I_0[v,\Omega] \;=\; \frac{1}{3}\int_{\Omega \cap J_{\nabla v}} |[\nabla v]|^3\, d\mathcal{H}^1$$

on an appropriate space of functions $v$ solving the eikonal equation $|\nabla v| = 1$. Here $J_{\nabla v}$ is the set where "$\nabla v$ jumps", and $[\nabla v]$ is the "jump".

A technique to control the functional from below was devised by Jin and Kohn [12], which introduced a class of "entropies" whose divergence is controlled, in an appropriate sense, by $F_\varepsilon$. Building upon this work, compactness with respect to the strong $W^{1,3}$ topology was then proven independently in [1, 7] and [10]. A lower bound was also obtained; which for the case that the limit is $BV$ coincides with the simple line integral (6), see [3]. Precisely:

**Theorem 1.** [From [1, 7]] *Let $\Omega \subset \mathbb{R}^2$ be a bounded Lipschitz domain, and let $\varepsilon_i \to 0$ and $u_i$ be such that $I_{\varepsilon_i}[u_i,\Omega] < C < \infty$. Then there is a subsequence converging strongly in $W^{1,3}$ to a function $u_0$ with $|\nabla u_0| = 1$. If additionally $\nabla u_0 \in BV$, then*

$$\liminf_{k\to\infty} I_{\varepsilon_{i_k}}[u_{i_k},\Omega] \geq \frac{1}{3}\int_{J_{\nabla u_0}} |\nabla^+ u_0 - \nabla^- u_0|^3 d\mathcal{H}^1\,.$$

Notice that the compactness result does not give $\nabla u_0 \in BV$. Indeed, whereas the functional (6) is lower semicontinuous on $BV$, it is not coercive in the same space, see [1, 7].

An upper bound matching this lower bound had already been obtained in [3] for the case that the limit is a single straight interface, and in [7] for the case that finitely many straight interfaces are present. The presence of the gradient structure made it however difficult to conclude by density. We present here the derivation of an upper bound under the assumption that the limit is in $BV$, which was discussed in detail in [5]. An independent proof of the same result was obtained by Poliakovsky [15, 16].

**Theorem 2.** [From [5]] *Let $\Omega \subset \mathbb{R}^2$ be a bounded $C^2$ set, let $u_0 \in W^{1,\infty}(\Omega, \mathbb{R})$ obey $\nabla u_0 \in BV(\Omega, S^1)$, and let $\varepsilon_i \to 0$. Then there is a sequence $u_i \in C^\infty(\Omega)$ such that $u_i \to u_0$ in $W^{1,p}(\Omega)$ for every $p < \infty$ and*

$$\limsup_{i \to \infty} I_{\varepsilon_i}[u_i, \Omega] \le \frac{1}{3} \int_{J_{\nabla u_0} \cap \Omega} |\nabla^+ u_0 - \nabla^- u_0|^3 d\mathcal{H}^1 \,.$$

The full determination of the $\Gamma$-limit, i.e., removing the assumption $\nabla u_0 \in BV$ in both Theorem 1 and Theorem 2, is open. Notice that if $\nabla u_0$ is not in BV but is the limit of a sequence bounded in energy, one can still give a meaning to the expression on the right hand side (see [8]): a natural conjecture is that this quantity coincides with the supremum among all lower bounds obtained with all entropies and that the optimal sequence exists also in this case.

The proof of Theorem 2 is based on taking a mollification of $u$ (after an appropriate continuation outside $\Omega$) and improving it locally, a technique already used in [4] to obtain $\Gamma$-convergence for a vectorial problem motivated by the theory of elasticity. Precisely, we fix a family of mollifiers $\phi_\varepsilon$, and define

$$(7) \qquad\qquad\qquad\qquad u_i = \phi_{\varepsilon_i} * u_0 \,.$$

Since $\nabla u_0 \in BV$, the sequence $u_i$ is automatically bounded in energy, and only the jump part of $D^2 u_0$ contributes to the limit.

The function $u_i$ is then modified around points of $J_{\nabla u_0}$ where the convergence of the blow-ups at scale $k\varepsilon$ is already "good enough", by replacing $u_i$ by the optimal single-interface profile of (5). The convergence of the blow-ups permits to show that the energy of the boundary layer is a small fraction of the total energy, and to conclude the proof.

### LITERATUR

[1] L. Ambrosio, C. De Lellis, and C. Mantegazza, *Line energies for gradient vector fields in the plane*, Calc. Var. Part. Diff. Eq. **9** (1999), 327–355.

[2] P. Aviles and Y. Giga, *A mathematical problem related to the physical theory of liquid crystal configurations*, Proc. Centre Math. Anal. Austr. Nat. Univ. **12** (1987), 1–16.

[3] ———, *On lower semicontinuity of a defect energy obtained by a singular limit of the Ginzburg-Landau type energy for gradient fields*, Proc. Roy. Soc. Edin. Sect. A **129** (1999), 1–17.

[4] S. Conti, I. Fonseca, and G. Leoni, *A Γ–convergence result for the two-gradient theory of phase transitions*, Comm. Pure Appl. Math. **55** (2002), 857–936.

[5] S. Conti and C. De Lellis, *Sharp upper bounds for a variational problem with singular perturbation*, preprint, to appear in Math. Ann. (2006).

[6] S. Conti and B. Schweizer, *Rigidity and Gamma convergence for solid-solid phase transitions with SO(2)-invariance*, Comm. Pure Appl. Math. **59** (2006), 830–868.

[7] C. De Lellis, *Energie di linea per campi di gradienti*, Tesi di Laurea, Università di Pisa, Pisa, 1999.

[8] C. De Lellis and F. Otto, *Structure of entropy solutions to the Eikonal equation*, J. Eur. Math. Soc. **5** (2003), 107–145.

[9] A. DeSimone, R. V. Kohn, S. Müller, and F. Otto, *Magnetic microstructures—a paradigm of multiscale problems*, ICIAM 1999, vol. 131, Oxford University Press, 1999, pp. 833–844.

[10] ———, *A compactness result in the gradient theory of phase transitions*, Proc. Roy. Soc. Edin. A **131** (2001), 833–844.

[11] N. M. Ercolani, R. Indik, A. C. Newell, and T. Passot, *The geometry of the phase diffusion equation*, J. Nonlinear Sci. **10** (2000), 223–274.

[12] W. Jin and R. V. Kohn, *Singular perturbation and the energy of folds*, J. Nonlinear Sci. **10** (2000), 355–390.

[13] L. Modica and S. Mortola, *Un esempio di Γ-convergenza*, Boll. Un. Mat. Ital. (5) **14-B** (1977), 285–299.

[14] M. Ortiz and G. Gioia, *The morphology and folding patterns of buckling-driven thin-film blisters*, J. Mech. Phys. Solids **42** (1994), 531–559.

[15] A. Poliakovsky, *A method for establishing upper bounds for singular perturbation problems*, C. R. Math. Acad. Sci. Paris **341** (2005), 97–102.

[16] ———, *Upper bounds for singular perturbation problems involving gradient fields*, preprint, 2005.

# Modeling and numerical solutions for shape-memory materials

Ferdinando Auricchio

(joint work with A.Reali, U.Stefanelli)

The great and always increasing interest in SMA materials and their industrial applications in many branches of engineering is deeply stimulating the research on constitutive laws. As a consequence, many models able to reproduce SMA macroscopic behaviours, i.e. *pseudo-elasticity* and *shape-memory effect*, have been proposed in the literature in the last years.

In particular, the constitutive law proposed in Reference [6], improved in References [1, 2] and studied from a more mathematical perspective in Reference [4], seems to be attractive. Developed within the theory of irreversible thermodynamics, this model is in fact able to describe both pseudo-elasticity and shape-memory effect and the corresponding solution algorithm is simple and robust being based on a plasticity-like return map procedure.

In the talk I tried to present an extension of such a model, able to reproduce also other experimentally observed SMA behaviours such as permanent inelasticity and degradation effects [3].

In particular, the model assumes total strain $\boldsymbol{\varepsilon}$ and absolute temperature $T$ as control variables, transformation strain $\boldsymbol{e}^{tr}$ and permanent inelastic strain $\boldsymbol{q}$ as internal ones. As in [1], the second-order tensor $\boldsymbol{e}^{tr}$ describes the strain associated to the transformation between the two solid phases referred to as martensite and austenite. Here, this quantity has no fully reversible evolution and the permanent inelastic strain $\boldsymbol{q}$ gives a measure of the part of $\boldsymbol{e}^{tr}$ that cannot be recovered when unloading to a zero stress state. Moreover, we require that

$$\|\boldsymbol{e}^{tr}\| \leq \varepsilon_L, \tag{1}$$

where $\|\cdot\|$ is the usual Euclidean norm and $\varepsilon_L$ is a material parameter corresponding to the maximum transformation strain reached at the end of the transformation during an uniaxial test.

Assuming a small strain regime, we may also consider the standard additive decomposition $\boldsymbol{\varepsilon} = \mathbf{1}\theta/3 + \boldsymbol{e}$, where $\theta = \text{tr}(\boldsymbol{\varepsilon})$ and $\boldsymbol{e}$ are respectively the volumetric and the deviatoric part of the total strain $\boldsymbol{\varepsilon}$, while $\mathbf{1}$ is the second-order identity

tensor. The free energy density function $\Psi$ for a polycrystalline SMA material is then expressed as the convex potential

$$\Psi(\theta, \boldsymbol{e}, T, \boldsymbol{e}^{tr}, \boldsymbol{q}) = \frac{1}{2}K\theta^2 + G\|\boldsymbol{e} - \boldsymbol{e}^{tr}\|^2 + \beta\langle T - M_f\rangle\|\boldsymbol{e}^{tr} - \boldsymbol{q}\| +$$

(2)
$$+ \frac{1}{2}h\|\boldsymbol{e}^{tr}\|^2 + \frac{1}{2}H\|\boldsymbol{q}\|^2 - A\boldsymbol{e}^{tr} : \boldsymbol{q} + \mathcal{I}_{\varepsilon_L}(\boldsymbol{e}^{tr}),$$

where $K$ and $G$ are respectively the bulk and the shear modulus, $\beta$ is a material parameter related to the dependence of the critical stress on the temperature, $M_f$ is the temperature below which only martensite phase is stable, $h$ defines the hardening of the phase transformation, $H$ controls the saturation of the permanent inelastic strain evolution, and $A$ controls the degradation of the model. Moreover, we make use of the indicator function

$$\mathcal{I}_{\varepsilon_L}(\boldsymbol{e}^{tr}) = \begin{cases} 0 & \text{if } \|\boldsymbol{e}^{tr}\| < \varepsilon_L \\ +\infty & \text{otherwise,} \end{cases}$$

in order to satisfy the transformation strain constraint (1); we also introduce the positive part function $\langle\cdot\rangle$.

We wish to note that, since we use only a single internal variable second-order tensor to describe phase transformations, at most it is possible to distinguish between a generic parent phase (not associated to any macroscopic strain) and a generic product phase (associated to a macroscopic strain). Accordingly, the model does not distinguish between the austenite and the twinned martensite, as both these phases do not produce macroscopic strain. We furthermore highlight that, for the sake of simplicity, the present model does not reflect the difference existing between the austenite and the martensite elastic properties.

Starting from the free energy function $\Psi$ and following standard arguments, we can derive the constitutive equations

(3)
$$\begin{cases} p &= \dfrac{\partial\Psi}{\partial\theta} &= K\theta, \\[2mm] \boldsymbol{s} &= \dfrac{\partial\Psi}{\partial\boldsymbol{e}} &= 2G(\boldsymbol{e} - \boldsymbol{e}^{tr}), \\[2mm] \eta &= -\dfrac{\partial\Psi}{\partial T} &= -\beta\|\boldsymbol{e}^{tr} - \boldsymbol{q}\|\dfrac{\langle T - M_f\rangle}{|T - M_f|}, \\[2mm] \boldsymbol{X} &= -\dfrac{\partial\Psi}{\partial\boldsymbol{e}^{tr}} &= \boldsymbol{s} - \beta\langle T - M_f\rangle\dfrac{\boldsymbol{e}^{tr} - \boldsymbol{q}}{\|\boldsymbol{e}^{tr} - \boldsymbol{q}\|} - h\boldsymbol{e}^{tr} + A\boldsymbol{q} - \gamma\dfrac{\boldsymbol{e}^{tr}}{\|\boldsymbol{e}^{tr}\|}, \\[2mm] \boldsymbol{Q} &= -\dfrac{\partial\Psi}{\partial\boldsymbol{q}} &= \beta\langle T - M_f\rangle\dfrac{\boldsymbol{e}^{tr} - \boldsymbol{q}}{\|\boldsymbol{e}^{tr} - \boldsymbol{q}\|} - H\boldsymbol{q} + A\boldsymbol{e}^{tr}, \end{cases}$$

where $p = \mathrm{tr}(\boldsymbol{\sigma})/3$ and $\boldsymbol{s}$ are respectively the volumetric and the deviatoric part of the stress $\boldsymbol{\sigma}$, $\boldsymbol{X}$ is a thermodynamic stress-like quantity associated to the transformation strain $\boldsymbol{e}^{tr}$, $\boldsymbol{Q}$ is a thermodynamic stress-like quantity associated to the permanent inelastic strain $\boldsymbol{q}$, and $\eta$ is the entropy. The variable $\gamma$ results from the

indicator function subdifferential $\partial \mathcal{I}_{\varepsilon_L}(\boldsymbol{e}^{tr})$ and it is defined as

$$\begin{cases} \gamma = 0 & \text{if } \|\boldsymbol{e}^{tr}\| < \varepsilon_L, \\ \gamma \geq 0 & \text{if } \|\boldsymbol{e}^{tr}\| = \varepsilon_L, \end{cases}$$

so that $\partial \mathcal{I}_{\varepsilon_L}(\boldsymbol{e}^{tr}) = \gamma \dfrac{\boldsymbol{e}^{tr}}{\|\boldsymbol{e}^{tr}\|}.$

To describe phase transformation and inelasticity evolution, we choose (following a plasticity-like terminology) a limit function $F$ defined as

$$(4) \qquad\qquad F(\boldsymbol{X}, \boldsymbol{Q}) = \|\boldsymbol{X}\| + \kappa\|\boldsymbol{Q}\| - R,$$

where $\kappa$ is a material parameter defining a scaling modulus between the inelastic effect and the phase transformation, while $R$ is the radius of the elastic domain. To reproduce the asymmetric behaviour in tension and compression shown by SMA in many experiments, different and more complicate choices for $F$ could be introduced in (4), [1].

Considering an associative framework, the flow rules for the internal variables take the form

$$(5) \qquad\qquad \begin{cases} \dot{\boldsymbol{e}}^{tr} & = & \dot{\zeta}\dfrac{\partial F}{\partial \boldsymbol{X}} & = & \dot{\zeta}\dfrac{\boldsymbol{X}}{\|\boldsymbol{X}\|}, \\[2mm] \dot{\boldsymbol{q}} & = & \dot{\zeta}\dfrac{\partial F}{\partial \boldsymbol{Q}} & = & \dot{\zeta}\kappa\dfrac{\boldsymbol{Q}}{\|\boldsymbol{Q}\|}. \end{cases}$$

The model is finally completed by the classical Kuhn-Tucker conditions

$$(6) \qquad\qquad \begin{cases} \dot{\zeta} \geq 0, \\ F \leq 0, \\ \dot{\zeta}F = 0. \end{cases}$$

**Observation 1.** By exploiting basic Convex Analysis tools, we can rewrite our constitutive model (3)-(6) in the equivalent form

$$(7) \qquad\qquad \begin{pmatrix} -p \\ -\boldsymbol{s} \\ \eta \\ \partial D \begin{pmatrix} \dot{\boldsymbol{e}}^{tr} \\ \dot{\boldsymbol{q}} \end{pmatrix} \end{pmatrix} + \partial \Psi \begin{pmatrix} \theta \\ \boldsymbol{e} \\ T \\ \boldsymbol{e}^{tr} \\ \boldsymbol{q} \end{pmatrix} \ni \boldsymbol{0}.$$

Here $\partial D$ stands for the subdifferential of the function $D$ defined as

$$(8) \qquad\qquad D(\boldsymbol{e}^{tr}, \boldsymbol{q}) = \sup_{F(\boldsymbol{A},\boldsymbol{B})\leq 0} \left\{ \boldsymbol{A} : \boldsymbol{e}^{tr} + \boldsymbol{B} : \boldsymbol{q} \right\},$$

which is the dissipation function associated to the phase transformation mechanism. It can be shown that

$$D(\boldsymbol{e}^{tr}, \boldsymbol{q}) = \begin{cases} \max\left\{ \dfrac{R||\boldsymbol{q}||}{\kappa}, \, R||\boldsymbol{e}^{tr}|| \right\} & \text{if } \kappa \neq 0, \\ R||\boldsymbol{e}^{tr}|| & \text{if } \kappa = 0 \text{ and } ||\boldsymbol{q}|| = 0, \\ +\infty & \text{if } \kappa = 0 \text{ and } ||\boldsymbol{q}|| \neq 0, \end{cases}$$

as well as that $D$ is the Fenchel-Legendre conjugate of the indicator function of the non-empty, convex, and closed domain

$$\mathcal{E} = \{(\boldsymbol{A}, \boldsymbol{B}) \, : \, F(\boldsymbol{A}, \boldsymbol{B}) \leq 0\}.$$

Hence, it is easy to check that $D$ is positively 1-homogeneous, that is

$$D(\lambda(\boldsymbol{e}^{tr}, \boldsymbol{q})) = \lambda D(\boldsymbol{e}^{tr}, \boldsymbol{q}) \quad \forall \lambda > 0.$$

Namely, the time-evolution of $(\boldsymbol{e}^{tr}, \boldsymbol{q})$ is of rate-independent type since we readily have that

$$\partial D(\lambda(\boldsymbol{e}^{tr}, \boldsymbol{q})) = \partial D(\boldsymbol{e}^{tr}, \boldsymbol{q}) \quad \forall \lambda > 0.$$

The formulation of rate-independent evolution problems in terms of a doubly-nonlinear differential inclusion as in (7) has recently attracted a good deal of attention. In particular, the mathematical treatment of relations as (7) is nowadays fairly settled and existence, uniqueness, and time-discretization results are available. The interested reader is referred to the recent survey by [5] where a comprehensive collection of mathematical results on doubly-nonlinear rate-independent problems is provided.

**Observation 2.** The proposed model is thermodynamically consistent. In the current temperature-parameterized situation, we are classically asked to check for the mechanical dissipation inequality

$$\dot{\psi} - \boldsymbol{s} : \dot{\boldsymbol{e}} - p\dot{\theta} \leq 0,$$

at least for sufficiently smooth evolutions. Taking (7) into account and owing to standard Convex Analysis results, we compute that

$$\dot{\psi} - \boldsymbol{s} : \dot{\boldsymbol{e}} - p\dot{\theta} = -(\boldsymbol{X}, \boldsymbol{Q}) \cdot (\dot{\boldsymbol{e}}^{tr}, \dot{\boldsymbol{q}}) \geq D(\dot{\boldsymbol{e}}^{tr}, \dot{\boldsymbol{q}}) \geq 0,$$

and the assertion follows.

## Literatur

[1] F. Auricchio, L. Petrini *A three-dimensional model describing stress-temperature induced solid phase transformations. Part I: solution algorithm and boundary value problems*, International Journal for Numerical Methods in Engineering, **61** (2004) 807–836.

[2] F. Auricchio, L. Petrini *A three-dimensional model describing stress-temperature induced solid phase transformations. Part II: thermomechanical coupling and hybrid composite applications*, International Journal for Numerical Methods in Engineering, **61** (2004) 716–737.

[3] F. Auricchio, A. Reali, U. Stefanelli, *A three-dimensional model describing stress-induced solid phase transformation with permanent inelasticity*, International Journal of Plasticity, **23** (2007), 207–226.

[4] F. Auricchio, A. Mielke, U. Stefanelli, *A rate-independent model for the isothermal quasi-static evolution of shape-memory materials*, submitted for publication (2007).

[5] A. Mielke, *Evolution of rate-independent systems*, In: C. Dafermos, E. Feireisl (Eds.), Handbook of Differential Equations. Elsevier (2005).

[6] A. C.Souza, E. N.Mamiya, N. Zouain, *Three-dimensional model for solids undergoing stress-induced phase transformations. European Journal of Mechanics*, **A: Solids 17** (1998) 789–806.

# Thermally driven phase transformation in shape-memory alloys

ADRIEN PETROV

(joint work with Alexander Mielke)

## 1. MATHEMATICAL FORMULATION

We consider a body with reference configuration $\Omega \subset \mathbb{R}^d$. This body may undergo phase transformation and deformations $u : \Omega \to \mathbb{R}^d$. The phase transformation will be characterized by the internal variable $z : \Omega \to \mathbb{R}^{d \times d}_{\mathrm{dev}}$ denoting the mesoscopic transformation strain where $\mathbb{R}^{d \times d}_{\mathrm{dev}}$ is the space of symmetric $d \times d$ tensors such that the trace of $z$ vanishes. The set of admissible deformations $\mathcal{F}$ is chosen as a suitable subspace of $W^{1,2}(\Omega; \mathbb{R}^d)$ by describing Dirichlet data at the part $\Gamma_{\mathrm{Dir}}$ of $\partial \Omega$ and the internal variable $z$ lives in $\mathcal{Z} = L^1(\Omega; \mathbb{R}^{d \times d}_{\mathrm{dev}})$. We assume also that the material behavior depends on the temperature $\theta$, which will be considered as a time dependent given parameter. Then we will not solve an associated heat equation but we will treat $\theta$ as an applied load and we denote it by $\theta_{\mathrm{appl}} : [0, T] \times \Omega \to [\theta_{\min}, \theta_{\max}]$. This approximation for the temperature is used in engineering models and we may justify it in the case where the changes of the loading are slow and the body is small in at least one direction such that excess of heat can be transported very fast to the surface and then radiated into the environment. We denote by $e(u) := \frac{1}{2}(\nabla u + \nabla u^T)$ and $\mathbb{C}(\theta)$ respectively the linearized strain tensor and the elasticity tensor that depends on the temperature $\theta$. The potential energy takes then the following form

$$(1) \qquad \mathcal{E}(t, u, z) := \int_\Omega W(e(u), z, \theta) + \frac{\sigma}{2}|\nabla z|^2 \, \mathrm{d}x - \langle l(t), u \rangle,$$

where $W(e(u), z, \theta) := \frac{1}{2}(e(u) - z) : \mathbb{C}(\theta) : (e(u) - z) + h(z, \theta)$. Here $\sigma$ is positive coefficient that is expected to measure some nonlocal interaction effect for the internal variable $z$ and $l(t)$ denotes the applied mechanical loading. In this work, we assume that $h(z, \theta) := c_1(\theta)|z|^2 + c_2(\theta)\sqrt{\delta^2 + |z|^2} + \frac{1}{\delta}\big(|z|^2 - c_3(\theta)\big)^3_+$, where $c_i(\theta) > 0$, $i = 1, 2, 3$, are given and depending on the temperature $\theta$. Observe that $c_1(\theta)$ measures the occurence of some hardening phenomenon with respect to the internal variable $z$, $c_2(\theta)$ is an activation threshold for initiation of martensitic phase transformations and $c_3(\theta)$ represents the maximum modulus of transformation strain that can be obtained by alignment of martensitic variants. We define

the dissipation potential by

$$(2) \qquad \mathcal{R}(\dot{z}) := \int_{\Omega} \rho |\dot{z}| \, \mathrm{d}x = \rho \|\dot{z}\|_{L^1(\Omega)}, \ \rho > 0.$$

This model was initiated in [8] and further developed in [1, 2]. The original model is obtained in the limit $\delta \to 0$ and $\sigma \to 0$. For mathematical purposes we need to keep $\delta, \sigma > 0$ fixed. Finally our problem is assumed to be governed by the *energetic formulation* of rate-independent problems, for the details the reader is referred to [5, 6, 4, 3, 7]. A function $(u, z) : [0, T] \to \mathcal{F} \times \mathcal{Z}$ is called an *energetic solution* of the rate-independent problem associated with $\mathcal{E}$ and $\mathcal{R}$ if for all $t \in [0, T]$, the *global stability condition* $(S)$ and the *global energy conservation* $(E)$ are satisfied, i.e.

$$(S) \ \ \forall (u, z) \in \mathcal{F} \times \mathcal{Z} : \mathcal{E}(t, u(t), z(t)) \leq \mathcal{E}(t, \bar{u}, \bar{z}) + \mathcal{R}(\bar{z} - z(t)),$$

$$(E) \ \ \mathcal{E}(t, u(t), z(t)) + \int_0^t \mathcal{R}(\dot{z}(s)) \, \mathrm{d}s = \mathcal{E}(0, u_0, z_0) + \int_0^t \partial_s \mathcal{E}(s, u(s), z(s)) \, \mathrm{d}s.$$

Here we assume to be given initial data $(u(0), z(0)) = (u_0, z_0) \in \mathcal{F} \times \mathcal{Z}$.

## 2. Existence result

We clarify now the assumptions. The applied temperature $\theta_{\mathrm{appl}}$ will extract or insert energy thanks to $\partial_\theta W(e(u), z, \theta_{\mathrm{appl}}) \dot{\theta}_{\mathrm{appl}}$. One can prove that the derivatives $\partial_\theta^j W(e(u), z, \theta_{\mathrm{appl}})$ exist for $j = 1, 2$ and using Young's inequality that there exist $c_0^W, c_1^W > 0$ such that

$$(3) \qquad |\partial_\theta^j W(e(u), z, \theta)| \leq c_1^W (W(e(u), z, \theta) + c_0^W).$$

Then $\partial_\theta^j W(e(u), z, \theta_{\mathrm{appl}}) \dot{\theta}_{\mathrm{appl}}$ is controled if we assume that $\theta_{\mathrm{appl}}$ is smooth enough. According to (3) with $j = 1$ and Gronwall's lemma, we have the following lemma.

**Lemma 2.1.** *If (3) holds, for all $\theta_1 \in [\theta_{\min}, \theta_{\max}]$, we have*

$$(4) \qquad W(e(u), z, \theta_1) + c_0^W \leq \exp(c_1^W |\theta_1 - \theta|)(W(e(u), z, \theta) + c_0^W).$$

For a given temperature profile $\theta_{\mathrm{appl}} \in C^1([0, T]; L^\infty(\Omega; [\theta_{\min}, \theta_{\max}]))$ and a given external loading $l \in C^1([0, T]; W^{1,2}(\Omega; \mathbb{R}^d)^*)$, we will study the potential energy $\mathcal{E}$ as defined in (1).

**Proposition 2.1.** *Under the above assumptions the following holds:*app

  (i) *If for some $(t_*, u, z) \in [0, T] \times \mathcal{F} \times \mathcal{Z}$ we have $\mathcal{E}(t_*, u, z) < +\infty$, then $\mathcal{E}(\cdot, u, z) \in C^1([0, T])$ and $\partial_t \mathcal{E}(t, u, z) = \int_\Omega \partial_\theta W(e(u), z, \theta_{\mathrm{appl}}(t)) \dot{\theta}_{\mathrm{appl}}(t) \, \mathrm{d}x - \langle \dot{l}(t), u \rangle$.*
  (ii) *There exist $c_0^E, c_1^E > 0$ such that $\mathcal{E}(t, u, z) < +\infty$ implies $|\partial_t \mathcal{E}(t, u, z)| \leq c_1^E(\mathcal{E}(t, u, z) + c_0^E)$.*
  (iii) *For each $\varepsilon > 0$ and $E \in \mathbb{R}$ there exists $\delta > 0$ such that $\mathcal{E}(t_1, u, z) \leq E$ and $|t_1 - t_2| < \delta$ imply $|\partial_t \mathcal{E}(t_1, u, z) - \partial_t \mathcal{E}(t_2, u, z)| \leq \varepsilon$.*

We prove now that the *energetic formulation* $(S)$ and $(E)$ has at least one solution $(u, z) : [0, T] \to \mathcal{F} \times \mathcal{Z}$ for a given stable initial datum $(u_0, z_0) \in \mathcal{F} \times \mathcal{Z}$, i.e. $(u_0, z_0)$ satisfies the *global stability condition* $(S)$ at $t = 0$. The existence theory for $(S)$ and $(E)$ was developed [2, 1, 5] and it is based on the incremental minimization problem. More precisely, for a given partition $\Pi = \{0 = t < t_1 < \ldots < t_N = T\}$, we define the incremental problem as follows:

$$(IP)_\Pi \quad \left\{ \begin{array}{l} \text{for } k = 1, \ldots, d \text{ find} \\ (u_k, z_k) \in \operatorname{Argmin}\{\mathcal{E}(t_k, \widetilde{u}, \widetilde{z}) + \mathcal{R}(\widetilde{z} - z_k) : (\widetilde{u}, \widetilde{z}) \in \mathcal{F} \times \mathcal{Z}\}. \end{array} \right.$$

One can observe that $(IP)_\Pi$ has always solutions. We define the piecewise constant interpolant $(u^\Pi, z^\Pi) : [0, T] \to \mathcal{F} \times \mathcal{Z}$ with $(u^\Pi(t), z^\Pi(t)) = (u_j, z_j)$ for $t \in [t_{j-1}, t_j)$ for $j = 0, \ldots, N$. Then we show that the limit function satisfies the *energetic formulation* $(S)$ and $(E)$ using Lemma 2.1, which gives the following Theorem:

**Theorem 2.2.** *Assume that $\mathcal{E}$, $\mathcal{R}$ and $(u_0, z_0)$ satisfy the assumptions from above. Then there exists an energetic solution $(u, z) : [0, T] \to \mathcal{F} \times \mathcal{Z}$ such that $(u(0), z(0)) = (u_0, z_0)$ and*

$$u \in L^\infty([0, T]; W^{1,2}(\Omega; \mathbb{R}^d)),$$
$$z \in L^\infty([0, T]; W^{1,2}(\Omega; \mathbb{R}^{d \times d}_{\mathrm{dev}})) \cap BV([0, T]; L^1(\Omega; \mathbb{R}^{d \times d}_{\mathrm{dev}})).$$

In futur work we will investigate the question of uniqueness by using the theory developed in [5]. For this it is necessary to establish smoothness of $\mathcal{E}$ as a function of $(u, z) \in \mathcal{F} \times H^1(\Omega; \mathbb{R}^{d \times d}_{\mathrm{dev}})$.

## LITERATUR

[1] F. Auricchio, A. Mielke, U. Stefanelli, *A rate-independent model for the isothermal quasi-static evolution of shape-memory materials*, M$^3$AS Math. Models Meth. Appl. Sci., (2006), to appear.

[2] F. Auricchio, L. Petrini, *A three-dimensional model describing stress-temperature induced solid phase transformations. Part II: thermomechanical coupling and hybrid composite applications*, Int. J. Numer. Meth. Engrg., **61** (2004), 716–737.

[3] G. Francfort, A. Mielke, *Existence results for a class of rate-independent material models with nonconvex elastic energies*, J. reine angew. Math., **595** (2006), 55–91.

[4] A. Mainik, A. Mielke, *Existence results for energetic models for rate–independent systems*, Calc. Var. PDEs, **22** (2005), 73–99.

[5] A. Mielke, F. Theil, *On rate–independent hysteresis models*, Nonl. Diff. Eqns. Appl. (NoDEA), **11** (2004), 151–189.

[6] A. Mielke, F. Theil, V.I. Levitas, *A variational formulation of rate–independent phase transformations using an extremum principle*, Arch. Rational Mech. Anal., **162** (2002), 137–177.

[7] A. Mielke, *Evolution in rate-independent systems (Ch. 6)*, In C.M. Dafermos and E. Feireisl, editors Handbook of Differential Equations, Evolutionary Equations, **vol. 2**, Elsevier B.V., Amsterdam (2005), 461–559.

[8] A. Souza, E. Mamiya, N. Zouain, *Three-dimensional model for solids undergoing stress-induced phase transformations*, Europ. J. Mech., A/Solids, **17** (1998), 789–806.

# Evolution of martensitic phase boundaries in heterogeneous media
## Patrick W. Dondl

The motivation for this problem lies in the question of whether, and how, hysteresis can arise from a linear microscopic kinetic relation through the effect of defects such as precipitates in the medium. Hysteresis in the physical problems considered stems from a stick-slip behavior of phase boundaries with respect to an applied force; this behavior is therefore often assumed in macroscopic models. The goal of my research is to show how it arises through homogenization from the interplay of a linear microscopic evolution law with the heterogeneities that are always present in a physical material.

For the basic model we consider an elastic solid occupying a domain $\Omega$ with a bulk energy of the form

$$\text{(1)} \qquad \mathcal{F}_{\text{elastic}} = \int_\Omega W(\nabla u, x),$$

where $u \colon \Omega \to \mathbb{R}^n$ is the displacement of the body. The domain is split into a subdomain $E$ and its complement, separated by a phase boundary $\Gamma$—this represents the two phases the material can be in. There may also be inclusions $A = \bigcup_i A_i$ present in $\Omega$. The elastic energy density $W(\nabla u, x)$ depends explicitly on the position $x$: its minimum, the transformation strain, is constant on the domains occupied by each phase or the inclusions and jumps across their respective boundaries. A surface energy of the form

$$\text{(2)} \qquad \mathcal{F}_{\text{surface}} = c \int_\Omega |\nabla \chi_E|$$

penalizing the length of the phase boundary can also be added.

Assuming smoothness of the involved quantities, one can calculate the rate of change of the energy in the system, depending on the normal velocity $v_n$ of the phase boundary, to be

$$\text{(3)} \qquad \frac{\mathrm{d}}{\mathrm{d}t}\left(\mathcal{F}_{\text{elastic}} + \mathcal{F}_{\text{surface}}\right) = -\int_\Gamma f\, v_n,$$

where $f$ is the thermodynamic driving force. The goal is to analyze the free boundary problem arising from the kinetic assumption

$$\text{(4)} \qquad v_n = f.$$

The main difficulty herein stems from the nonlocal coupling of the driving force to the elliptic problem of calculating the displacement. My first approach to an analysis uses an approximate elastic energy for a phase boundary with small slope; the second treats the general problem by considering the evolution of sets of finite perimeter.

**Small slope approximation.** Assuming that the phase boundary can be described by the graph of a shallow function $g$ with periodic boundary conditions, one can formally approximate the model. The resulting problem is given in Fourier space by the equation

$$(5) \qquad \widehat{g}_t(k) = -|k|\,\widehat{g}(k) + \widehat{\varphi}(k) + \widehat{F}(k).$$

Here, the effect of the precipitates and that of an applied stress on the driving force are collected into the local forcing $\varphi = \varphi(x, g(x))$ and a constant external load $F$.

We have proven existence of a solution to this problem, existence of a threshold force $F^*$ up to which there is a stationary solution to the problem and existence of time-space periodic solutions for $F > F^*$. The physical implication of this is that the phase boundary is stuck up to a critical applied force and moves freely with a macroscopic average velocity thereafter.

The general proof of existence of a solution to the equation uses semigroup methods. In order to assert the existence of a threshold force and that of a time-space periodic solution, we use the Schauder fixed point theorem together with compact embeddings of fractional Sobolev spaces. The latter work follows [1], where the reaction-diffusion equation is considered with $|k|$ replaced by $|k|^2$. However, in our case, one cannot use elliptic or parabolic regularity.

In current work, we are examining the depinning transition of these interfaces both numerically and analytically. A critical power law behavior for the average velocity of the interface can be seen in simulations.

**The general problem.** For the full model, we have proven the existence of a solution on a bounded domain $\Omega$ for non-zero surface energy. We rely on an implicit time discretization for a set evolution model as employed in [2] for a purely curvature driven interface. The main difficulty here lies in the nonlocality of the problem due to the coupling with the elliptic equation, since it is necessary to obtain uniform bounds on the $L^\infty$ norm of the forcing.

Given an initial condition, we build a piecewise constant approximation of the evolving set $E(t)$ (and thus of the evolving phase boundary) by minimizing the set function

$$(6) \qquad \mathcal{F}^h(E, E_0) = \mathcal{F}_{\text{elastic}}(E) + c \int_\Omega |\nabla \chi_E| + \frac{1}{h} \int_{E \triangle E_0} \text{dist}(x, \partial E_0)\, \mathrm{d}x$$

at each timestep of duration $h$. The first term in this energy is the already familiar elastic energy. The second term is equal to the surface energy term introduced before, written now as the variation of a characteristic function. The third term—an integral over the symmetric set difference $E \triangle E_0$—is chosen such that its variation produces a discretized normal velocity of the interface.

For given $h > 0$ and $E_0$ of finite perimeter, existence of a minimizer follows from the boundedness of all involved energies and the SBV compactness and closedness theorems. One must now establish convergence as $h \to 0$ of the piecewise constant approximation $\chi_{E(t)}$ to a function

$$(7) \qquad X \colon \Omega \times [0, T] \longrightarrow \{0, 1\},$$

which requires strong convergence of the family of characteristic functions. To this end, we introduce a further regularization of the elastic energy $\mathcal{F}^\varepsilon_{\text{elastic}}$ through mollification of the transformation strain. We then have $\mathcal{F}^{\varepsilon,h} \xrightarrow{\Gamma} \mathcal{F}^h$ and the piecewise constant approximation obtained from sequentially minimizing $\mathcal{F}^{\varepsilon,h}$, for $\varepsilon = h^{1/n}$, converges strongly as $h \to 0$. For a uniformly smooth phase boundary, the resulting normal velocity equals the one in (4).

Current work focuses on numerics and establishing an existence result for time-space periodic solutions. The nature of pinned solutions under a finite applied stress which comprise local energy minima is also being examined.

## Literatur

[1] N. Dirr and N. K. Yip. Pinning and de-pinning phenomena in front propagation in heterogeneous media. *Interfaces Free Bound.*, 8(1):79–109, 2006.
[2] Stephan Luckhaus and Thomas Sturzenhecker. Implicit time discretization for the mean curvature flow equation. *Calc. Var. Partial Differential Equations*, 3(2):253–271, 1995.

## Regularity in Prandtl-Reuss perfect plasticity

### Alexey Demyanov

**Statement of the problem.** The strong formulation of the Prandt-Reuss model of perfect plasticity is the following: given a domain $\Omega \subset \mathbb{R}^n$, a partition of its boundary $\partial\Omega$ into two sets $\Gamma_0$ and $\Gamma_1$

> a body force $f(t,x) : [0,T] \times \Omega \to \mathbb{R}^n$,
> a boundary displacement $w(t,x) : [0,T] \times \Gamma_0 \to \mathbb{R}^n$,
> and a surface force $F(t,x) : [0,T] \times \Gamma_1 \to \mathbb{R}^n$,

the problem is to find functions

$$u(t,x),\ e(t,x),\ p(t,x) \quad \text{and } \sigma(t,x)$$

such that for every $t \in [0,T]$, for every $x \in \Omega$ the following conditions hold:

(1) kinematic admissibility: $\varepsilon(u(t,x)) = e(t,x) + p(t,x)$ in $\Omega$, $u(t,x) = w(t,x)$ on $\Gamma_0$
(2) constitutive equation: $\sigma(t,x) = \mathbb{A}^{-1} e(t,x)$,
(3) equilibrium: $\operatorname{div}_x \sigma(t,x) = -f(t,x)$ in $\Omega$, $\sigma(t,x)\nu(x) = g(t,x)$ on $\Gamma_1$,
(4) stress constraint $\sigma^D(t,x) \in \mathbb{K}$,
(5) associative flow rule: $(\xi - \sigma(t,x)) : \dot{p}(t,x) \leq 0$ for every $\xi \in \mathbb{K}$,

where $\varepsilon(u) = \frac{1}{2}(\nabla u + \nabla u^T)$, $\sigma^D$ denotes the deviatoric part of $\sigma$

$$\mathbb{K} = \{\tau \in \mathbb{M}^{n \times n}_{sym} \ : \ |\tau^D| \leq \sqrt{2}k_*\}$$

and $\mathbb{A}$ is the elasticity tensor defined as

$$\mathbb{A}\sigma = \frac{\operatorname{tr}\sigma}{n^2 K_0}\mathbf{1} + \frac{1}{2\mu}\sigma^D.$$

The problem is supplemented by initial conditions at time $t = 0$.

Because of the linear growth, with respect to $\varepsilon(u)$, of the functional arising in variational formulation of the problem one looks for displacements $u$ in the space $BD(\Omega)$ and for stresses $\sigma$ in the space $L^2(\Omega; \mathbb{M}^{n \times n}_{sym})$. However, one can expect better regularity of the stress tensor $\sigma$. Namely, as it was shown in [3, 5, 6, 7], in some stationary situations the stress belongs to the space $W^{1,2}_{loc}(\Omega; \mathbb{M}^{n \times n}_{sym})$.

Here we address the issue of $W^{1,2}_{loc}$ regularity, with respect to spatial variables, of the stress tensor $\sigma(t)$ in the Prandtl-Reuss model. The main result (see Theorem 1 below) states, that one has

$$\sigma \in L^\infty([0,T]; W^{1,2}_{loc}(\Omega; \mathbb{M}^{n \times n}_{sym})).$$

A similar result was obtained in [1], where the authors have used Norton-Hoff approximations. We remark, however, that our proof is based on a completely different approach, developed by G. Seregin for proving regularity of stresses in the case of Hencky perfect plasticity (see for example [3, 5, 6]). Observe, that due to this fact, our assumptions on the data of the problem are different from those of [1].

We believe, that the method proposed can be used for proving differentiability of stresses for other models occurring in plasticity theory.

**The main result.** We impose the following assumptions on the data of the problem

(1)
$$f \in AC([0,T]; L^n(\Omega; \mathbb{R}^n)) \cap L^\infty([0,T]; C^1_{loc}(\Omega; \mathbb{R}^n))$$
$$F \in AC([0,T]; L^\infty(\Gamma_1))$$
$$w \in AC([0,T]; W^{1,2}(\Omega; \mathbb{R}^n)).$$

Assume also the so-called uniform safe-load condition:

(2)
there exists a function $\varrho \in AC([0,T]; L^2(\Omega; \mathbb{M}^{n \times n}_{sym}))$, such that
$\operatorname{div}_x \varrho(t) = -f(t)$ in $\Omega$ and $[\varrho\nu] = F(t)$ on $\Gamma_1$ for every $t \in [0,T]$,
$|\varrho^D(t,x)| \leq \lambda\sqrt{2}k_*$ a.e. $x \in \Omega$,
for some $0 < \lambda < 1$, for every $t \in [0,T]$,
and $\varrho^D \in AC([0,T]; L^\infty(\Omega; \mathbb{M}^D))$.

Suppose, that $\partial\Omega \in C^2$ is partitioned into two disjoint open sets $\Gamma_0$, $\Gamma_1$ and their common interface $\gamma = \partial\Gamma_0 = \partial\Gamma_1$:

$$\partial\Omega = \Gamma_0 \cup \gamma \cup \Gamma_1.$$

Further, we assume that

(3)
for each $x \in I$, there exists a $C^2$ diffeomorphism defined in a neighborhood of $x$ which maps $\partial\Omega$ to an $(n-1)$−dimensional hyperplane, and $\gamma$ to an $(n-2)$-dimensional plane.

**Theorem 1.** *Suppose that $n = 2, 3$ and the assumptions* (1)- (3) *are satisfied. Then for a solution $(u, e, p)$ of the quasistatic problem we have*

$$\sigma \in L^\infty([0,T]; W^{1,2}_{loc}(\Omega; \mathbb{M}^{n \times n}_{sym})),$$

*with $\sigma(t,x) = \mathbb{A}^{-1}e(t,x)$.*

**The idea of the proof.** Shortly, the strategy of proving Theorem 1 consists in refining the proof of the existence of solution to the quasistatic problem, carried out in [2], by generalizing the estimates obtained in [3] and [5] for establishing the regularity of stresses in the case of Hencky perfect plasticity.

More precisely, we follow the general scheme for proving the existence of weak solutions of continuous-time energy formulation of rate-independent processes described in [4] (see the references therein). We perform a standard time-discretization procedure, and for chosen in a suitable way approximate solutions $(u_N(t), e_N(t), p_N(t), \sigma_N(t))$, that converge to a weak solution of the quasistatic problem, we obtain the estimate

$$(4) \qquad \sup_{N \in \mathbb{N}} \sup_{t \in [0,T]} \|\sigma_N(t)\|_{W^{1,2}_{loc}(\Omega; \mathbb{M}^{n \times n}_{loc})} \leq C,$$

which yields Theorem 1. To get (4), we look for solutions $(u_N^m, e_N^m, p_N^m)$ of the incremental problems (see [2] for the details and definitions)

$$(5) \qquad \min \left\{ \mathcal{Q}(e) + \mathcal{H}(p - p_N^{m-1}) + L_N^m(u) : (u, e, p) \text{ admissible for } w_N^m \right\}$$

as for saddle points of a Lagrangian (details can be found in [3, 5])

$$\ell(v, \tau) = \int_\Omega (\varepsilon(v) + e_N^{m-1}) : \tau \, dx - \int_\Omega g^*(\tau) \, dx - \int_\Omega f_N^m \cdot \tau \, dx - \int_{\Gamma_1} F_N^m \cdot v \, dx,$$

which is similar to the one considered in the static case of Hencky perfect plasticity, but takes into account the preceding history of plastic deformation through the term $e_N^{m-1}$. Using the abstract relaxation scheme, see [3], one considers an appropriate relaxation of this Lagrangian and shows that its saddle points $(u, \sigma)$ generate solutions of the incremental problem (5). Then we consider certain regularized problems and show, that their solutions $\sigma^\delta$ are smooth enough and

$$\sigma^\delta \rightharpoonup \sigma_N^m \quad \text{in } L^2(\Omega; \mathbb{M}^{n \times n}_{sym}) \text{ and } \|\sigma^\delta\|_{W^{1,2}_{loc}(\Omega; \mathbb{M}^{n \times n}_{sym})} \leq C(m, N).$$

Thus one concludes that for the approximate solutions $\sigma^N(t)$, obtained from $\sigma_N^m$ by piecewise-constant interpolations, the following is valid

$$(6) \qquad \sup_{t \in [0,T]} \|\sigma_N(t)\|_{W^{1,2}_{loc}(\Omega; \mathbb{M}^{n \times n}_{sym})} = \max_{m=0,\dots,N} \|\sigma_N^m\|_{W^{1,2}_{loc}(\Omega; \mathbb{M}^{n \times n}_{sym})} \leq C(N),$$

however, without any uniformity with respect to $N$. Finally, by using the fact that $\sigma_N^m$ is a Sobolev function, we manage to improve estimate (6), showing that (4) holds.

### LITERATUR

[1] Bensoussan A., Frehse J, *Asymptotic behaviour of the time-dependent Norton-Hoff law in plasticity theory and $H^1$ regularity.* Comment. Math. Univ. Carolinae **37** (1996), no. 2, 285–304.

[2] Dal Maso G., DeSimone A., Mora M.G., *Quasistatic evolution problems for linearly elastic-perfectly plastic materials.* Arch. Ration. Mech. Anal. **180** (2006), no. 2, 237–291.

[3] Fuchs M., Seregin G.A., *Variational methods for problems from plasticity theory and for generalized Newtonian fluids.* Springer-Verlag, Berlin, 2000.

[4] Mielke A., *Evolution of rate-independent systems.* In: Evolutionary equations. Vol. II. Edited by M. Dafermos and E. Feireisl, 461–559, Handbook of Differential Equations. Elseveir/North-Holland, Amsterdam, 2005.

[5] Seregin G.A., *Twodimensional variational problems in plasticity theory.* Izvestiya: Mathematics **60** (1996) no.1, 179–216.

[6] Seregin G.A., *On regularity of minimizers of certain variational problems in plasticity theory.* St. Petersburg Math. J. **4** (1993), 1257–1272.

[7] Seregin G.A., *Diferentiability properties of weak solutions of certain variational problems in the theory of perfect elasticplastic plates* Appl. Math. Optim. **28** (1993), 307–335.

# Discontinuous Hysteresis

Augusto Visintin

## 1. Hysteresis Operators

Hysteresis occurs in ferromagnetism, ferroelectricity, plasticity, pseudo-elasticity, superconductivity, phase transitions, porous media filtration, and in several other phenomena, cf. e.g. [2],[5],[6],[10]. A classical example is provided by the dependence of the (uniform) magnetization $\vec{M}$ on a (uniform) magnetic field $\vec{H}$ in a univariate experiment. This relation may be represented in the form $\vec{M}(t) = [\mathcal{F}(\vec{H})](t)$ for any $t \in [0,T]$, where $\mathcal{F}$ is a *hysteresis operator,* namely it has *memory* and is *rate-independent.*

The functional analyical approach to hysteresis and its applications to differential equations were pioneered by Bouc in the 1960s [1]. The notion of hysteresis operator was thoroughly investigated by Krasnosel'skiĭ, Pokrovskiĭ and co-workers in the 1970s and 1980s [5]. Since the 1980s some west-European analysts also began to study hysteresis models, especially in connection with P.D.E.s and applications, see e.g. the monographs [2],[6],[10]. Since the late 1990s a new approach to hysteresis was studied under the keywords of *rate-independence* and *energetic formulation,* see e.g. [3],[4],[7],[8]. (The latter approach might be compared with the system (7) and (8) below.)

The first formulation of the model that is outlined below dates back to [9]; more recently in [10],[11],[12] it was applied to first- and second-order quasilinear hyperbolic equations with hysteresis, respectively of the form

$$(1) \qquad u_t + \mathcal{F}(u)_t + \vec{v} \cdot \nabla u = f, \qquad u_{tt} + \mathcal{F}(u)_{tt} + Au = f,$$

$\vec{v}$ being a prescribed vector field and $A$ a linear elliptic operator.

## 2. Discontinuous Hysteresis

Here we review a model of discontinuous hysteresis, that is the basic element for the construction of the Preisach operator.

**Relay.** Let us fix any $\rho := (\rho_1, \rho_2) \in \mathbf{R}^2$ with $\rho_1 < \rho_2$. For any $u \in C^0([0,T])$ and any $\xi \in \{-1, 1\}$, let us set $X_u(t) := \{\tau \in \,]0,t] : u(\tau) = \rho_1 \text{ or } \rho_2\}$, and after [9] and [10] (Chap. VI) define the function $w = h_\rho(u, \xi) : [0,T] \to \{-1, 1\}$ as follows:

$(2)$  $w(0) := -1$ if $u(0) \leq \rho_1$, $w(0) := \xi$ if $\rho_1 < u(0) < \rho_2$, $w(0) := 1$ if $u(0) \geq \rho_2$,

$$(3) \qquad w(0) := \begin{cases} w(0) & \text{if } X_u(t) = \emptyset \\ -1 & \text{if } X_u(t) \neq \emptyset \text{ and } u(\max X_u(t)) = \rho_1 \\ 1 & \text{if } X_u(t) \neq \emptyset \text{ and } u(\max X_u(t)) = \rho_2 \end{cases}$$

cf. the first figure below. We call $h_\rho$ a (delayed) *relay operator*.

Any function $u \in C^0([0,T])$ is uniformly continuous, hence it can only oscillate at most a finite number of times between the thresholds $\rho_1$ and $\rho_2$. Therefore $w$ can jump just a finite number of times between $-1$ and $1$, if at all; thus $w \in BV(0,T)$.

**Closure.** The relay operator $h_\rho : C^0([0,T]) \to L^1(0,T)$ is not closed. Following [9] and [10] (Chap. VI), we then introduce the *completed relay operator, $k_\rho$*. For any $u \in C^0([0,T])$ and any $\xi \in [-1,1]$, we set $w \in k_\rho(u,\xi)$ if and only if $w$ is measurable in $]0,T[$ and

$$(4) \qquad w(0) := \begin{cases} -1 & \text{if } u(0) < \rho_1 \\ \xi & \text{if } \rho_1 \le u(0) \le \rho_2 \\ 1 & \text{if } u(0) > \rho_2 \end{cases}$$

$$(5) \qquad w(0) := \begin{cases} \{-1\} & \text{if } u(0) < \rho_1 \\ [-1,1] & \text{if } \rho_1 \le u(0) \le \rho_2 \qquad \forall t \in ]0,T], \\ \{1\} & \text{if } u(0) > \rho_2 \end{cases}$$

$$(6) \qquad \begin{cases} \text{if } u(t) \neq \rho_1, \rho_2, \text{ then } w \text{ is constant in a neighbourhood of } t \\ \text{if } u(t) = \rho_1, \text{ then } w \text{ is nonincreasing in a neighbourhood of } t \\ \text{if } u(t) = \rho_2, \text{ then } w \text{ is nondecreasing in a neighbourhood of } t \end{cases}$$

for any $t \in ]0,T]$. Still $w \in BV(0,T)$ for any $u \in C^0([0,T])$. The graph of $k_\rho$ in the $(u,w)$-plane invades the whole rectangle $[\rho_1,\rho_2] \times [-1,1]$, cf. the second figure below. This operator is the closure of $h_\rho$ w.r.t. the strong topology of $C^0([0,T])$ and the sequential weak star topology of $BV(0,T)$, cf. [10] (Chap. VI).



(a) (b)
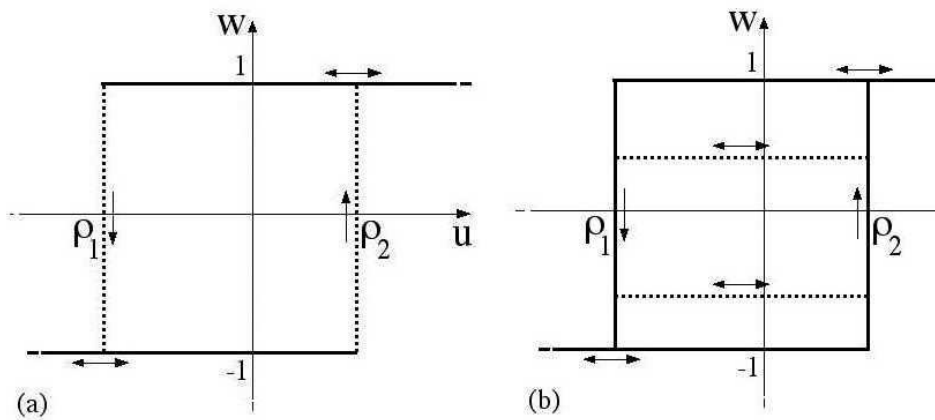
**Reformulation of the Scalar Relay.** (5) and (6) are respectively equivalent to

$$(7) \qquad |w| \le 1, \quad (w-1)(u-\rho_2) \ge 0, \quad (w+1)(u-\rho_1) \ge 0 \qquad \text{a.e. in } ]0,T[,$$

$$(8) \qquad \int_0^t u \, \mathrm{d}w = \int_0^t \rho_2 \, (\mathrm{d}w)^+ - \int_0^t \rho_1 \, (\mathrm{d}w)^- =: \Psi_\rho(w; [0,t]) \qquad \forall t \in ]0,T].$$

**Vector Relay.** For any $\rho := (\rho_1, \rho_2)$ and any $\vec{\theta} := (\theta_1, \theta_2, \theta_3) \in S^2 := \{\vec{\theta} \in \mathbf{R}^3 : |\vec{\theta}| = 1\}$ we introduce the *vector-relay operator*

$$(9) \qquad \vec{h}_{(\rho,\theta)} : C^0([0,T])^3 \times \{\pm 1\} \to L^\infty(0,T) : (\vec{u}, \xi) \mapsto h_\rho(\vec{u} \cdot \vec{\theta}, \xi) \vec{\theta}.$$

The component of the input $\vec{u}$ in the direction $\vec{\theta}$ is thus assumed as input for the scalar relay $h_\rho$; the output of the latter is then applied to the same direction $\vec{\theta}$. The operator $\vec{h}_{(\rho,\theta)}$ inherits several properties from $h_\rho$. Its closure $\vec{k}_{(\rho,\theta)}$ is simply obtained by replacing $h_\rho$ by $k_\rho$ in (9).

**Reformulation of the Vector Relay.** After [10] the characterization (7), (8) of the scalar relay may be extended to the vector relay. For any $(\vec{u}, \xi) \in C^0([0,T])^3 \times [-1,1]$ and any $(\rho, \vec{\theta}) \in \mathcal{P} \times S^2$, $\vec{w} \in \vec{k}_{(\rho,\theta)}(\vec{u}, \xi)$ if and only if $\vec{w}(t) := w(t)\vec{\theta}$ for any $t$, and

$$(10) \qquad w(0) := \begin{cases} -1 & \text{if } \vec{u}(0) \cdot \vec{\theta} < \rho_1 \\ \xi_{(\rho,\theta)} & \text{if } \rho_1 \leq \vec{u}(0) \cdot \vec{\theta} \leq \rho_2 \\ 1 & \text{if } \vec{u}(0) \cdot \vec{\theta} > \rho_2 \end{cases}$$

$$(11) \qquad \begin{cases} |w(t)| \leq 1 \\ (w(t) - 1)\big(\vec{u}(t) \cdot \vec{\theta} - \rho_2\big) \geq 0 \qquad \forall t \in ]0,T], \\ (w(t) + 1)\big(\vec{u}(t) \cdot \vec{\theta} - \rho_1\big) \geq 0 \end{cases}$$

$$(12) \qquad \int_0^t \vec{u} \cdot \vec{\theta} \, \mathrm{d}w \geq \Psi_\rho(w; [0,t]) \qquad \forall t \in ]0,T].$$

This formulation of the vector-relay operator can also be extended to space-distributed systems just by inserting the variable $x$ as a parameter [11], [12].

## Literatur

[1] R. Bouc, *Modèle mathématique d'hystérésis.* Acustica **24** (1971), 16–25.

[2] M. Brokate, J. Sprekels, *Hysteresis and Phase Transitions.* Springer, Berlin 1996.

[3] G. Dal Maso, R. Toader, *A model for the quasi-static growth or brittle fractures: existence and approximation results.* Arch. Rat. Mech. Anal. **162** (2002), 101-135.

[4] G.A. Francfort, J.-J. Marigo, *Revisiting brittle fracture as an energy minimization problem: existence and approximation results.* J. Mech. Phys. Solids **46** (1998), 1319-1342.

[5] M.A. Krasnosel'skiĭ, A.V. Pokrovskiĭ, *Systems with Hysteresis.* Springer, Berlin 1989 (Russian ed. Nauka, Moscow 1983).

[6] P. Krejčí, *Convexity, Hysteresis and Dissipation in Hyperbolic Equations.* Gakkotosho, Tokyo 1997.

[7] A. Mielke, F. Theil, *On rate-independent hysteresis models.* Nonl. Diff. Eqns. Appl. **11** (2004), 151–189.

[8] A. Mielke, F. Theil, V. Levitas, *A variational formulation of rate-independent phase transformations using an extremum principle.* Arch. Rational Mech. Anal. **162** (2002), 137–177.

[9] A. Visintin, *On hysteresis in phase transitions.* Control and Cybernetics **14** (1985), 297–307.

[10] A. Visintin, *Differential Models of Hysteresis.* Springer, Berlin 1994.

[11] A. Visintin, *Quasilinear hyperbolic equations with hysteresis.* Ann. Inst. H. Poincaré. Analyse non linèaire **19** (2002), 451-476.
[12] A. Visintin, *Maxwell's equations with vector hysteresis.* Arch. Rat. Mech. Anal. **175** (2005), 1–38 .

# On Configurational-Force-Driven Crack Propagation

Christian Miehe

(joint work with E. Gürses, D. Zimmermann)

**Keywords:** Fracture, configurational forces, energy minimization, finite elements, crack simulations

**Abstract:** The paper outlines a variational formulation of brittle fracture in solids and considers its numerical implementation by a distinct finite element method. The starting point is a variational setting of fracture mechanics that recasts a monotonic quasistatic fracture process into a sequence of incremental energy minimization problems. The proposed numerical implementation introduces discretized crack patterns with material-force-driven incremental crack-segment releases. These releases of crack segments constitute a sequence of positive definite subproblems with successively decreasing overall stiffness, providing an extremely robust algorithmic setting in the postcritical range. The formulation is embedded into accompanying r-adaptive crack-pattern reorientation procedures with material-force-based indicators, providing reorientations of finite elements at the crack-tip.

## 1. Variational Formulation of Brittle Crack Propagation

The coordinates $\mathbf{X} \in \mathcal{B}_\Gamma$ of the solid in its reference configuration $\mathcal{B}_\Gamma$ are referred to as the material coordinates. In a deformed configuration at the time $t \in \mathcal{R}_+$, these coordinates are mapped by the deformation map

$$(1) \qquad \varphi_t : \begin{cases} \mathcal{B}_\Gamma \to \mathcal{S}_\Gamma \\ \mathbf{X} \mapsto \mathbf{x} = \varphi_t(\mathbf{X}) \end{cases}$$

onto the spatial coordinates $\mathbf{x} \in \mathcal{S}_\Gamma$, where $\mathcal{S}_\Gamma \subset \mathcal{R}^3$ denotes the current configuration of the solid. This deformation is assumed to be prescribed on the part $\partial \mathcal{B}_\varphi \subset \partial \mathcal{B}$ of the exterior surface by the Dirichlet condition in a monotonous format with given velocity function $\bar{\mathbf{v}}$. In the interior domain $\mathcal{B}_\Gamma$, the deformation map is constrained by the condition $\det \mathbf{F} > 0$ at $\mathbf{X} \in \partial \mathcal{B}_\Gamma$ with $\mathbf{F} = \nabla \varphi_t(\mathbf{X})$, where $\mathbf{F}$ denotes the deformation gradient of the solid at $\mathbf{X} \in \partial \mathcal{B}_\Gamma$ and time $t \in \mathcal{R}_+$.

Consider a one-to-one piecewise differentiable transformation $\boldsymbol{\Xi_t} : \Omega_\Gamma \to \mathcal{B}_\Gamma$ of the reference configuration onto itself. This mapping is considered as the time-dependent *parameterization of the medium* that accounts for *material structural changes in the form of a crack propagation*. It reflects a time-dependent change of the Lagrangian coordinates $\boldsymbol{\theta} \in \Omega_\Gamma$ to $\mathbf{X} \in \mathcal{B}_\Gamma$ in a sense of a change of material
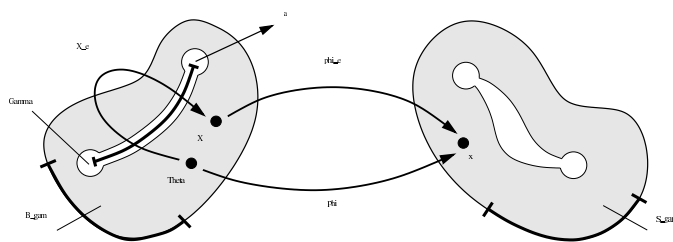
ABBILDUNG 1. Structural changes and deformation. Both, reference and spatial configurations are independently parameterized by material and spatial maps $\boldsymbol{\Xi_t}$ and $\boldsymbol{\xi_t}$. The change of $\boldsymbol{\Xi_t}$ in time describes material structural changes.

structure. With this viewpoint at hand, we introduce the material and spatial coordinate maps

$$(2) \qquad \boldsymbol{\Xi}_t : \left\{ \begin{array}{l} \Omega_\Gamma \to \mathcal{B}_\Gamma \\ \boldsymbol{\theta} \mapsto \mathbf{X} = \boldsymbol{\Xi}_t(\boldsymbol{\theta}) \end{array} \right. \quad \text{and} \quad \boldsymbol{\xi}_t : \left\{ \begin{array}{l} \Omega_\Gamma \to \mathcal{S}_\Gamma \\ \boldsymbol{\theta} \mapsto \mathbf{x} = \boldsymbol{\xi}_t(\boldsymbol{\theta}) \end{array} \right.$$

at time $t \in \mathcal{R}_+$ and express the deformation map defined in (1) by the composition $\boldsymbol{\varphi}_t(\mathbf{X}) = \boldsymbol{\xi}_t(\boldsymbol{\theta}) \circ \boldsymbol{\Xi}_t^{-1}(\mathbf{X})$ as visualized in Figure 1. As a consequence, the deformation gradient $\mathbf{F}$ appears as the composition

$$(3) \qquad \mathbf{F} = \mathbf{j} \cdot \mathbf{J}^{-1} \quad \text{with} \quad \mathbf{j} = \nabla_{\boldsymbol{\theta}} \boldsymbol{\xi}_t \quad \text{and} \quad \mathbf{J} = \nabla_{\boldsymbol{\theta}} \boldsymbol{\Xi}_t$$

of the gradients of the material and spatial coordinate maps introduced in (2). Furthermore, the volume element of the Lagrangian reference configuration is now defined in terms of the material coordinate map, i.e. $dV = \det \mathbf{J} d\Omega$. With these definitions at hand, we obtain the total time derivative of the above kinematic objects by

$$(4) \qquad \dot{\boldsymbol{\varphi}} = \mathbf{v} - \mathbf{F} \cdot \mathbf{V} \quad , \quad \dot{\mathbf{F}} = \nabla \mathbf{v} - \mathbf{F} \cdot \nabla \mathbf{V} \quad , \quad \dot{dV} = (\mathbf{1} : \nabla \mathbf{V}) dV$$

in terms of the spatial and material velocity fields $\mathbf{v} := \frac{\partial}{\partial t} \boldsymbol{\xi}_t$ and $\mathbf{V} := \frac{\partial}{\partial t} \boldsymbol{\Xi}_t$, respectively. These fields govern possible variations of both the Lagrangian as well as the Eulerian coordinates $\mathbf{X} \in \mathcal{B}_\Gamma$ and $\mathbf{x} \in \mathcal{S}_\Gamma$.

We focus on an elastic response of the solid with evolving cracks. In order to set up the global constitutive equations for the crack evolution in the elastic solid, we consider a global dissipation analysis in the sense of Coleman's method. This includes a comparison of the global power $\mathcal{P}$ applied to the solid by external tractions on its boundary with the global energy storage of the solid. We have the global postulate

$$(5) \qquad \mathcal{D} := \mathcal{P} - \frac{d}{dt}\Psi = \int_{\partial \mathcal{B}_\Gamma} \mathbf{t} \cdot \mathbf{v} dA - \frac{d}{dt} \int_{\mathcal{B}_\Gamma} \widehat{\psi}(\mathbf{F}) dV \geq 0 \ .$$

where $\widehat{\psi}$ denotes the free energy function and $\mathbf{t}$ is the traction vector on $\partial \mathcal{B}_\Gamma$. This statement is the demand of the second axiom of thermodynamics in the pure mechanical context. It is the global counterpart to the classical Clausius-Duhem inequality of continuum thermodynamics. The insertion of the kinematic
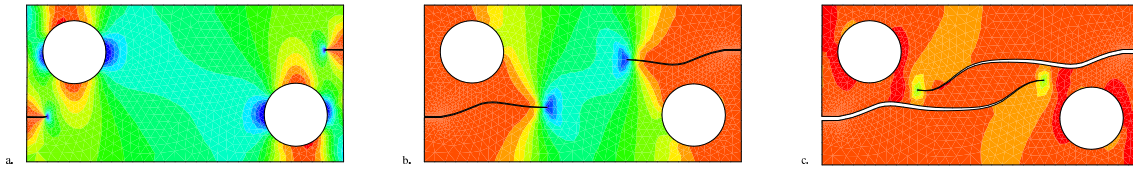
ABBILDUNG 2. a.) - c.) The tensile stress during the crack evolu-
tion in a notched specimen under tension.

relationships (4) into (5) with the application of generalized Gauss theorem results in

$$\text{(6)} \qquad \text{Div}\mathbf{P} = \mathbf{0} \text{ in } \mathcal{B}_\Gamma \quad , \quad \text{Div}\mathbf{\Sigma} = \mathbf{0} \text{ in } \mathcal{B}_\Gamma$$

along with additional traction conditions on the crack surfaces and outer boundaries, see also [3] for a similar discussion. These equations cover the equilibrium condition and the local equation for the Eshelby stress field in the bulk $\mathcal{B}_\Gamma$ of the homogeneous elastic solid. Taking into account the conditions (6), we obtain the *reduced global dissipation inequality* as an integral over the crack tips, $\mathcal{D} = \int_{\partial\Gamma} \mathbf{g} \cdot \dot{\mathbf{a}}dS \geq 0$ . Here, $\mathbf{g} := \lim_{|C| \to 0} \int_C \boldsymbol{\varphi} \cdot \mathbf{n}dS$ and $\dot{\mathbf{a}}$ are the crack driving force and crack tip velocity, respectively. The crack propagation rate $\dot{\mathbf{a}}$ needs to be specified by a constitutive assumption. To this end, consider the classical isotropic Griffith-type crack criterion function $\widehat{\phi}(\mathbf{g}) = |\mathbf{g}| - g_c \leq 0$ , where $g_c$ is a material parameter specifying the critical energy release per unit length of the crack. With this notion at hand, an associated evolution equation for the crack evolution may be constructed by introducing an *elastic domain* for the material forces at the crack tip and a local principle of maximum dissipation. The evolution equation for the local crack propagation reads

$$\text{(7)} \qquad \dot{\mathbf{a}} = \dot{\gamma}\partial_{\mathbf{g}}\widehat{\phi}(\mathbf{g}) = \dot{\gamma}\frac{\mathbf{g}}{|\mathbf{g}|}$$

along with the crack loading-unloading conditions. The algorithmic counterpart of the formulation outlined above requires the spatial discretizations of the domain, configurational maps $\mathbf{\Xi}_t$, $\boldsymbol{\xi}_t$ and temporal discretization of the evolution equation (7), respectively. In order to obtain a stable setting for this incremental scenario in a typical time interval $[t_n, t_{n+1}]$, we apply a staggered scheme of energy minimization at frozen crack pattern and a successive crack release by single nodal doubling. We refer to [2] for the computation of configurational forces in the finite element context and to [1] for details of the algorithm. Here, as an example we consider a specimen with two holes under tension where two symmetric cracks evolve. In Fig. 2 the crack trajectories and the maximum tensile stresses at different level of loads are presented.

## LITERATUR

[1] C. Miehe, E. Gürses, A Robust Algorithm for Configurational-Force-Driven Brittle Crack Propagation with R-Adaptive Mesh Alignment, *published online in Int. J. Numer. Meth. Engng.* (2006).

[2] P. Steinmann, D. Ackermann, and F. Barth Application of material forces to hyperelasto-static fracture mechanics II. Computational setting, *Int. J. Solids Structures,* **38**, (2000), 5509–5526.

[3] H. Stumpf, and K.Ch Le, Variational Principles of Nonlinear Fracture Mechanics, *Acta Mech.,* **83**, (1990), 25–37.

## Numerical implementation of the variational brittle fracture formulation

### Blaise Bourdin

### 1. The variational formulation of brittle fracture

The variational formulation of brittle fracture mechanics proposed in [6] relies in computing the time evolution of global minimizers of a total energy functional under unilaterality constraints. For the sake of brevity, we quickly recall the formulation without getting into the details. In particular, we do not state the proper function spaces.

We consider an open bounded connected domain $\Omega \subset \mathbb{R}^N$ ($N = 1, 2, 3$) with Lipschitz boundary $\partial\Omega$ representing the crack-free reference configuration of an elastic body. We consider a discretization of the time interval $[0, T]$ into $p + 1$ time steps $0 = t_0 < t_1 < \cdots < t_p = T$. At each time step, we apply a *time-dependent displacement* boundary condition $g(t; x)$ on a part $\partial\Omega_D \subset \partial\Omega$ with non-null measure, while the remaining part of $\partial\Omega_N := \partial\Omega \setminus \partial\Omega_D$ remains traction free. For technical reasons better exposed in [2, 5], we consider an extended domain $\widetilde{\Omega}$ such that $\bar{\Omega} \subset \widetilde{\Omega}$, and an extension (still noted $g$) of the Dirichlet boundary condition to $\widetilde{\Omega}$. By $\mathcal{K}_A(t_i)$ we denote the set of all kinematicaly admissible displacement fields for time step $t_i$, and define the total jump set

$$\Gamma(u(t_i)) := \bigcup_{0 \leq j \leq i} J_{u(t_j)},$$

where $J_v$ is the jump set of a function $v$. Remark that $\Gamma(u(t))$ is monotonically increasing. Roughly speaking, at any given time, it is the set of all points across which $u$ has been discontinuous in the past. It represents the crack set associated to the time-dependent deformation, accounting for the irreversible nature of fracture.

Indeed, to any $u$ be such that $u(t) \in \mathcal{K}_A(t)$ for all $0 < t \leq T$ and its associated total jump set $\Gamma(u(t))$, Francfort and Marigo propose to associate the total energy

$$(1) \qquad E(u(t), \Gamma(u(t))) = \int_\Omega W(\mathbf{e}(u(t))\,dx + G_c \mathcal{H}^{N-1}(\Gamma(u(t)) \setminus \partial\Omega_N),$$

where $G_c$ is the *fracture toughness* of the material considered, $\mathbf{e}(u)$ is the symmetrized gradient of $u$, $W(\mathbf{e})$ is the classical linear elastic potential, and $\mathcal{H}^{N-1}$ denotes the $N-1$–dimensional Haussdorf measure. Then, at each time step $t_i$, the displacement field $u(t_i)$ minimizes $E$ under unilaterality condition, *i.e.*

$$(2) \qquad \min_{v \in \mathcal{K}_A(t)} \int_\Omega W(\mathbf{e}(v))\,dx + G_c \mathcal{H}^{N-1}\left(J_v \setminus [\Gamma(u(t_i)) \cup \partial\Omega_N]\right),$$

with the convention that $\Gamma(u(t_{-1})) = \emptyset$.

The actual implementation of (2) is a challenging problem. The kinematically displacement fields are discontinuous, but the location of their discontinuities is of course not known in advance, which is a requirement of most classical discretization methods. Following an approach originally devised in [1] for an image segmentation problem, we introduce a secondary variable $v$, representing in some sense the jumps of $u$, and for any $\varepsilon > 0$, and $\eta_\varepsilon \ll \varepsilon$, the regularized functional

$$
(3) \qquad E_\varepsilon(u, v) := \int_\Omega \left(v^2 + \eta_\varepsilon\right) W(\mathbf{e}(u))\, dx + G_c \int_{\widetilde{\Omega} \setminus \partial\Omega_N} \frac{(1-v)^2}{4\varepsilon} + \varepsilon |\nabla v|^2\, dx,
$$

which approximates $E$ in the sense of the $\Gamma$–convergence.

## 2. Numerical implementation

The regularized functional $E_\varepsilon$ is the basis of our the numerical implementation. For the first time step, a classical result shows that the minimizers of $E_\varepsilon$ converge to that of $E$ when $\varepsilon \to 0$. Practically, we minimize $E_\varepsilon$ for a fixed but "small" $\varepsilon$.

In order to approximate of the solution of the next steps, we minimize $E_\varepsilon$ under the constraint that $v_\varepsilon^i = 0$ whenever $v_\varepsilon^{i-1} \leq \alpha_\varepsilon$, $\alpha_\varepsilon = O(\varepsilon)$ being a fixed parameter. This approach derives slightly from the one studied in [7] (which relies on enforcing the constraint $v_\varepsilon^i \leq v_\varepsilon^{i-1}$), is practically more efficient to implement but can not be justified. Numerical experiments indicates that the solution obtained using both methods are similar.

Like $E$, $E_\varepsilon$ is non-convex, and computing its global minimizers is a challenge. As an algorithm provably converging to the global minimizer of $E_\varepsilon$ is out of reach, a classical strategy is to establish necessary conditions for optimality and to devise an algorithm converging to a point satisfying these conditions.

At each time step, we alternate minimizations with respect to $u$ and $v$. One can prove that this algorithm always converges to a critical point for $E_\varepsilon$, which can be a local or global minimizer or even a critical point. It is proved in [4, Theorem 2] that the alternate minimization algorithm, initialized "close enough" from an *isolated* local minimizer of $F_\varepsilon$, will converge to the said local minimizer. As a corollary, as long as the crack propagation is smooth and if the time discretization is fine enough, the alternate minimization properly initialized converges towards a global minimizer of $E_\varepsilon$.

In order to detect potential local minimizers or saddle points, we study an optimality condition for the whole evolution. We assume that $W$ is homogeneous of degree 2, and that the loads are monotonically increasing (*i.e.* that $g(t; x) = tg(x)$). Let $(u_\varepsilon(t_i), v_\varepsilon(t_i))_{i=0,\ldots,p}$ be a family of critical points for $F_\varepsilon$. For any $j \leq i$, $\left(\frac{t_j}{t_i} u_\varepsilon(t_i), v_\varepsilon(t_i)\right)$ is admissible for the time step $t_j$, and we have

$$
E_\varepsilon\left(\frac{t_j}{t_i} u_\varepsilon(t_i), v_\varepsilon(t_i)\right) = \frac{t_j^2}{t_i^2} E_\varepsilon^b\left(\frac{t_j}{t_i} u_\varepsilon(t_i), v_\varepsilon(t_i)\right) + E_\varepsilon^s\left(\frac{t_j}{t_i} u_\varepsilon(t_i), v_\varepsilon(t_i)\right),
$$

where $E_\varepsilon^b$ and $E_\varepsilon^b$ refer to the first and second terms in (3). From this, we deduce that if $(u_\varepsilon(t_i), v_\varepsilon(t_i))$ is a global minimizer of $F_\varepsilon$ at time step $t_i$:

$$\frac{t_j^2}{t_i^2} E_\varepsilon^b \left( \frac{t_j}{t_i} u_\varepsilon(t_i), v_\varepsilon(t_i) \right) + E_\varepsilon^s \left( \frac{t_j}{t_i} u_\varepsilon(t_i), v_\varepsilon(t_i) \right) \geq E_\varepsilon(u_\varepsilon(t_j), v_\varepsilon(t_j)) \ \forall 0 \leq j \leq i. \tag{4}$$

This necessary condition for optimality is the foundation of the backtracking algorithm: at each time step $t_i$ after computing a critical point using the alternate minimization algorithm, we check if condition (4) is satisfied for each $t_j$ with $0 \leq j < i$. If it is not, then $(u_\varepsilon(t_i), v_\varepsilon(t_i))$ cannot be a global minimizer for time step $t_i$, and we restart the minimization process from time step $t_i$, using $\left( \frac{t_j}{t_i} u_\varepsilon(t_i), v_\varepsilon(t_i) \right)$ as the initial point of the alternate minimization algorithm.

The following figure represents the evolution of the bulk, surface and total energies for a traction experiment on a fiber–reinforced square matrix with (thick lines) and without (thin lines) backtracking, adapted from [2, 3]. Indeed, the total energy associated to the solution computed using the backtracking algorithm is less than that of the evolution computed without it. Moreover, the total energy of the backtracking solution is continuous with respect to time, which is known to be true of the actual global minimizer (see [5]), while the other is not.
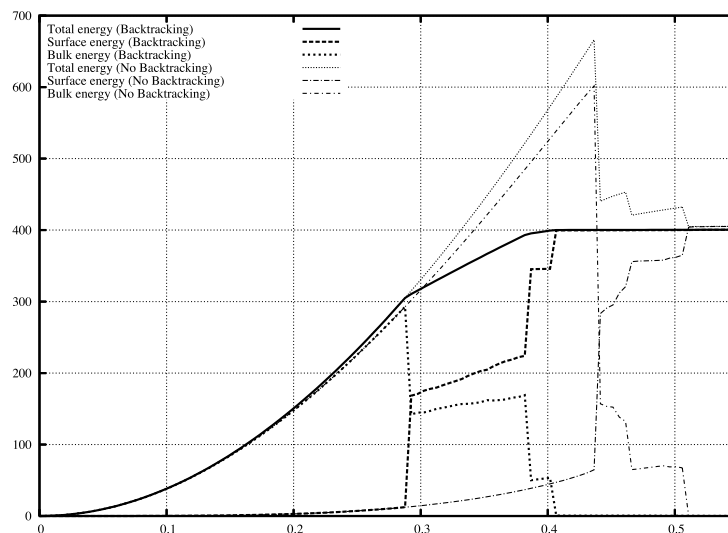
## Literatur

[1] L. Ambrosio and V.M. Tortorelli, *Approximation of functionals depending on jumps by elliptic functionals via Γ-convergence*, Comm. Pure Appl. Math. **43** (1990), no. 8, 999–1036.

[2] B. Bourdin, G.A. Francfort, and J.-J. Marigo, *Numerical experiments in revisited brittle fracture*, J. Mech. Phys. Solids **48** (2000), no. 4, 797–826.

[3] B. Bourdin, J.-J. Marigo, and G.A. Francfort, *The variational approach to fracture*, Springer, to appear.

[4] B. Bourdin, *Numerical implementation of the variational formulation of quasi-static brittle fracture*, To appear.

[5] G.A. Francfort and C. Larsen, *Existence and convergence for quasi-static evolution in brittle fracture*, Comm. Pure Appl. Math. **56** (2003), no. 10, 1465–1500.

[6] G.A. Francfort and J.-J. Marigo, *Revisiting brittle fracture as an energy minimization problem*, J. Mech. Phys. Solids. **46** (1998), no. 8, 1319–1342.

[7] A. Giacomini, *Ambrosio-Tortorelli approximation of quasi-static evolution of brittle fractures*, Calc. Var. Partial Differential Equations **22** (2005), no. 2, 129–172.

## A variational principle in non-smooth Mechanics

ULISSE STEFANELLI

Let $Y$ be a Banach space with dual $Y^*$, $\psi : Y \to (-\infty, \infty]$ be convex, proper, and lower semicontinuous dissipation potential, $\phi \in C^1(Y; \mathbb{R})$ be an energy, and the load $\ell \in L^\infty(0, T; Y^*)$ and the initial state $y_0 \in Y$ be given. A variety of non-smooth (thermo-)mechanical evolution models can be represented by the relation

$$(1) \qquad\qquad \partial\psi(\dot{y}) + D\phi(y) \ni \ell \quad \text{a.e. in } (0, T), \quad y(0) = y_0,$$

where $\partial$ stands for the subdifferential in the sense of Convex Analysis and $t \mapsto y(t)$ is meant to be in $W^{1,1}(0, T; Y)$. Here $\partial\psi$ represents the system of dissipative forces whereas $D\phi - \ell$ stands for the conservative forces instead. Relation (1) appears in connection with many different applicative situations among which plasticity, visco-elasticity, friction [6], heat conduction, and phase change.

Fenchel's inequality $\psi(u) + \psi^*(v) \geq \langle v, u \rangle$ holds for all $u \in Y$ and $v \in Y^*$ where $\langle \cdot, \cdot \rangle$ stands for the duality pairing between $Y^*$ and $Y$ and $\psi^*$ is the conjugate of $\psi$. Moreover, the latter inequality reduces to an equality iff $v \in \partial\psi(u)$. Hence, by defining the *Lagrangian* $L : (0, T) \times Y \times Y \to \mathbb{R}$ as

$$L(t, y, p) := \psi(p) + \psi^*(\ell(t) - D\phi(y)) - \langle \ell(t) - D\phi(y), p \rangle$$

for almost every $t \in (0, T)$, one readily checks that $L(t, y, p) \geq 0$ and

$$L(t, y, p) = 0 \quad \text{iff} \quad \partial\phi(p) \ni \ell(t) - D\phi(y).$$

Let now the functional $F : W^{1,1}(0, T; Y) \to [0, \infty]$ be defined as

$$F(y) := \int_0^T L(t, y(t), \dot{y}(t))\, dt + \phi(y(0) - y_0).$$

Then, minimizers of $F$ and solutions to (1) coincide. Indeed, as $y$ solves (1), we have that $L(t, y(t), \dot{y}(t)) = 0$ for almost every $t \in (0, T)$ and $y(0) = y_0$. That is $F(y) = 0$. On the contrary, if $F(y) = 0$, then $L(t, y(t), \dot{y}(t)) = 0$ for almost every $t \in (0, T)$ and $\phi(y(0) - y_0) = 0$ and (1) follows. Hence, we have the following.

**Theorem 0.1.** *$y$ solves* (1) *iff* $F(y) = 0 = \min F$.

The characterization of solutions of differential problems driven by convex potentials as minimizers of functionals via the Fenchel approach is rather classical and has to be traced back to Brezis & Ekeland [1, 2]. In the referred papers, the Authors provide some similar variational characterization for gradient flows of

convex functionals in Hilbert spaces. I have recently extended these ideas to the case of doubly nonlinear equations [7].

In order to extract some information from the variational characterization of Theorem 1, it is convenient to focus on some more specific situation. I shall in particular consider the case of linearized hardening elasto-plasticity [4] by additionally requiring

$\psi$ positively 1-homogeneous and $\phi$ quadratic and coercive on $D(\psi)$,

namely the domain of $\psi$. In this specific situation $D\phi$ is linear and Theorem 1 is providing a useful tool in order to deal with limiting procedures. Indeed, since one reinterprets the equation as a minimum problem, it is clear that the natural concept to be considered is that of $\Gamma$-convergence [3]. More precisely, as Theorem 1 directly quantifies the value of the minimum to be 0, what is actually needed are so-called $\Gamma$-$\liminf$ inequalities only.

The variational approach by Theorem 1 provides the possibility of recovering convergence in a variety of approximated situations.

**Space approximation.** Conformal finite elements and data approximations can be considered. In particular, one can easily handle by means of this variational approach the case where $Y$ is replaced by a nested sequence of finite dimensional subspaces $Y_h$ such that $\cup_h Y_h$ is dense in $Y$, $\phi_h$ is the restriction of $\phi$ to $Y_h$, and $\psi_h \to \psi$ in the sense of Mosco in $Y$ [3].

**Time discretization.** One can provide a discrete analogue to Theorem 1. Namely, it is possible to variationally characterize solutions of the so-called $\theta$-scheme

$$y^0 = y_0, \quad \psi(y^i - y^{i-1}) + A\big(\theta y^i + (1-\theta)y^{i-1}\big) \ni \ell_\theta^i \quad \text{for} \quad i = 1, \dots, N,$$

where $\ell_\theta^i = \ell(\theta t^i + (1-\theta)t^{i-1})$ for $0 = t^0 < t^1 < \cdots < t^N = T$, as minimizers of a suitable discrete functional tailored on $F$. This approach can be exploited in order to prove the unconditional stability of the scheme in $W^{1,\infty}(0, T; Y)$ and its convergence with respect to the corresponding weak-star topology as the diameter of the partition goes to 0. Finally, the discrete functional itself can be used in order to control the discretization error.

**Fully discrete schemes.** The above-mentioned techniques for space and time discretization can be combined in order to provide the weak-star convergence in $W^{1,\infty}(0, T; Y)$ of some fully discretized solutions as well. This result has to be compared with the former analysis in [5], where a stronger convergence in proved by means of a somehow more complicated argument.

### Literatur

[1] H. Brezis and I. Ekeland, *Un principe variationnel associé à certaines équations paraboli-ques. Le cas dépandant du temps.* C. R. Acad. Sci. Paris Sér. A-B, **282** (1976), A1197–A1198.

[2] H. Brezis and I. Ekeland, *Un principe variationnel associé à certaines équations paraboli-ques. Le cas indépandant du temps*, C. R. Acad. Sci. Paris Sér. A-B, **282** (1976), A971–A974.

[3] G. Dal Maso, *An introduction to $\Gamma$-convergence*, Progress in Nonlinear Differential Equations and their Applications, 8. Birkhäuser Boston, Inc., Boston, MA, 1993.

[4] W. Han and B. D. Reddy, *Plasticity. Mathematical theory and numerical analysis*, Inter-disciplinary Applied Mathematics, 9. Springer-Verlag, New York, 1999.
[5] W. Han and B. D. Reddy, *Convergence of approximations to the primal problem in plasticity under conditions of minimal regularity*, Numer. Math. **87** (2000), 2:283–315.
[6] J.-J. Moreau, *Sur les lois de frottement, de viscosité et plasticité*, C. R. Acad. Sci. Paris Sér. II Méc. Phys. Chim. Sci. Univers Sci. Terre, **271** (1970), 608–611.
[7] U. Stefanelli, *The Brezis-Ekeland principle for doubly nonlinear equations*, Preprint IMATI - CNR, 41-PV, 2006.

## Global energetic approach to stochastic damage evolution in lattice structures

### Jan Zeman

### (joint work with Ron H.J. Peerlings, Marc G.D. Geers)

Lattice models of fracture represent a heterogeneous material as discrete units interacting via brittle elements. By *randomizing* the individual links' properties and repeated Monte-Carlo type analyses, the models are able to simulate very complex phenomena using few parameters; e.g. [1]. Such numerical simulations, however, do not provide any insight into the governing equations of the collective behavior, in particular long-range interactions among fractured elements. Therefore, the present contribution can be seen as the first step in the direction of a consistent derivation of non-local damage theories from stochastic discrete models.

In the adopted "global energetic" philosophy [5, 6], the system is assumed to be described by a *globally stored* elastic energy and a *global energy dissipation*. Consider first a *deterministic system* consisting of $N$ brittle units connecting $M$ nodes in a $n$-dimensional space. Similarly to [3], the state of the $e$-th element is specified by a *displacement vector* $\boldsymbol{d}_e \in \mathbb{R}^{2n}$ storing the displacement of the nodes associated with the element and an internal variable $\chi_e \in \{0, 1\}$ providing the fracture state of the unit; $\chi_e = 0$ describes an intact unit while $\chi_e = 1$ corresponds to a failed element. The energy stored in the $e$-th element $E_e : \mathbb{R}^{2n} \times \{0, 1\} \to \mathbb{R}$ is then provided by

$$(1) \qquad E_e(\boldsymbol{d}_e, \chi_e) := \tfrac{1}{2}\left(1 - \chi_e\right)\boldsymbol{d}_e^\mathsf{T}\mathsf{B}_e^\mathsf{T}C_e\mathsf{B}_e\boldsymbol{d}_e,$$

where $\mathsf{B}_e \in \mathbb{M}^{1 \times 2n}$ denotes the displacement-to-strain matrix and $C_e$ stands for the axial element stiffness; e.g. [2]. The irreversible processes are quantified by the dissipation distance $D_e : \{0, 1\} \times \{0, 1\} \to \overline{\mathbb{R}}$

$$(2) \qquad D_e(\chi_e^1, \chi_e^2) := \begin{cases} \kappa_e(\chi_e^2 - \chi_e^1) & \text{for } \chi_e^1 \leq \chi_e^2, \\ +\infty & \text{otherwise,} \end{cases}$$

where $\kappa_e$ denotes an energy dissipated by the failure of the element.

Now consider behavior of the whole structure on a time interval $[0; T]$ when subject to a hard-device loading imposed by a prescribed displacement $\overline{\boldsymbol{d}}(t) \in \mathbb{R}^{\overline{M}}$, applied to the nodes indexed by a set $\overline{I} \subset \{1, 2, \ldots, M\}$. Introducing a partition of the time domain $0 = t_0 < t_1 < \ldots < t_F = T$ and an initial datum $(\boldsymbol{d}(0), \boldsymbol{\chi}(0))$,

the time-discretized evolution of the system is provided by an *incremental* minimization principle [5, 6]:

$$(3) \qquad (\boldsymbol{d}(t_{i+1}), \boldsymbol{\chi}(t_{i+1})) = \arg\min_{(\boldsymbol{d}, \boldsymbol{\chi}) \in \mathbb{K}(t_{i+1}) \times \mathbb{S}} E(\boldsymbol{d}, \boldsymbol{\chi}) + D(\boldsymbol{\chi}(t_i), \boldsymbol{\chi})$$

with the set of kinematically admissible displacements defined as

$$(4) \qquad \mathbb{K}(t) := \left\{ \boldsymbol{d} \in \mathbb{R}^{nM} : \boldsymbol{d}_{\overline{I}} = \overline{\boldsymbol{d}}_{\overline{I}}(t) \right\}$$

and the set of admissible internal variables $\mathbb{S} := \{0, 1\}^N$. The terms appearing in (3) without the index $e$ correspond to the global quantities, obtained by the assembly of individual elements contributions [2]. In this setting, the incremental evolution problem (3) coincides with the weakest link algorithm used as the basic component of statistical simulations of fracture [1].

Uncertainty is incorporated into the model by treating the energy thresholds $\kappa_e$ as *independent random* variables $K_e$ with a probability distribution $F_{K_e}(\kappa_e)$. As the result of randomization, each internal variable appears only with a certain probability. In particular, taking into account the discrete nature of the system, all internal variables can be enumerated by an index $\omega = 1, 2, \ldots, 2^N = |\mathbb{S}|$. The probability distribution of internal variables is fully specified by *discrete* values $\mu(\omega) \geq 0$, $\sum_{\omega=1}^{|\mathbb{S}|} \mu(\omega) = 1$. Hence, the full statistical description would require to provide a time-dependent evolution of probabilities $\boldsymbol{\mu}(t)$ as a result of prescribed loading and a particular choice of randomization. Such characterization is, however, rather difficult to obtain as the number of probabilities grows exponentially with $N$ and the influence of $F_{K_e}$ is very complex.

An alternative approach, inspired by the Young-measure relaxation of rate independent problems [5], is to characterize the stochastic evolution using *statistics* of internal variables. The simplest choice allowing to account for binary interactions between units is provided by a *two-unit probability matrix* $\mathsf{P}$:

$$(5) \qquad \mathsf{P}(\boldsymbol{\mu}) := \sum_{\omega=1}^{|\mathbb{S}|} \boldsymbol{\chi}(\omega) \boldsymbol{\chi}^{\mathsf{T}}(\omega) \mu(\omega) \in \mathcal{S} \subset \mathbb{M}^{N \times N},$$

where the set of admissible two-unit probability matrices $\mathcal{S}$ coincides with the *Boolean quadratic polytope* characterized in [7]. Moreover, we introduce a set

$$(6) \qquad \Omega(\overline{\mathsf{P}}) := \{ \mu(\omega) \geq 0, \sum_{\omega=1}^{|\mathbb{S}|} \mu(\omega) = 1 : \mathsf{P}(\boldsymbol{\mu}) = \overline{\mathsf{P}} \}$$

collecting the probability distributions compatible with a probability matrix $\overline{\mathsf{P}}$.

Such a re-definition of internal variables allows us to introduce a relaxed version of the incremental minimization principle. In the first step, we rewrite (3) as

$$(7) \qquad \boldsymbol{\chi}(t_{i+1}) \in \arg\min_{\boldsymbol{\chi} \in \mathbb{S}} H(t_{i+1}, \boldsymbol{\chi}) + D(\boldsymbol{\chi}(t_i), \boldsymbol{\chi}),$$

with the "condensed" energetic function $H : [0; T] \times \mathbb{S} \to \mathbb{R}$ defined by

$$(8) \qquad H(t, \boldsymbol{\chi}) := \min_{\boldsymbol{d} \in \mathbb{K}(t)} E(\boldsymbol{d}, \boldsymbol{\chi}).$$

The relaxed function $\mathcal{H} : [0; T] \times \mathcal{S} \to \mathbb{R}$ is introduced via:

$$(9) \qquad \mathcal{H}(t, \mathsf{P}) := \min_{\boldsymbol{\mu} \in \Omega(\mathsf{P})} \sum_{\omega=1}^{|\mathbb{S}|} \min_{\boldsymbol{d}(\omega) \in \mathbb{K}(t)} E(\boldsymbol{d}, \boldsymbol{\chi}(\omega))\mu(\omega).$$

Adapting the methods developed in [4] to the discrete setting, the energetic term $\mathcal{H}$ can bounded from above by

$$(10) \qquad \mathcal{H}(t, \mathsf{P}) \leq H^0(t) + \tfrac{1}{2}(\boldsymbol{\tau}(\mathsf{P}) \bullet \mathrm{diag}(\mathsf{P}))^{\mathsf{T}}(\mathsf{B}\boldsymbol{d}^0(t))$$

where $H^0$ denotes the minimum energy for an original (intact) structure when subjecting the selected nodes to displacement $\overline{\boldsymbol{d}}(t)$, $\boldsymbol{d}^0$ is the corresponding displacement of all nodes in the structure, $\bullet$ denotes the Hadamard product and the $\boldsymbol{\tau}(t)$ is the optimal stress polarization defined by a system of linear equations

$$(11) \qquad \left[\mathsf{P} \bullet \left(\mathsf{C}^{-1} - \mathsf{\Gamma}^0(t)\right)\right] \boldsymbol{\tau}(t) = \mathrm{diag}(\mathsf{P}) \bullet (\mathsf{B}\boldsymbol{d}^0(t))$$

where the matrix $\mathsf{\Gamma}^0 \in \mathbb{M}^{N \times N}$ is introduced in [4].

Derivation of the *relaxed dissipation distance* is currently under development and only few preliminary results are available. In particular, it can be shown that for $N = 1$

$$(12) \qquad \mathcal{D}_1(P_{11}^1, P_{11}^2) = \begin{cases} \int_{P_{11}^1}^{P_{11}^2} F_{K_1}^{-1}(P)\,\mathrm{d}P & \text{for } P_{11}^1 \leq P_{11}^2, \\ +\infty & \text{otherwise,} \end{cases}$$

which generalizes the local relations used in [3]. For a two-element structure and deterministic values of thresholds, the Wasserstein distance approach introduced in [5, Section 5.2], resulting in a linear programming problem, leads to an additive expression

$$(13) \qquad \mathcal{D}(\mathsf{P}^1, \mathsf{P}^2) = \mathcal{D}_1(P_{11}^1, P_{11}^2) + \mathcal{D}_2(P_{22}^1, P_{22}^2).$$

For a general distribution of thresholds, however, the additivity of dissipation contributions is no longer valid as easily verified by the analysis of serial and parallel system of two units.

Finally note that assuming $\mathcal{D}(\mathsf{P}^1, \mathsf{P}^2)$ is a function convex in $\mathsf{P}^2$, the relaxed version of (7) assumes the form of a convex incremental problem

$$(14) \qquad \mathsf{P}(t_{i+1}) \in \arg\min_{\mathsf{P} \in \mathcal{S}} \mathcal{H}(t_{i+1}, \mathsf{P}) + \mathcal{D}(\mathsf{P}(t_i), \mathsf{P})$$

efficiently solvable by modern tools of mathematical programming.

LITERATUR

[1] M. J. Alava, P. K. V. V. Nukala, and S. Zapperi, *Statistical models of fracture*, Advances in Physics **55** (2006), 349–476.
[2] Z. Bittnar and J. Šejnoha, *Numerical methods in structural mechanics*, ASCE Press and Thomas Telford (1996).
[3] G.A. Francfort and J.J. Marigo, *Stable damage evolution in a brittle continuous medium*, European Journal of Mechanics A-Solids **12** (1993), 149–189.

[4] R. Luciano and J. R. Willis, *FE analysis of stress and strain fields in finite random composite bodies*, Journal of the Mechanics and Physics of Solids **53** (2005), 1505–152.

[5] A. Mielke, *Deriving new evolution equations for microstructures via relaxation of variational incremental problems*, Computer Methods in Applied Mechanics and Engineering, **193** (2004), 5095–5127.

[6] A. Mielke, *Evolution of rate-independent systems*, In C. Dafermos and E. Feireisl, editors, Handbook of Differential Equations: Evolutionary Equations II, Elsevier (2005), 461–559.

[7] M. Padberg, *Boolean quadric polytope: Some characteristics, facets and relatives*, Mathematical Programming, Series B **45** (1989), 139–172.

## Energy release rate for cracks in finite–strain elasticity

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(joint work with Alexander Mielke)

Griffith's fracture criterion describes in a quasistatic setting whether or not a pre–existing crack in an elastic body is stationary for given external forces. In the two dimensional case and assuming that the crack path is a smooth curve which is known in advance, this fracture criterion can be reformulated in terms of the energy release rate (ERR). The ERR is defined as the derivative of the deformation energy of the body with respect to the crack length. In this note we describe sufficient conditions on polyconvex energy densities which guarantee that the ERR is well defined in the finite–strain case.

Let $\Omega_* \subset \mathbb{R}^2$ be a bounded Lipschitz domain with $0 \in \Omega_*$. For $\delta \in \mathbb{R}$ we define $S_\delta = \{x \in \mathbb{R}^2; \; x_1 \leq \delta, \; x_2 = 0\}$ and consider cracked domains $\Omega_\delta = \Omega_* \backslash S_\delta$ with cracks $C_\delta = \overline{\Omega_*} \cap S_\delta$. It is assumed that $\partial \Omega_\delta = \overline{\Gamma}_{\mathrm{Dir}} \cup \overline{\Gamma}_{\mathrm{N}} \cup C_\delta$, where $\Gamma_{\mathrm{Dir}}$ and $\Gamma_N$ are the Dirichlet and Neumann boundary, respectively, and that there exists a $\delta_0 > 0$ such that $\Omega_\delta$ is a connected domain for every $\delta \leq \delta_0$.

The behavior of the body is described in the framework of finite–strain elasticity. Let $\varphi : \Omega_\delta \to \mathbb{R}^2$ be a deformation field. Assuming vanishing volume forces, the deformation energy is given by

$$I(\Omega_\delta, \varphi) = \int_{\Omega_\delta} W(\nabla \varphi) \mathrm{d}x - \langle h, \varphi \rangle_{\Gamma_N},$$

where $W : \mathbb{R}^{2,2} \to [0, \infty]$ is the elastic energy density and $h \in \left( W^{1-\frac{1}{p}, p}(\Gamma_N) \right)'$ is a prescribed surface force density on $\Gamma_N$. We have the following conditions on $W$

**A1 Polyconvexity:** $W : \mathbb{R}^{2,2} \to [0, \infty]$ is polyconvex with $W(F_n) \to \infty$ as $\det F_n \searrow 0$ and $W(F) = \infty$ if $\det F \leq 0$. Here, $F, F_n \in \mathbb{R}^{2,2}$.

**A2 Coercivity:** For every $F \in \mathbb{R}^{2,2}$ we have $W(F) \geq c_1 |F|^p - c_2$ with $p > 2$ and $c_i > 0$.

Let $g \in W^{1-\frac{1}{p}, p}(\Gamma_{\mathrm{Dir}})$. The set of admissible deformation fields is denoted by

$$V_{\mathrm{ad}}(\Omega_\delta) = \{\varphi \in W^{1,p}(\Omega_\delta); \; \varphi|_{\Gamma_{\mathrm{Dir}}} = g\}.$$

For every $\delta \leq \delta_0$ Ball's fundamental theorem guarantees that there exists a minimizer $\varphi_\delta \in V_{\mathrm{ad}}(\Omega_\delta)$ with

$$I(\Omega_\delta) \equiv I(\Omega_\delta, \varphi_\delta) = \min_{\psi \in V_{\mathrm{ad}}(\Omega_\delta)} I(\Omega_\delta, \psi).$$

**Definition.** *The energy release rate corresponding to the domain $\Omega_0$ with crack $C_0$ is defined as*

$$ERR(\Omega_0) = \lim_{\delta \searrow 0} \tfrac{1}{\delta} \big( I(\Omega_0) - I(\Omega_\delta) \big) = -\frac{\mathrm{d}I(\Omega_\delta)}{\mathrm{d}\delta}\Big|_{\delta = 0+}.$$

With this definition the Griffith fracture criterion takes the form

If $ERR(\Omega_0) < 2\gamma$, then the crack is stationary.

The constant $\gamma > 0$ is the fracture toughness and depends on the material. For linear elastic models, Destuynder/Djaoua [3] were the first who proved rigorously that the $ERR$ is well defined and that it can be expressed through formulas which are based on the Eshelby tensor. Similar formulas are stated as well for the nonlinear case, but they are in general derived under the assumption that the deformation gradients and the stress fields have a certain singular behavior near the crack tip. However, in the finite–strain case such regularity results have not been proved yet. We formulate now additional conditions on the energy density $W$ which allow us to show, without making any assumptions on the smoothness of the minimizers, that the $ERR$ is well defined in the finite–strain case.

**A3:** $W$ is differentiable on $\mathbb{R}_+^{2,2}$ and for every $F \in \mathbb{R}_+^{2,2}$ we have

$$\left| F^\top DW(F) \right| \leq \kappa_1 (1 + W(F)).$$

**A4:** $W$ is twice differentiable on $\mathbb{R}_+^{2,2}$ and for every $F \in \mathbb{R}_+^{2,2}$, $B, C \in \mathbb{R}^{2,2}$ we have

$$\left| D^2 W(F)[FB, FC] \right| \leq \kappa_2 (1 + W(F)) |B| |C|.$$

Condition **A3** was first introduced and discussed in [2, 1]. Note that conditions **A3** and **A4** are compatible with the assumption that $W(F) = \infty$ if $\det F \leq 0$. For example let $p > 1$, $c_i > 0$ and $r > 0$. The function $W(F) = c_1 |F|^p + c_2 (\det F)^{-r}$ if $\det F > 0$, $W(F) = \infty$, otherwise, is polyconvex and satisfies **A3** and **A4**.

Based on assumptions **A3** and **A4** we proved a weak convergence theorem for Eshelby tensors, which is the key for our further analysis. Let

$$E(\nabla \varphi) = -\nabla \varphi^\top DW(\nabla \varphi) + W(\nabla \varphi)\mathbf{1}$$

denote the Eshelby tensor corresponding to the deformation field $\varphi$.

**Theorem 1.** [5] *Let $\Omega$ be a bounded, open subset of $\mathbb{R}^2$, $p > 2$ and assume that $W : \mathbb{R}^{2,2} \to [0, \infty]$ satisfies assumptions **A1**, **A3** and **A4**. For every sequence*

$(\varphi_n)_{n \in \mathbb{N}_0} \subset W^{1,p}(\Omega)$ *with*

$$\varphi_n \rightharpoonup \varphi_0 \ \text{weakly in } W^{1,p}(\Omega),$$

$$\int_\Omega W(\nabla \varphi_n) \to \int_\Omega W(\nabla \varphi_0)\mathrm{d}x < \infty \quad \text{for } n \to \infty$$

*it follows that* $E(\nabla \varphi_n) \rightharpoonup E(\nabla \varphi_0)$ *weakly in* $L^1(\Omega)$.

**Remark on the proof.** In order to show that $\nabla \varphi_n^\top DW(\nabla \varphi_n) \rightharpoonup \nabla \varphi_0^\top DW(\nabla \varphi_0)$ weakly in $L^1(\Omega)$, we consider a parameter dependent energy for $B \in L^\infty(\Omega)$:

$$J_B(t, \varphi) = \int_\Omega W(\nabla \varphi(x)(\mathbf{1} + tB(x)))\, \mathrm{d}x.$$

The above assumptions guarantee that $J_B$ is differentiable with respect to $t$ with $\partial_t J_B(0, \varphi) = \int_\Omega \left( \nabla \varphi^\top DW(\nabla \varphi) \right) : B\, \mathrm{d}x$. An abstract convergence lemma by Francfort/Mielke [4] on the convergence of derivatives of parameter dependent energies implies that $\partial_t J_B(0, \varphi_n) \to \partial_t J_B(0, \varphi_0)$. Since $B \in L^\infty(\Omega)$ was arbitrarily chosen, we obtain the desired result.

We are now ready to formulate our main result on the energy release rate for a two dimensional body with a straight crack.

**Theorem 2.** [Griffith formula] [5] *Let* **A1**–**A4** *be satisfied and assume that*

$$\inf_{\varphi \in V_{\mathrm{ad}}(\Omega_0)} I(\Omega_0, \varphi) < \infty.$$

*Let furthermore* $\theta \in C_0^\infty(\Omega_*)$ *with* $\theta = 1$ *near the crack tip* $(0,0)^\top$. *The energy release rate* $ERR(\Omega_0)$ *is well defined and a generalized Griffith formula is valid:*

(1) $\qquad ERR(\Omega_0) = \max\{\, G(\varphi, \theta)\,;\, \varphi \text{ minimizes } I(\Omega_0, \cdot) \text{ over } V_{\mathrm{ad}}(\Omega_0)\,\},$

*where*

(2) $$G(\varphi) := G(\varphi, \theta) = -\int_{\Omega_0} E(\nabla \varphi) : \nabla \left(\begin{smallmatrix} \theta \\ 0 \end{smallmatrix}\right)\, \mathrm{d}x.$$

*Formulas* (1) *and* (2) *are independent of the choice of* $\theta$. The energy release rate can also be expressed through the $J$–integral. Let $B_R(x_0) = \{\, x \in \mathbb{R}^d\,;\, |x - x_0| < R\,\}$.

**Theorem 3.** [5] *Let the assumptions from the previous theorem be satisfied and let* $R_0 > 0$ *such that* $\overline{B_{R_0}(0)} \subset \Omega_*$. *For every minimizer* $\varphi_0$ *of* $I(\Omega_0, \cdot)$ *and almost every* $R \in (0, R_0)$ *we have*

(3) $$G(\varphi_0) = -\int_{\partial B_R(0)} \left( E(\nabla \varphi_0)\vec{n} \right) \cdot \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)\, \mathrm{d}s,$$

*where* $\vec{n}$ *is the interior unit normal vector on* $\partial B_R(0)$. Formally, the $J$–integral is derived from the Griffith formula by integration by parts. For minimizers $\varphi_0$

assumption **A3** guarantees that $E(\nabla\varphi_0) \in L^1(\Omega_0)$. Moreover, the considerations in [2, 1] imply that div $E(\nabla\varphi_0) = 0$. If we knew in addition that $E(\nabla\varphi_0) \in L^q(\Omega_0)$ for some $q > 1$, then a suitable version of the Gauss theorem would allow us to pass from the Griffith formula to the $J$–integral with respect to arbitrary paths around the crack tip. In the case $q = 1$ a suitable Gauss theorem seems to be unknown, and we applied Fubini's theorem in order to obtain identity (3) at least for almost every circular path.

Let us finally remark that in the case of unique minimizers we recover the formulas proposed in the literature on fracture mechanics.

### LITERATUR

[1] J.M. Ball, *Some open problems in elasticity*, In Paul Newton, editor, Geometry, mechanics, and dynamics. Volume in honor of the 60th birthday of J.E. Marsden, New York, Springer (2002), 3–59.

[2] P. Bauman, N.C. Owen, D. Phillips, *Maximum principles and a priori estimates for a class of problems from nonlinear elasticity*, Ann. Inst. Henri Poincaré – Analyse non linéaire **8** (1991), 119–157.

[3] P. Destuynder, M. Djaoua, *Sur une interpretation mathématique de l'intégrale de Rice en théorie de la rupture fragile*, Math. Meth. Appl. Sci., **3** (1981), 70–87.

[4] G. Francfort, A. Mielke, *Existence results for a class of rate–independent material models with nonconvex elastic energies*, J. reine angew. Math., **595** (2006), 55–91.

[5] D. Knees, A. Mielke, *Energy release rate for cracks in finite–strain elasticity*, Preprint No. 1100, Weierstrass Institute for Appl. Analysis and Stochastics, Berlin, (2006). submitted

## Evolution of microstructures in shape memory alloys
### Klaus Hackl

### 1. General framework

Our modeling will be based on the general framework presented for example in [4], [5] and [7]. For this purpose we need a relaxed free energy $\Psi^{\mathrm{rel}}(\varepsilon, \lambda_{\boldsymbol{z}})$ dependent on the macroscopic strain $\varepsilon$ and on the Young-measure $\lambda_{\boldsymbol{z}}$, i.e. a probability distribution of the internal variable $\boldsymbol{z}$. Moreover we will assume a relaxed dissipation potential of the form $\Delta^*(\dot{\lambda}_{\boldsymbol{z}})$. We state that the total power is minimized by $\dot{\lambda}_{\boldsymbol{z}}$, where we have to respect the facts that $\lambda_{\boldsymbol{z}} \geq 0$ and $\int \lambda_{\boldsymbol{z}}\, \mathrm{d}\boldsymbol{z} = 1$. Introducing this constraints via Langrange- and Kuhn-Tucker-multipliers, respectively, we formulate a Lagrange functional of the form

$$(1) \qquad \mathcal{L}(\varepsilon, \lambda_{\boldsymbol{z}}, \dot{\lambda}_{\boldsymbol{z}}) = \frac{d}{dt}\,\Psi^{\mathrm{rel}}(\varepsilon, \lambda_{\boldsymbol{z}}) + \Delta^*(\dot{\lambda}_{\boldsymbol{z}}) + \alpha \int \dot{\lambda}_{\boldsymbol{z}}\, \mathrm{d}\boldsymbol{z} - \int \beta_{\boldsymbol{z}} \dot{\lambda}_{\boldsymbol{z}}\, \mathrm{d}\boldsymbol{z},$$

and we get the Kuhn-Tucker conditions

$$(2) \qquad\qquad \dot{\lambda}_{\boldsymbol{z}} \geq 0, \quad \beta_{\boldsymbol{z}} \geq 0, \quad \dot{\lambda}_{\boldsymbol{z}}\beta_{\boldsymbol{z}} = 0.$$

By minimization of $\mathcal{L}$ with respect to $\dot{\lambda}_{\boldsymbol{z}}$ we are now able to derive evolution equations for $\lambda_{\boldsymbol{z}}$. For details see the references above. We are going to specify $\Psi^{\mathrm{rel}}$ and $\Delta^*$ for two different models of shape memory alloys.

## 2. Polycrystal model

An ideal polycrystalline shape memory alloy consists of an infinite number of randomly oriented grains, which means we have $\boldsymbol{z} = \boldsymbol{R} \in \mathrm{SO}_3$. For modeling purposes, however, the number of different crystal orientations is restricted to a large, but finite number $N$. Starting from an arbitrary fixed coordinate system, every crystal orientation $j$ is described by a rotational tensor $\boldsymbol{R}_j$. Together with the linearized Bain strain $\boldsymbol{\varepsilon}_t$ describing the transformation from the undeformed austenite reference configuration to the lower symmetry martensitic structure, the transformation strain for the orientation $j$ is

$$(3) \qquad \boldsymbol{\eta}_j = \boldsymbol{R}_j^T \boldsymbol{\varepsilon}_t \boldsymbol{R}_j .$$

The volume fraction corresponding to the $j$th martensite orientation is now denoted by $\lambda_j$, $j = 1, \ldots, N$, whereas $\lambda_0$ corresponds to the transformation strain $\boldsymbol{\eta}_0 = \boldsymbol{0}$ of the austenite. We assume a simple linear elastic material law,

$$(4) \qquad \Psi_j \left( \boldsymbol{\varepsilon}_j, \boldsymbol{\eta}_j \right) = \frac{1}{2} \left( \boldsymbol{\varepsilon}_j - \boldsymbol{\eta}_j \right) : \mathbb{C}_j : \left( \boldsymbol{\varepsilon}_j - \boldsymbol{\eta}_j \right) + \alpha_j ,$$

where $\mathbb{C}_j$ is the elasticity tensor correponding to orientation $\boldsymbol{R}_j$, "$:$" means contraction with respect to two indices, and $\alpha_j$ denotes the chemical energy of the $j$th variant, which only differs from austenite to martensite but is the same for all martensite variants for reasons of symmetry.

In our energy formulation (4), we introduced the strain $\boldsymbol{\varepsilon}_j$ of the crystals of orientation $j$. The global strain $\boldsymbol{\varepsilon}$ is then given as the volume average of the local ones, which leads to the following formulation of the global energy for fixed volume fractions:

$$(5) \qquad \Psi^{\mathrm{rel}} \left( \boldsymbol{\varepsilon}, \boldsymbol{\lambda} \right) = \inf \left\{ \sum_{j=0}^{N} \lambda_j \Psi_j \left( \boldsymbol{\varepsilon}_j, \boldsymbol{\eta}_j \right) \middle| \boldsymbol{\varepsilon}_j, \boldsymbol{\varepsilon} = \sum_{j=0}^{N} \lambda_j \boldsymbol{\varepsilon}_j \right\} .$$

This way of calculating the free energy corresponds to a relaxation by convexification, which is actually a very crude way of obtaining lower bounds as estimates to the energy of a multivariant material. For a comparison of upper and lower bounds to the free energy in order to estimate the quality of the convexification bound, see [2], [3], and [6].

Minimizing (5) over the crystal strains $\boldsymbol{\varepsilon}_j$ yields the straightforward expression for the relaxed energy

$$(6) \qquad \Psi^{\mathrm{rel}} \left( \boldsymbol{\varepsilon}, \boldsymbol{\lambda} \right) = \frac{1}{2} \left( \boldsymbol{\varepsilon} - \boldsymbol{\eta}_{\mathrm{eff}} \right) : \mathbb{C}_{\mathrm{eff}} : \left( \boldsymbol{\varepsilon} - \boldsymbol{\eta}_{\mathrm{eff}} \right) + \alpha_{\mathrm{eff}} ,$$

with the effective elasticity tensor, transformation strain and chemical energy

$$(7) \qquad \mathbb{C}_{\mathrm{eff}} = \left( \sum_{j=0}^{N} \lambda_j \mathbb{C}^{-1} \right)^{-1} , \qquad \boldsymbol{\eta}_{\mathrm{eff}} = \sum_{j=0}^{N} \lambda_j \boldsymbol{\eta}_j , \qquad \alpha_{\mathrm{eff}} = \sum_{j=0}^{N} \lambda_j \alpha_j .$$

The crystal strains for which this minimal energy is achieved are $\boldsymbol{\varepsilon}_j = \boldsymbol{\varepsilon} + \boldsymbol{\eta}_j - \boldsymbol{\eta}_{\mathrm{eff}}$. Since changes in the orientation distribution correspond to a growth and shrinking

of domains containing certain variants, an intuitional assumption is the dissipation function

$$(8) \qquad \Delta^* \left( \dot{\boldsymbol{\lambda}} \right) = r \left| \dot{\boldsymbol{\lambda}} \right|$$

which connects the Euclidian norm of the rate of change of the orientation distributions linearly to the dissipated energy. The orientation distributions obtained by solving the evolution equations corresponding to this model compare well with $\gamma$-ray diffraction experiments, see [8].

## 3. Single-crystal model

For the single-crystal model we can approximate the relaxed energy in a more accurate way by a so-called lamination, where the local displacement–field is perturbed subjected to a prescribed microstructure on a representative volume element. For more details on this approach, see [1]. Precisely, the strains are determined as

$$(9) \qquad \varepsilon_A \;=\; \varepsilon + \frac{1}{\lambda_A}\, \mathbf{n}_A \otimes_S \mathbf{u}_A,$$

$$(10) \qquad \varepsilon_I \;=\; \varepsilon - \frac{1}{\sum \lambda_I}\, \mathbf{n}_A \otimes_S \mathbf{u}_A + \frac{1}{\lambda_I}\, \mathbf{n}_M \otimes_S \left( \mathbf{u}_I - \mathbf{u}_{I-1} \right)$$

with $\mathbf{a} \otimes_S \mathbf{b} := \frac{1}{2} \left( \mathbf{a} \otimes \mathbf{b} + \mathbf{b} \otimes \mathbf{a} \right)$, where $\mathbf{u}_A, \mathbf{u}_I$ are referred to as amplitudes of perturbation and $\mathbf{n}_A, \mathbf{n}_M$ symbolize the laminate–directions. The relaxed energy is now given as

$$(11) \qquad \Psi^{\text{rel}}(\varepsilon, \boldsymbol{\lambda}, \mathbf{n}_A, \mathbf{n}_M) = \inf \left\{ \left. \sum_{j=0}^{N} \lambda_j \Psi_j \left( \varepsilon_j, \eta_j \right) \right| \mathbf{u}_A, \mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_{NV-1} \right\}.$$

In our case, this energy can be represented analytically by

$$\begin{aligned}
\Psi^{\text{rel}} \;=\;& \frac{1}{2}\varepsilon : \bar{\mathbb{C}} : \varepsilon + \varepsilon : \left[ (\Delta\mathbb{C} \cdot \mathbf{n}_A) \cdot \mathbf{u}_A \right] + \frac{1}{2}\mathbf{u}_A \cdot \widehat{\mathbb{C}} \cdot \mathbf{u}_A - \bar{\boldsymbol{\tau}} : \varepsilon \\
&+ \frac{1}{\lambda_M} \left( \bar{\boldsymbol{\tau}} \cdot \mathbf{n}_A \right) \cdot \mathbf{u}_A - \frac{1}{2} \sum_{I=1}^{NV} \left\{ \boldsymbol{\tau}_i \cdot (\mathbf{u}_i - \mathbf{u}_{I-1}) \right\} \cdot \mathbf{n}_M + \bar{\alpha},
\end{aligned}$$

where

$$\mathbf{u}_A \;=\; -\widehat{\mathbb{C}}^{-1} \cdot \left( \Delta\mathbb{C} : \varepsilon + \frac{1}{\lambda_M}\bar{\boldsymbol{\tau}} \right) \cdot \mathbf{n}_A,$$

$$\mathbf{u}_I \;=\; -\frac{1}{\lambda_M} \mathbb{C}_M^{-1} \cdot \left( \sum_{i=1}^{I} \sum_{j=I+1}^{NV} \left\{ \lambda_i\, \lambda_j \left( \boldsymbol{\tau}_j - \boldsymbol{\tau}_i \right) \right\} \right) \cdot \mathbf{n}_M$$

symbolize optimal amplitudes of the applied perturbations determined by the minimization. The quantities $\bar{\mathbb{C}} := \lambda_A\, \mathbb{C}_A + \sum \lambda_I\, \mathbb{C}_M$, $\Delta\mathbb{C} := \mathbb{C}_A - \mathbb{C}_M$, $\widehat{\mathbb{C}} := \mathbf{n}_A \cdot \mathbb{C} \cdot \mathbf{n}_A$, $\boldsymbol{\tau}_I := \varepsilon_I^t : \mathbb{C}_I$, $\bar{\boldsymbol{\tau}} := \sum \{ \lambda_I\, \boldsymbol{\tau}_I \}$, $\bar{\alpha} = \lambda_A\, \alpha_A + \sum \lambda_I\, \alpha_M + \frac{1}{2} \sum \{ \boldsymbol{\tau}_I : \varepsilon_I^t \}$ just represent abbreviations, [1].

A suitable relaxed dissipation functional is then be given for example by

$$(12) \qquad \Delta^* = k_1 \, |\dot{\boldsymbol{\lambda}}| + k_2 \left( |\dot{\mathbf{n}}_A| + |\dot{\mathbf{n}}_M| \right),$$

which leads to evolution equations of a classical elasto–plastic type, see [1].

## Literatur

[1] T. Bartel, K. Hackl, *A micromechanical model for martensitic transformations in single-crystals*, manuscript, submitted for publication (2007).

[2] S. Govindjee, K. Hackl, R. Heinen, *An upper bound to the free energy of mixing by twin-compatible lamination for n-variant martensitic phase transformations*, Continuum Mechanics and Thermodynamics, **18, No. 7-8** (2007) 443–453.

[3] S. Govindjee, A. Mielke, G. J. Hall, *J. Mech. Phys. Solids*, **51** (2003), 763+.

[4] K. Hackl, *Relaxation and evolution of microstructures – some conceptual ideas*, Oberwolfach Reports **52** (2005) 10-ï¿½2.

[5] K. Hackl, R. Heinen, *A micromechanical model for pre-textured polycrystalline shape memory alloys including elastic anisotropy*, manuscript, submitted for publication (2007).

[6] R. Heinen, K. Hackl, U. Hoppe, *Prediction of microstructural patterns in shape memory alloys using global energy minimization*, Mat. Sci. Eng. A, in print (2007).

[7] K. Hackl, M. Schmidt-Baldassari, W. Zhang, *A micromechanical model for polycrystalline shape-memory alloys*, Materials Science and Engineering A **378** (2003) 503–506.

[8] K. Hackl, R. Heinen, W. W. Schmahl, M. Hasan, *Experimental verification of a micromechanical model for polycrystalline shape memory alloys in dependence of martensite orientation distributions*, Mat. Sci. Eng. A, in print (2007).

# The Kurzweil integral approach to discontinuous rate independent processes

## Pavel Krejčí

Consider a real separable Hilbert space $X$ endowed with a scalar product $\langle \cdot, \cdot \rangle$, and a family $Z(v)$ of nonempty convex closed sets parameterized by elements $v$ from a closed subset $V$ of a Banach space $Y$. For a given mapping $u : [0, T] \to V$, we look for a solution $\xi : [0, T] \to X$ of the sweeping process

$$(1) \qquad \dot{\xi}(t) + \partial I_{Z(u(t))}(\xi(t)) \;\ni\; 0 \,,$$

$$(2) \qquad \xi(0) = \xi^0 \in Z(u(0)) \,,$$

where $I_{Z(u(t))}$ is the indicator function of the set $Z(u(t))$, and $\partial I_{Z(u(t))}$ is its subdifferential. Our aim is to extend the results of [11, 8] to discontinuous inputs $u$ with locally unbounded variation. More specifically, we deal with the so-called *regulated functions*, that is, functions $u$ that admit both one-sided limits $u(t-)$, $u(t+)$ at each point $t \in [0, T]$, with the convention $u(0-) = u(0)$, $u(T+) = u(T)$. Such functions were introduced in [1] and further investigated in [4, 5, 12]. We denote by $G(0, T; X)$ the Banach space of regulated functions $[0, T] \to X$ endowed with the sup-norm. If $V$ is not a linear subspace of $Y$, the set $G(0, T; V)$ with the natural metric induced by the norm of $Y$ can still be treated as a complete metric space. The space $BV(0, T; X)$ of functions of bounded variation is a dense

subspace of $G(0, T; X)$. Alternatively, $G(0, T; X)$ can be defined as the closure of $BV(0, T; X)$ in the sup-norm topology.

We restrict ourselves to left continuous inputs $u$, that is, $u(t-) = u(t)$ for all $t \in [0, T]$. The space of all left continuous regulated functions is denoted by $G_L(0, T; X)$. We restate the inclusion (1) in the form

$$(3) \quad \xi(t) \in Z(u(t)) \qquad \forall t \in [0, T] \,,$$

$$(4) \quad \int_0^T \langle w(t) - \xi(t+), d\xi(t) \rangle \geq 0 \quad \forall w \in G(0, T; X) : w(t) \in Z(u(t)) \quad \forall t \in [0, T] \,,$$

with the Kurzweil integral (the original reference goes back to [9]) on the left hand side of (4). The advantage of this setting is that the convergence properties of the Kurzweil integral are compatible with the natural topologies of $G(0, T; X)$ (see [2], where the Young integral as a special case of the Kurzweil integral was used instead). The main result for the problem (2)–(4) reads as follows.

**Theorem 1.** *Let the mapping $v \mapsto Z(v)$ be continuous with respect to the Hausdorff distance. Then problem (2)–(4) has a unique solution $\xi \in BV_L(0, T; X)$ for every $u \in BV_L(0, T; V)$ and $\xi^0 \in Z(u(0))$. If moreover $Z(v)$ has nonempty interior for every $v \in V$, then (2)–(4) has a unique solution $\xi \in BV_L(0, T; X)$ for every $u \in G_L(0, T; V)$, and the solution mapping $\mathcal{S} : G_L(0, T; V) \to G_L(0, T; X) : u \mapsto \xi$ is continuous.*

The implicit problem, which consists in complementing (2)–(4) with an additional constitutive equation

$$(5) \qquad\qquad\qquad u(t) = g(t, \xi(t))$$

with a given function $g$, deserves special attention. Existence can be established by the Schauder fixed point principle under fairly general assumptions. Uniqueness and Lipschitz continuous data dependence is obtained by the Banach contraction principle, provided the distance of convex sets is measured in terms of a stronger concept than the Hausdorff one, and additional regularity of $g$ with respect to both $t$ and $u$ is required, see [3].

Quite surprisingly, there are two independent weak convergence concepts in $G(0, T; X)$: the one induced by the dual space, which can be identified with a slight extension of $BV(0, T; X)$, and the one related to the Helly selection principle. Rate independent variational inequalities of the above type together with the Kurzweil (Young) integral calculus provide a tool for extending Fraňková's generalization of the Helly selection principle proposed in [4], to the so-called *functions of $\Phi$-bounded variation*, see [2]. A detailed survey about regulated functions, rate independent variational inequalities, and the Kurzweil integral, is given in [7].

An interesting special case corresponds to the choice $V = Y = X$ and $Z(v) = v - K$, where $K \subset X$ is a fixed convex set. Then Eq. (1) can be written in the form

$$(6) \qquad\qquad\qquad \dot{\xi}(t) - \partial I_K(u(t) - \xi(t)) \ni 0 \,,$$

or, formally equivalently, as

(7) $$\partial M_{K^*}(\dot{\xi}(t)) + \xi(t) \ni u(t),$$

where $M_{K^*}$ is the Minkowski functional of the polar set $K^*$ to $K$. The Young integral counterpart of (4) proposed in [6] reads

(8) $$\int_0^T \langle u(t+) - \xi(t+) - w(t), d\xi(t)\rangle \geq 0 \quad \forall w \in G(0,T;K).$$

Following the energetic approach to rate-independent evolutions suggested in [10] and using the Kurzweil integration-by-parts formula, we rewrite Eq. (8) as

(9) $$\frac{1}{2}|\xi(t)|^2 - \langle u(t), \xi(t)\rangle + \frac{1}{2}\sum_{\tau \in [s,t]} |\xi(\tau+) - \xi(\tau)|^2 + \operatorname*{Var}_{\substack{K^* \\ [s,t]}} \xi$$

$$A = \frac{1}{2}|\xi(s)|^2 - \langle u(s), \xi(s)\rangle - \int_s^t \langle \xi(t), \mathrm{d}u(t)\rangle$$

for every $0 \leq s < t \leq T$, where we set

$$\operatorname*{Var}_{\substack{K^* \\ [s,t]}} \xi = \sup \sum_{i=1}^p M_{K^*}(\xi(\sigma_i) - \xi(\sigma_{i-1})),$$

the supremum being taken over all divisions $s = \sigma_0 < \sigma_1 < \cdots < \sigma_p = t$. This term corresponds to the "hysteresis dissipation". There is a difference here with respect to the continuous case (cf. [10]), namely the additional dissipation term $\frac{1}{2}\sum_{\tau \in [s,t]} |\xi(\tau+) - \xi(\tau)|^2$ in the energy balance. Note that only countably many $\tau$'s enter into the sum, which is finite due to the bounded variation of $\xi$. It is interesting to compare identity (9) with the one corresponding to the "viscous" regularization as $\varepsilon \searrow 0$

(10) $$\partial M_{K^*}(\dot{\xi}_\varepsilon(t)) + \varepsilon\dot{\xi}_\varepsilon(t) + \xi_\varepsilon(t) \ni u(t),$$

which has the form

(11) $$\frac{1}{2}|\xi_\varepsilon(t)|^2 - \langle u(t), \xi_\varepsilon(t)\rangle + \varepsilon\int_s^t |\dot{\xi}_\varepsilon(\tau)|^2\mathrm{d}\tau + \operatorname*{Var}_{\substack{K^* \\ [s,t]}} \xi_\varepsilon$$

$$= \frac{1}{2}|\xi_\varepsilon(s)|^2 - \langle u(s), \xi_\varepsilon(s)\rangle - \int_s^t \langle \xi_\varepsilon(t), \mathrm{d}u(t)\rangle$$

for every $0 \leq s < t \leq T$. The following result holds.

**Theorem 2.** *Let $K$ have nonempty interior in $X$, and let $u \in G_L(0,T;X)$ be arbitrary. Let $\xi, \xi_\varepsilon$ be solutions to (8) and (10), respectively, with the same initial conditions. Then*

(12) $$\lim_{\varepsilon \to 0+} |\xi_\varepsilon(t) - \xi(t)| = 0 \qquad \forall t \in [0,T].$$

*In particular, for every $0 \leq s < t \leq T$, we have*

(13) $$\lim_{\varepsilon \to 0+} \left(\varepsilon\int_s^t |\dot{\xi}_\varepsilon(\tau)|^2\mathrm{d}\tau + \operatorname*{Var}_{\substack{K^* \\ [s,t]}} \xi_\varepsilon\right) = \frac{1}{2}\sum_{\tau \in [s,t]} |\xi(\tau+) - \xi(\tau)|^2 + \operatorname*{Var}_{\substack{K^* \\ [s,t]}} \xi.$$

## Literatur

[1] G. Aumann: Reelle Funktionen. Springer-Verlag, Berlin – Göttingen – Heidelberg, 1954 (in German).

[2] M. Brokate, P. Krejčí: Duality in the space of regulated functions and the play operator. *Math. Z.* **245** (2003), 667–688.

[3] M. Brokate, P. Krejčí, H. Schnabel: On uniqueness in evolution quasivariational inequalities. *J. Convex Anal.* **11** (2004), 111–130.

[4] D. Fraňková: Regulated functions. *Math. Bohem.* **119** (1991), 20–59.

[5] C. S. Hönig: Volterra Stieltjes-Integral Equations. North-Holland Math. Studies, Amsterdam, 1975.

[6] P. Krejčí, Ph. Laurençot: Generalized variational inequalities. *J. Convex Anal.* **9** (2002), 159–183.

[7] P. Krejčí: Regulated evolution quasivariational inequalities. Lectures held at the University of Pavia, May 2003, `http://www.math.cas.cz/%7Ekrejci/pa7.pdf`.

[8] M. Kunze, M. Monteiro Marques: An introduction to Moreau's sweeping process. In: *Impacts in Mechanical Systems - Analysis and Modelling* (B. Brogliato ed.), LN Physics 551, Springer 2000, 1–60.

[9] J. Kurzweil: Generalized ordinary differential equations and continuous dependence on a parameter. *Czechoslovak Math. J.* **7** (**82**) (1957), 418–449.

[10] A. Mielke, F. Theil: On rate-independent hysteresis models. *NoDEA Nonlinear Differential Equations Appl.* **11** (2004), 151–189.

[11] J.-J. Moreau: Evolution problem associated with a moving convex set in a Hilbert space, J. Diff. Eq. 26 (1977), 347–374.

[12] M. Tvrdý: Differential and integral equations in the space of regulated functions. *Memoirs Diff. Equations and Math. Phys.* **25** (2002), 1–104.

## Piecewise rigidity

Antonin Chambolle

(joint work with Alessandro Giacomini, Marcello Ponsiglione)

In an open connected set $\Omega$ of $\mathbb{R}^N$, it is well known that if $\nabla u = 0$ ($u$ a distribution), then $u$ is constant; if $e(u) = (\nabla u + \nabla u^T)/2 = 0$ ($u$ $\mathbb{R}^N$-valued distribution) then $u$ is a rigid displacement $Ax + b$ ($A + A^T = 0$). A classical result due to Liouville (extended by Reshetnyak to Sobolev maps) shows that if $\nabla u \in SO(N)$ a.e., where $u \in W^{1,\infty}(\Omega)$, then $u$ is again affine: $u = Rx + b$ for some $R \in SO(N)$.

Our purpose is to extend such results to functions with discontinuities, in the class $SBV$ or $SBD$. If $u$ is a function, displacement, or deformation with a closed discontinuity set $\Gamma$, it is clear that the results above remain true, up to the fact that $\Omega \setminus \Gamma$ might be no more connected: for instance, if $\nabla u \in SO(N)$ a.e., one deduces $u = \sum_i (R_i x + b_i)\chi_{E_i}$, where $R_i$ are rotations, $b_i$ $N$-vectors, and $E_i$ the connected components of $\Omega \setminus \Gamma$. We want to extend this to situations where the jump set $\Gamma$ is just a rectifiable set, not necessarily closed (and possibly dense).

A function in $L^1(\Omega)$ is said to be in $SBV(\Omega)$ if its distributional derivative is a measure

$$Du = \nabla u\, dx + (u^+ - u^-) \otimes \nu_u \mathcal{H}^{N-1} \llcorner J_u$$

whereas it is of class $SBD(\Omega)$ if (it is $\mathbb{R}^N$-valued and)

$$\mathcal{E}(u) = Du + Du^T = e(u)\,dx + (u^+ - u^-) \odot \nu_u \mathcal{H}^{N-1} \llcorner J_u\,.$$

Here, $\nabla u, e(u) \in L^1$, $J_u$ is a $(N-1)$-rectifiable set of normal $\nu_u$ (defined $\mathcal{H}^{N-1}$-a.e.), $u^\pm$ are the traces of $u$ on both sides of $J_u$.

It is known (*cf* [1, Thm. 4.23]) that if $\nabla u = 0$ and $\mathcal{H}^{N-1}(J_u) < +\infty$, $u = \sum_i a_i \chi_{E_i}$ where $(E_i)_i$ is a "Caccioppoli partition", that is, a partition (up to a negligible set) of $\Omega$ such that each $E_i$ has finite perimeter in $\Omega$ ($\chi_{E_i} \in BV(\Omega)$), and $\sum_i \mathrm{Per}(E_i, \Omega) < +\infty$. The assumption $\mathcal{H}^{N-1}(J_u) < +\infty$ is here essential, as shows the following example: $u(x) := \mu([0, x])$ where $\mu = \sum_{n=1}^\infty \frac{1}{2^n} \delta_{r_n}$, with $(r_n)_{n \geq 1} = \mathbb{Q} \cap (0, 1)$. This function is in $SBV(0, 1)$, its derivative is a pure jump, though, it is constant on no set of positive measure, it is even strictly increasing from 0 to 1 on $(0, 1)$.

We have provided in this talk a new proof of this result, based on a discretization/interpolation argument (inspired from [3, 4]) that provides us with an approximation $(u_\varepsilon)$ of $u$ (with $u_\varepsilon \to u$ in $L^1(\Omega)$), such that $\nabla u_\varepsilon = 0$, $J_{u_\varepsilon}$ is a quite simple closed set (made of a finite union of facets of hypercubes), and $\mathcal{H}^{N-1}(J_{u_\varepsilon}) \leq c\mathcal{H}^{N-1}(J_u) + \varepsilon < +\infty$. Hence for each $\varepsilon$, it is obvious that $u_\varepsilon = \sum_i a_i^\varepsilon \chi_{E_i^\varepsilon}$. We get the result in the limit $\varepsilon \to 0$.

Which is interesting in this proof is that it easily extends to the case of $SBD$ displacements. Then, we find that $u \in SBD(\Omega)$ with $e(u) = 0$ a.e. and $\mathcal{H}^{N-1}(J_u) < +\infty$ is approximated with $u_\varepsilon$ such that $e(u_\varepsilon) = 0$ a.e., $J_{u_\varepsilon}$ is a nice closed set made of a finite union of facets of hypercubes, with $\mathcal{H}^{N-1}(J_{u_\varepsilon}) \leq c\mathcal{H}^{N-1}(J_u) + \varepsilon < +\infty$. Again, it follows that $u_\varepsilon = \sum_i (A_i^\varepsilon x + b_i^\varepsilon)\chi_{E_i^\varepsilon}$, with $A_i^\varepsilon$ skew-symmetric and $(E_i^\varepsilon)_i$ a Caccioppoli partition with uniformly bounded perimeter. In the limit, we get $u = \sum_i (A_i x + b_i)\chi_{E_i}$.

In the nonlinear case, that is, for $u \in SBV(\Omega; \mathbb{R}^N)$, with $\nabla u \in SO(N)$ a.e. in $\Omega$ and $\mathcal{H}^{N-1}(J_u) < +\infty$, the proof is more involved. We show, again, that $u = \sum_i (R_i x + b_i)\chi_{E_i}$ with $R_i$ a rotation for each $i$.

The proof is as follows: With the same discretization/reinterpolation argument as before, we can show that $u$ is approximated with functions with "nice" jump and equibounded gradient (in $L^\infty$). It follows, by approximation, that $\mathrm{curl}\, u$ is a measure with $|\mathrm{curl}\, u| \leq C\mathcal{H}^{N-1} \llcorner J_u$. This curl measures how far $\nabla u$ is from a true gradient. Using an appropriate Helmoltz decomposition, the approximate rigidity estimate of Friesecke, James and Müller [5] and a Sobolev-type estimate for divergence-free fields whose curl is a measure, we deduce that on each cube $Q \subset \Omega$ of side $h$, there exists a rotation $R_Q$ such that

$$\|\nabla u - R_Q\|_{L^p(Q)} \leq C\frac{h^{N/p}}{h^{N-1}}\mathcal{H}^{N-1}(Q \cap J_u)\,,$$

where $p \in (1, N/(N-1))$ and $C$ is a constant depending only on $p$ and the dimension $N$. We then cover most of $\Omega$ with such cubes, and define a function $\Psi_h$ as the piecewise constant rotation $R_Q$ in each cube $Q$, given by the above estimate. It turns out that we can estimate the variation of $\Psi_h$ (in each open set $A \subset\subset B \subset \Omega$, by $C\mathcal{H}^{N-1}(B \cap J_u)$ if $h$ is small enough), and that $\Psi_h \to \nabla u$

as $h \to 0$. We find in the limit that $D\nabla u$ is a measure absolutely continuous with respect to $\mathcal{H}^{N-1} \llcorner J_u$. This shows that $\nabla u = \sum_i R_i \chi_{E_i}$, from which follows $u = \sum_i (R_i x + b_i)\chi_{E_i}$.

Most of these results have appeared in [2] (see also [3, 4]).

## Literatur

[1] L. Ambrosio, N. Fusco, D. Pallara, *Functions of Bounded Variations and Free Discontinuity Problems*, Clarendon Press, Oxford, 2000.
[2] A. Chambolle, A. Giacomini and M. Ponsiglione, *Piecewise Rigidity*, J. Funct. Anal. **244** (2007), 134–153.
[3] A. Chambolle, *An approximation result for special functions with bounded deformation*, J. Math. Pures Appl. (9) **83** (2004) 929–954.
[4] A. Chambolle, *Addendum to "An approximation result for special functions with bounded deformation"*, J. Math. Pures Appl. (9) **84** (2005) 137–145.
[5] G. Friesecke, R.D. James, S. Müller, *A theorem on geometric rigidity and the derivation of nonlinear plate theory from three-dimensional elasticity*, Comm. Pure Appl. Math. **55** (2002) 1461–1506.

# Experiments with Local Minimizers in the Griffith Model

## Christoph Ortner

### (joint work with Matteo Negri)

We consider the rate-independent propagation of a crack in a brittle solid in anti-plane deformation with prescribed crack path. The goal of the study is to exploit the simplicity of this model problem in order to understand the problem of crack evolution in the setting of Griffith [2] and of Francfort and Marigo [3] in full detail.

Let $\Omega = (-L, L) \times (-1, 1)$ and let $K(l) = \{(x, 0) : -l \le x \le l\}$ denote the crack with length $l$. The problem can be now be reduced to computing only the variable $\ell(t)$ denoting the length of the crack at time $t$. The elastic energy $\mathcal{E}(t, l)$ and the fracture energy $\mathcal{F}(t, l)$ are, respectively, given by

$$\mathcal{E}(t, l) = \inf_{u \in \mathrm{H}^1(\Omega), u|_{\Gamma_D} = g(t)} \frac{1}{2} \int_\Omega |\nabla u|^2 \, \mathrm{d}x, \qquad \text{and } \mathcal{F}(t, l) = \mathcal{E}(t, l) + G_c l,$$

where $G_c$ is the fracture toughness and $g(t)$ the displacement applied on the Dirichlet boundary $\Gamma_D = \{(x, \pm 1) : -L \le x \le L\}$.

We present two constructions of crack evolutions based on the equilibrium condition $\frac{\partial F}{\partial l} \ge 0$, usually written as $G \le G_c$ where $G = -\frac{\partial \mathcal{E}}{\partial l}$, instead of the global minimality condition in the model of Francfort and Marigo [3]. The first construction is based on time-discretization: fix $h > 0$ and set $t_j = hj$, $j = 0, 1, \ldots$. Furthermore, let $\ell_h$ be the piecewise constant interpolant of the nodal values $\ell_h(t_j)$ given by $\ell_h(0) = l_0$ and

$$\ell_h(t_j) = \inf\{l \ge \ell_h(t_{j-1}) : G(t, l) > G_c\}.$$

Letting $h \to 0$, we can extract a pointwise converging subsequence with a limit $\ell : [0, \infty) \to [l_0, L]$ satisfying the evolution law

(1) $\qquad G(t, \ell(t)) \leq G_c$

(2) $\qquad \ell(t + \tau) - \ell(t - \tau) > 0 \, \forall \tau > 0 \Rightarrow G(t, l) \geq G_c \, \forall l \in [\ell(t-), \ell(t+)].$

When $g$ is a monotone increasing load, i.e. $g(t) = tg(1)$, the solution is almost everywhere unique. This can be seen by writing $G(t, l) = t^2 G(1, l) =: t^2 \widehat{G}(l)$. We then show that, for

$$\tau(l) = \sqrt{G_c / \widehat{G}_m(l)}$$

where $\widehat{G}_m$ is the monotone decreasing envelope of $\widehat{G}$ in $[l_0, L]$, the set of all solutions is given by all possible monotone inverses of $\tau$ which also satisfy the stability condition. This provides a particularly simple geometric construction of crack evolutions for pre-defined crack paths which we use to give a detailed comparison between the Griffith model and the Francfort–Marigo model.

Finally, we discuss the modified energy balance formula, which solutions to (1) and (2) satisfy:

(3) $\qquad \mathcal{F}(t_1, \ell(t_1)) = \mathcal{F}(t_2, \ell(t_2)) + \int_{t_1}^{t_2} \mathcal{E}_t(t, \ell(t)) \, \mathrm{d}t - \sum_{t \in S(\ell) \cap (t_1, t_2)} \mathcal{D}(t),$

where

$$\mathcal{D}(t) = \int_{\ell(t-)}^{\ell(t+)} \big[ G(t, l) - G_c \big] \, \mathrm{d}l.$$

This clearly shows that the assumption of rate independence is justified if, and only if, $\ell$ is continuous. When it jumps, several interpretations of (3) are possible. In essence, one has to ask the question, whether elastic waves are dissipated throughout the body in which case the model may be considered correct. On the other hand, if kinetic energy is dissipated into the crack tip only, then one should require an energy balance formula to hold and thus the crack should propagate until $\mathcal{D}(t) = 0$.

The talk concludes with some numerical examples which show a good correspondence of an implementation of the Ambrosio–Tortorelli energy (see [1] for a detailed description and applications in fracture mechanics) based on local minimization with the exact solutions of the Griffith model.

<div align="center">LITERATUR</div>

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

[2] A. A. Griffith, *The phenomenon of rupture and flow in solids*, Philos. Trans. R. Soc. London **A221** (1921)

[3] G. A. Francfort and J.-J. Marigo, *Revisiting brittle fracture as an energy minimization problem*, Topology **32** (1990), 100–120.

## Quasistatic evolution in plasticity with softening

Maria Giovanna Mora

(joint work with G. Dal Maso, A. DeSimone, and M. Morini)

In plasticity theory the term *softening* refers to the reduction of the yield stress as plastic deformation proceeds. We deal with this problem in the *quasistatic* case, in the framework of *small strain associative elastoplasticity* in a bounded and Lipschitz domain $\Omega \subset \mathbb{R}^n$.

The linearized strain $Eu$, defined as the symmetric part of the spatial gradient of the displacement $u$, is decomposed as $Eu = e + p$, where $e$ and $p$ are the elastic and plastic strains. The stress $\sigma$ depends only on $e$, through the formula $\sigma = \mathbb{C}e$, where $\mathbb{C}$ is the elasticity tensor. The *elastic domain* – the set of admissible stresses enclosed by the yield surface – depends on an internal parameter $\zeta$ and it has the form $\{\sigma \in \mathbb{M}^{n \times n}_{sym} : \sigma_D \in K(\zeta)\}$, where $\sigma_D$ denotes the deviatoric part of $\sigma$ and $K(\zeta)$ is a subset of the subspace $\mathbb{M}^{n \times n}_D$ of trace-free symmetric matrices. To simplify the mathematics of the problem, we assume that the set

$$K := \{(\sigma, \zeta) \in \mathbb{M}^{n \times n}_D \times \mathbb{R} : \sigma \in K(\zeta)\}$$

is a *compact convex neighbourhood* of $(0,0)$ in $\mathbb{M}^{n \times n}_D \times \mathbb{R}$.

To express the evolution laws, it is convenient to introduce an internal variable $z$, related to $\zeta$ by the equation $\zeta = -V'(z)$, where $V : \mathbb{R} \to \mathbb{R}$ is a given function of class $C^2$ with bounded second derivatives, called the *softening potential*.

The strong formulation of the quasistatic evolution problem consists in finding functions $\boldsymbol{u}(t,x)$, $\boldsymbol{e}(t,x)$, $\boldsymbol{p}(t,x)$, and $\boldsymbol{z}(t,x)$ satisfying the following conditions for every $t \in [0, +\infty)$ and every $x \in \Omega$:

(1) additive decomposition: $E\boldsymbol{u}(t,x) = \boldsymbol{e}(t,x) + \boldsymbol{p}(t,x)$,
(2) constitutive equations: $\boldsymbol{\sigma}(t,x) := \mathbb{C}\boldsymbol{e}(t,x)$ and $\boldsymbol{\zeta}(t,x) := -V'(\boldsymbol{z}(t,x))$,
(3) equilibrium: div $\boldsymbol{\sigma}(t,x) = 0$,
(4) stress constraint: $(\boldsymbol{\sigma}_D(t,x), \boldsymbol{\zeta}(t,x)) \in K$,
(5) associative flow rule: $(\dot{\boldsymbol{p}}(t,x), \dot{\boldsymbol{z}}(t,x)) \in N_K(\boldsymbol{\sigma}_D(t,x), \boldsymbol{\zeta}(t,x))$,

where dots denote time derivatives and $N_K(\sigma, \zeta)$ is the normal cone to $K$ at $(\sigma, \zeta)$. The evolution is driven by a prescribed time-dependent boundary condition

$$\boldsymbol{u}(t,x) = \boldsymbol{w}(t,x) \quad \text{for every } t \in [0, +\infty) \text{ and every } x \in \partial\Omega \,.$$

The problem is also supplemented by initial conditions at $t = 0$.

Introducing the support function $H(\xi, \theta) := \sup\{\xi \cdot \sigma + \theta \zeta : (\sigma, \zeta) \in K\}$, the flow rule (5) can be written in the equivalent form

(5′) dissipation potential formulation: $(\boldsymbol{\sigma}_D(t,x), \boldsymbol{\zeta}(t,x)) \in \partial H(\dot{\boldsymbol{p}}(t,x), \dot{\boldsymbol{z}}(t,x))$,

where $\partial H(\xi, \theta)$ denotes the subdifferential of $H$ at $(\xi, \theta)$.

If $V$ is strictly convex, this model describes plasticity with hardening, where the yield surface expands as $\dot{\boldsymbol{p}}(t,x) \neq 0$. In this case it is possible to give a variational formulation of the problem, according to the theory of rate-independent processes

developed in [5]. To this aim we introduce the energies

$$\mathcal{Q}(e) := \tfrac{1}{2} \int_\Omega \mathbb{C}e(x) \cdot e(x)\, dx\,, \qquad \mathcal{H}(p, z) := \int_\Omega H(p(x), z(x))\, dx\,,$$

$$\mathcal{V}(z) := \int_\Omega V(z(x))\, dx\,.$$

The term $\mathcal{H}(p, z)$ is used to define the notion of dissipation of a function $t \mapsto (\boldsymbol{p}(t), \boldsymbol{z}(t))$ on an interval $[a, b] \subset [0, +\infty)$, which is given by

$$\mathcal{D}_H(\boldsymbol{p}, \boldsymbol{z}; a, b) := \sup \sum_{j=1}^k \mathcal{H}(\boldsymbol{p}(t_j) - \boldsymbol{p}(t_{j-1}), \boldsymbol{z}(t_j) - \boldsymbol{z}(t_{j-1}))\,,$$

where the supremum is taken over all finite partitions $\{t_j\}$ of $[a, b]$.

The variational formulation of the quasistatic evolution problem consists in finding $\boldsymbol{u}(t, x)$, $\boldsymbol{e}(t, x)$, $\boldsymbol{p}(t, x)$, and $\boldsymbol{z}(t, x)$ satisfying the following conditions:

(a) global stability: for every $t \in [0, +\infty)$ we have $E\boldsymbol{u}(t) = \boldsymbol{e}(t) + \boldsymbol{p}(t)$ in $\Omega$, $\boldsymbol{u}(t) = \boldsymbol{w}(t)$ on $\partial\Omega$, and

$$\mathcal{Q}(\boldsymbol{e}(t)) + \mathcal{V}(\boldsymbol{z}(t)) \le \mathcal{Q}(\widehat{e}) + \mathcal{H}(\widehat{p} - \boldsymbol{p}(t), \widehat{z} - \boldsymbol{z}(t)) + \mathcal{V}(\widehat{z})$$

for every $\widehat{u}$, $\widehat{e}$, $\widehat{p}$, $\widehat{z}$ such that $E\widehat{u} = \widehat{e} + \widehat{p}$ in $\Omega$, $\widehat{u} = \boldsymbol{w}(t)$ on $\partial\Omega$;

(b) energy inequality: for every $t \in [0, +\infty)$ we have

$$\mathcal{Q}(\boldsymbol{e}(t)) + \mathcal{D}_H(\boldsymbol{p}, \boldsymbol{z}; 0, t) + \mathcal{V}(\boldsymbol{z}(t)) \le \mathcal{Q}(\boldsymbol{e}(0)) + \mathcal{V}(\boldsymbol{z}(0)) + \int_0^t \langle \mathbb{C}\boldsymbol{e}(s), E\dot{\boldsymbol{w}}(s) \rangle_{L^2}\, ds\,.$$

In the convex case, owing to the Euler-Lagrange equations, condition (a) is equivalent to the following property:

(a′) local stability: for every $t \in [0, +\infty)$ we have $E\boldsymbol{u}(t) = \boldsymbol{e}(t) + \boldsymbol{p}(t)$ in $\Omega$, $\boldsymbol{u}(t) = \boldsymbol{w}(t)$ on $\partial\Omega$, and

$$\operatorname{div} \boldsymbol{\sigma}(t, x) = 0\,, \quad (\boldsymbol{\sigma}_D(t, x), \boldsymbol{\zeta}(t, x)) \in K \quad \text{for } x \in \Omega\,,$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\zeta}$ are defined by (2).

In this work we assume $V$ to be *concave*, which reflects the fact that the yield surface shrinks as $\dot{\boldsymbol{p}}(t, x) \neq 0$. By lack of convexity condition (a′) is no longer equivalent to (a), but we only have (a) $\Rightarrow$ (a′). In this case the selection criterion provided by global minimality is not justified from the mechanical point of view. Indeed, as we shall show in [2], global minimality fails to capture the softening phenomenon altogether.

We explore a different selection criterion, based on the approximation by solutions of some regularized evolution problems, depending on a small *"viscosity"* parameter $\varepsilon > 0$. The $\varepsilon$-regularized problem consists in finding $\boldsymbol{u}_\varepsilon(t, x)$, $\boldsymbol{e}_\varepsilon(t, x)$, $\boldsymbol{p}_\varepsilon(t, x)$, and $\boldsymbol{z}_\varepsilon(t, x)$ satisfying conditions (1), (2), (3), and

($4_\varepsilon$) regularized flow rule: $(\dot{\boldsymbol{p}}_\varepsilon(t, x), \dot{\boldsymbol{z}}_\varepsilon(t, x)) = N_K^\varepsilon(\boldsymbol{\sigma}_\varepsilon(t, x)_D, \boldsymbol{\zeta}_\varepsilon(t, x))$,

where $N_K^\varepsilon(\sigma, \zeta) := \tfrac{1}{\varepsilon}\big((\sigma, \zeta) - P_K(\sigma, \zeta)\big)$ and $P_K$ is the projection onto $K$. We observe that condition ($4_\varepsilon$) is closely related to (5). It also acts as a penalization leading to the stress constraint (4) as $\varepsilon \to 0$.

The existence of a solution to the $\varepsilon$-regularized evolution problem can be proved by a variational method based on time discretization. One can also show that condition $(4_\varepsilon)$ is equivalent to the following two properties:

$(4'_\varepsilon)$ modified stress constraint: for every $t \in [0, +\infty)$ we have

$$(\boldsymbol{\sigma}_\varepsilon(t,x)_D - \varepsilon\dot{\boldsymbol{p}}_\varepsilon(t,x), \boldsymbol{\zeta}_\varepsilon(t,x) - \varepsilon\dot{\boldsymbol{z}}_\varepsilon(t,x)) \in K \quad \text{for } x \in \Omega\,,$$

$(4''_\varepsilon)$ energy balance: for every $t \in [0, +\infty)$ we have

$$\mathcal{Q}(\boldsymbol{e}_\varepsilon(t)) + \mathcal{D}_H(\boldsymbol{p}_\varepsilon, \boldsymbol{z}_\varepsilon; 0, t) + \mathcal{V}(\boldsymbol{z}_\varepsilon(t)) + \varepsilon \int_0^t \|\dot{\boldsymbol{p}}_\varepsilon(s)\|_{L^2}^2\, ds + \varepsilon \int_0^t \|\dot{\boldsymbol{z}}_\varepsilon(s)\|_{L^2}^2\, ds$$
$$= \mathcal{Q}(\boldsymbol{e}_\varepsilon(0)) + \mathcal{V}(\boldsymbol{z}_\varepsilon(0)) + \int_0^t \langle \boldsymbol{\sigma}_\varepsilon(s), E\dot{\boldsymbol{w}}(s) \rangle_{L^2}\, ds\,.$$

By accepting only those solutions of (a$'$) and (b) which can be approximated by solutions of (1), (2), (3), $(4_\varepsilon)$ we regard quasistatic evolution as the limiting case of a viscosity-driven dynamics. A similar approach in finite dimension was used in [4].

The main difficulty in our approach is due to the fact that, by the nonconvexity of the energy, the components $\boldsymbol{p}_\varepsilon$ and $\boldsymbol{z}_\varepsilon$ of the $\varepsilon$-regularized solution may develop stronger and stronger space oscillations as $\varepsilon \to 0$. As a consequence of this fact, their weak limits do not satisfy, in general, (a$'$) and (b). To overcome this difficulty, a weaker formulation in terms of Young measures is required. However, since the functionals $\mathcal{H}$ and $\mathcal{V}$ have linear growth, the classical notion of Young measure is not enough. To take into account possible concentrations at infinity, we use the notion of generalized Young measure introduced in [3].

In addition, to write the Young measure version of (b) we need to introduce a notion of dissipation for a time-dependent family of generalized Young measures. A natural definition can be given by taking the limit of the dissipations of suitable time-dependent generating functions. Unfortunately, this limit does not depend only on the values of the generalized Young measures at each time, but it also involves the mutual correlations between oscillations at different times. We solve this problem by using the notion of system of generalized Young measures introduced in [1]. This allows us to write a Young measure formulation of problem (a$'$), (b) and to prove an existence result.

## LITERATUR

[1] G. Dal Maso, A. DeSimone, M.G. Mora, M. Morini, *Time-dependent systems of generalized Young measures*, Netw. Heterog. Media **2** (2007), 1–36.

[2] G. Dal Maso, A. DeSimone, M.G. Mora, M. Morini, *Globally stable quasistatic evolution in plasticity with softening*, in preparation.

[3] R.J. DiPerna, A.J. Majda, *Oscillations and concentrations in weak solutions of the incompressible fluid equations*, Comm. Math. Phys. **108** (1987), 667–689.

[4] M. Efendiev, A. Mielke, *On the rate-independent limit of systems with dry friction and small viscosity*, J. Convex Anal. **13** (2006), 151–167.

[5] A. Mainik, A. Mielke, *Existence results for energetic models for rate-independent systems*, Calc. Var. Partial Differential Equations **22** (2005), 73–99.

# Micromechanical modelling of evolving laminates in SMA single crystals

STANISŁAW STUPKIEWICZ

(joint work with Henryk Petryk)

Laminated microstructures are common features accompanying stress-induced martensitic transformations in shape memory alloys (SMA), and their evolution is the main mechanism responsible for the interesting effects, such as pseudoelasticity, observed in these materials. Micromechanical modelling of several related effects has been the topic of our recent research. These results are summarized in this talk.

A micromechanical model of stress-induced phase transformation in SMA single crystals has been developed [1], starting from transformations of the atomic lattice structure and using exact compatibility conditions on the interfaces under stress. The transition to the behavior of a single crystal of a higher-rank laminated microstructure varying with the overall deformation has been made by combining the micro-macro transition for rank-one laminates with a local phase transformation criterion. The transformation criterion is rate-independent with a threshold value for the thermodynamic driving force acting on a phase transformation front. The intrinsic dissipation due to phase transition is thus naturally included in the model. The resulting pseudoelastic stress-strain response to a loading-unloading cycle exhibits a characteristic hysteresis loop. Extension of the model to the finite-strain framework is presented in [5].

Formation of untwinned internally-faulted martensite plates in Cu-based alloys and the effect of stacking fault energy on the microstructure of martensite plates have been studied in [2]. The microstructure, including the orientation of the martensite plate and the density of stacking faults, is obtained as a solution of a minimization problem for load multiplier.

The effect of martensite variant rearrangement (detwinning) during progressive transformation has been accounted for in [3] by considering the propagation of twin boundaries within twinned martensitic plates. Accordingly, the micro-macro transition is applied for an evolving rank-two laminate. The predicted material response corresponding to the development of a uniform laminated microstructure within the representative volume element is characterized by significant softening. It is thus concluded that such macroscopically uniform transformation pattern is unstable and localization of transformation is expected.

Our current research activities concentrate on the effects of interfacial energies of different origin and on the related size effects (initial results are presented in [4, 6]), as well as on the transition to the scale of a polycrystalline aggregate accounting for the interaction of neighbouring grains.

## LITERATUR

[1] S. Stupkiewicz and H. Petryk, *Modelling of laminated micro-structures in stress-induced martensitic transformation*, J. Mech. Phys. Solids **50** (2002), 2303–2331.

[2] S. Stupkiewicz, *The effect of stacking fault energy on the formation of stress-induced internally faulted martensite plates*, Eur. J. Mech. A/Solids **23** (2004), 107–126.

[3] S. Stupkiewicz and H. Petryk, *Micromechanical modelling of stress-induced martensitic transformation and detwinning in shape memory alloys*, Journal de Physique IV **115** (2004), 141–149.

[4] G. Maciejewski, S. Stupkiewicz, and H. Petryk, *Elastic micro-strain energy at the austenite–twinned martensite interface*, Arch. Mech. **57** (2005), 277–297.

[5] S. Stupkiewicz and H. Petryk, *Finite-strain micromechanical model of stress-induced martensitic transformations in shape memory alloys*, Mater. Sci. Eng. A **438–440** (2006), 126–130.

[6] H. Petryk, S. Stupkiewicz, and G. Maciejewski, *Modelling of austenite/martensite laminates with interfacial energy effect*, In P. Tong and Q.P. Sun, editors, Proc. IUTAM Symp. on Size Effects on Material and Structural Behaviour at Micron- and Nano-scales, pp. 151–162, Springer, 2006.

# Thin elastic sheets torn by a blunt tool: a simple crack model based on Griffith's propagation criterion

BASILE AUDOLY

Spectacular saw-tooth patterns are obtained when one tears through a thin sheet of plastic material clamped along its long sides, using a cylindrical tool. In the experiments reported in Refs. [1, 2], a 'blunt' cutting tool (with cylindrical or rectangular profile) is perpendicularly driven through a long, rectangular thin elastic sheet. We consider the case of a sheet that can be bent without breaking, but is not ductile: when brought back to their planar configuration, the two lips of the crack match perfectly. The sheet is clamped along its long edges while the tool is moved along centerline of the sheet. As the tip advances, it progressively cuts the material leaving behind a well defined and highly reproducible oscillatory path. Moreover, there is a threshold for the tip width, below which the crack paths are straight. We consider the geometric limit when the tool size is much larger than this threshold.

In reference [3], we proposed a simple geometrical model that accurately reproduces the crack morphology as well as the details of the crack tip motion. This model is first recalled shortly below. In the present contribution, we propose a reformulation of this geometric model, based on a simple expression for the elastic energy and on Griffith's criterion for crack propagation. We argue that the two formulations are roughly equivalent. Compared to the initial one, the advantage of the new formulation is that it is minimalist (it does not make use of a parameter, such as the angle of propagation $\beta$ of the initial formulation, that has to introduced by hand), and is based on a popular propagation criterion.

We shall start by recalling the main ingredients of the model proposed in reference [3]. This model was built on the remark that the typical bending energy involved in the deformation of the sheet is too low to make the crack propagate. The elastic sheet can be viewed as a membrane, and its bending modulus can effectively be set to zero as long as one is interested in predicting only the crack

motion. Whenever the intersection of the tool with the plane of strip is contained within the convex hull of the crack path, the presence of the tool can be accommodated by bending the strip. This involves no membrane energy, and so it cannot lead to crack propagation. The driving force for crack propagation comes from the stretching energy of the sheet, and the latter is only present when the intersection of the tool with the plane of the strip goes past the convex hull of the crack path. We called $\alpha$ the angle, measured at the crack tip, of the sector defined as the set difference of the convex hull of (the crack path union the tool) minus the convex hull of the the crack path. This angle $\alpha$ measures loosely how much the tool has moved beyond the convex hull of the crack path. Based on simple scaling arguments, we proposed that propagation occurs when this angle reaches a critical value $\alpha_c$. We also proposed that the direction of propagation of the crack takes place along a direction given by a fixed angle $\beta$ with respect to the edge of the crack path. Both the angles $\alpha_c$ and $\beta$ were assumed to depend on material parameters and on the film's thickness. We tuned these parameters so as to fit the experimental crack motion. Having only two adjustable parameters, this iterative geometrical construction does a surprisingly good job at predicting the crack motion: not only does it reproduce the detailed crack path morphology, including the presence of relatively sharp kinks every half period, it also explains the alternation of dynamic and quasi-static crack propagation observed in the experiments.

In the present contribution, we note that another measure of the penetration of the tool beyond the convex hull of the crack path is provided by the difference $\ell - \ell_0$, where $\ell$ is the perimeter of the 'big' convex hull (that is the convex hull of the union of the tool and the crack path), and $\ell_0$ is the perimeter of the 'small' convex hull (that is the convex hull of the crack path), see figure 2. In fact, in a simple geometry, the stretching energy of the membrane can be estimated as:

$$\mathcal{E} \sim E\,h\,w^2 \left(\frac{\ell - \ell_0}{w}\right)^{5/2},$$

in order of magnitude. In this expression, $E$ is Young's modulus of the strip, $h$ its thickness, $w$ the typical width of the tool. One can get rid of all constants by proper rescaling. We should alter slightly the value of the exponent with the aim to keep the numerical implementation as efficient as possible: we define the elastic energy of the system as

$$\mathcal{E} = (\ell - \ell_0)^2. \tag{1}$$

Note that this energy $\mathcal{E}$ is a function of the tool's position (through $\ell$), of the crack path (through $\ell$ and $\ell_0$) and of the tip position (through $\ell$ and $\ell_0$).

To start with, we shall analyze a simple crack geometry, sketched in Fig. 1: we compute the critical value of the penetration angle $\alpha$, and the direction of propagation $\beta$ predicted by our model. These angles are the two parameters of the model given in Ref. [3]. By computing the values of $\alpha_c$ and $\beta$ predicted by the new model, we shall show how two formulations are related. A simple geometric calculation yields the opposite of the gradient of the difference of perimeters $\ell - \ell_0$,
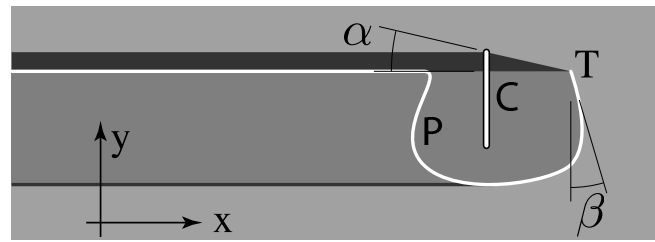
ABBILDUNG 1. Analysis of a simple crack geometry. The crack is made up of a semi-infinite straight line, connected to a U-shaped region. The tool is a straight blade, and penetrates by a small angle past the crack's convex hull.

with respect to the tool's position $T$, as:

$$-\nabla_T(\ell - \ell_0) = (1 - \cos\alpha)\,\underline{e}_x + \sin\alpha\,\underline{e}_y.$$

Up to a positive multiplicative constant, this is proportional to the energy release rate associated with the elastic energy (1). The direction of propagation is such that this release rate is maximum. This yields the equation for the direction of propagation $\beta$ as $\tan(-\beta) = (1 - \cos\alpha)/\sin\alpha$. For small $\alpha$, one has $\beta \approx -\alpha/2$ (note that the sign conventions for $\beta$ have been changed with respect to the initial paper [3]: the $\beta$ in the original article is the opposite of the new one, and so the latter reads $+\alpha/2$). This new equation relates the two 'free' parameters of the initial model. It is consistent with the values of $\alpha_c$ and $\beta$ obtained in the initial paper by fitting the experiments. By writing the magnitude of the energy release rate, one can similarly express the critical value of $\alpha$ in terms of the critical energy release rate, $G_c$.

We have made numerical simulations of the crack motion, based on the elastic energy (1) and on Griffith's criterion for crack propagation. Typical simulations are shown in Fig. 2. Like our original model, these simulations capture the striking saw-tooth crack pattern, as well as the alternation of quasi-static and dynamic regimes. The main difference with the previous model is that the present one has only one adjustable parameter, the dimensionless critical energy release rate, and can be expressed neatly using a single equation (1). A second asset is that the case of a 'large' convex hull extending on both sides of the crack tip is handled naturally; as a result, the kinks are smoothed out in the present simulation, much like in the experiments, while the previous model, which does not handle the case of two angles $\alpha$ gracefully, displayed sharp angles at the kinks.

I would like to thank Benoît Roman and Pedro M. Reis for stimulating (and ongoing) discussions on this topic.

LITERATUR

[1]  B. Roman, P. M. Reis, B. Audoly, S. De Villiers, V. Viguié and D. Vallet. *Oscillatory fracture paths in thin elastic sheets*. C. R. Mécanique **331** (2003), 811–816.
[2]  A. Ghatak and L. Mahadevan, *Crack street: the cycloidal wake of a cylinder tearing through a thin sheet*, Phys. Rev. Lett. **91** (2003), 215507.
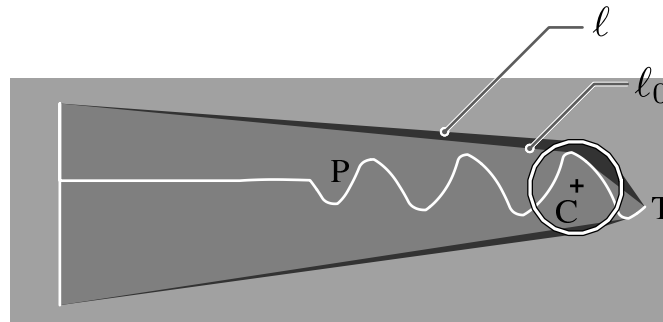
ABBILDUNG 2. Numerical simulation of the model with an initial T-shaped cut (seen on the left-hand side), and with dimensionless critical energy release rate $G_c = 0.04$.

[3] B. Audoly, P. M. Reis and B. Roman, *Cracks in thin sheets: when geometry rules the fracture path*, Phys. Rev. Lett. **95** (2005), 025502.

## Elastic energy stored in a crystal induced by screw dislocations
### MARCELLO PONSIGLIONE

This talk deals with energy minimization methods to model static elastic properties of *dislocations* in crystals. We present the results obtained in [11], concerning the asymptotic behavior of the elastic energy stored in a crystal, induced by a configuration of dislocations, as the atomic scale tends to zero. Our approach is completely variational, and is based on $\Gamma$-*convergence*. We consider the setting of *anti-planar* linear elasticity, so that all the physical quantities involved in our model will be defined on a domain $\Omega \subset \mathbb{R}^2$, which represents an horizontal section of an infinite cylindrical crystal. The elastic energy associated with a vertical *displacement* $u : \Omega \to \mathbb{R}$, in absence of dislocations, is given by

$$E(\nabla u) := \int_\Omega |\nabla u(x)|^2 \, dx.$$

Now we assume that vertical *screw dislocations* are present in the crystal. To model the presence of dislocations we follow the general theory of eigenstrains, namely to any dislocation corresponds a pre-existing strain in the reference configuration (we refer to [9] and [10] for details on this subject, and to the recent paper [2] where the pre-existing strain approach is developed in a discrete setting). In this framework a configuration of screw dislocations in the crystal can be represented by a measure on $\Omega$ which is a finite sum of *Dirac masses* of the type $\mu := \sum_i z_i |\mathbf{b}| \, \delta_{x_i}$. Here $x_i$'s represent the intersection of the dislocation lines with $\Omega$, $\mathbf{b}$ is the so-called *Burgers vector*, which in this anti-planar setting is a vertical fixed vector whose modulus depends on the specific crystal lattice, and $z_i \in \mathbb{Z}$ represent the multiplicity of the dislocations. The class of admissible strains associated with a dislocation $\mu$ is given by the fields whose circulation around the dislocations $x_i$ are equal to $z_i |\mathbf{b}|$. These fields by definition have a singularity at each $x_i$ and are not in $L^2(\Omega; \mathbb{R}^2)$. To set up a variational formulation it is then

convenient to introduce an internal scale $\varepsilon$ called core radius, which is comparable with the atomic scale, and to remove balls of radius $\varepsilon$ around each point of singularity $x_i$. More precisely to any admissible strain $\psi$ we associate the elastic energy

$$E_\varepsilon(\psi) := \int_{\Omega_\varepsilon(\mu)} |\psi(x)|^2 \, dx,$$

where $\Omega_\varepsilon(\mu) := \Omega \setminus \cup_i \overline{B}_\varepsilon(x_i)$. Given a dislocation $\mu$, the elastic energy induced by $\mu$, in the absence of external forces, is given by minimizing $E_\varepsilon(\psi)$ among all admissible strains.

This variational formulation has been recently considered in [4] to study the limit of the elastic energy induced by a fixed configuration of dislocations as the atomic scale $\varepsilon$ tends to zero. The authors prove in particular that the energy is of the order $|\log \varepsilon|$.

We study the asymptotic behavior of the elastic energy induced by the dislocations in terms of $\Gamma$-convergence, in this regime of energies, i.e., rescaling the energy functionals by $|\log \varepsilon|$, without assuming the dislocations to be fixed, uniformly bounded in mass nor *well separated*. We prove that the $\Gamma$-limit of the (rescaled) elastic energy functionals as $\varepsilon \to 0$, with respect to the convergence of the dislocations in a suitable topology (which turns out to be the *flat convergence*), is given by the functional $\mathcal{F}$ defined by

$$(1) \qquad\qquad\qquad \mathcal{F}(\mu) := \frac{1}{2\pi} |\mu|(\Omega).$$

The asymptotic elastic energy per unit volume is essentially proportional to the number (and hence to the length) of the screw dislocations. Then we recover in the limit as $\varepsilon \to 0$ a *line tension model*. A similar result was obtained in [7], [8], where the authors considered a phase field model for dislocations proposed by [6]. They study the asymptotic behavior, in different rescaling regimes, of the elastic energy given by the interaction of a non-local $H^{1/2}$ elastic energy, a non-linear *Peierls potential* and a *pinning condition*, under the assumption that only one *slip system* is active. In particular, in the energy regime corresponding to a rescaling of the order $1/|\log \varepsilon|$, their $\Gamma$-limit is given by the sum of a bulk term, taking in account the pinning condition, and a surface term concentrated on the dislocation lines. More in general energy concentration phenomena as a result of the logarithmic rescaling are nowadays classical in the theory of *Ginzburg-Landau* type functionals, to model vortices in superfluidity and superconductivity. We refer to [3], [5], [1] and to the references therein.

Even if we do not assume the dislocations to be fixed, our analysis shows that, as $\varepsilon_n \to 0$, the most convenient way to approximate a dislocation $\mu$ with multiplicity $z_i \equiv 1$, is the constant sequence $\mu_n \equiv \mu$. In this respect the main point is that there is no homogenization process able to approach an energy less then $1/2\pi \liminf_{\varepsilon_n} |\mu_n(\Omega)|$. The latter term can be interpreted as the quantity usually referred to as *geometrically necessary dislocations*. We conclude that in this energy regime there is no energetic advantage for the crystal to create micro-patterns of dislocations.

These considerations become trivial if one assumes a priori a uniform bound for the number of dislocations. However sequences $\{\mu_n\}$ with uniformly bounded energy are not in general bounded in mass. The main reason is that one can easily construct a *short dipole* $\mu_n := \delta_{x_n} - \delta_{y_n}$, with $|\mu_n|(\Omega) = 2$, $|x_n - y_n| \to 0$, and whose energetic contribution is vanishing. On the other hand, the flat norm of these dipoles is given exactly by $\|\mu_n\|_f = |x_n - y_n|$, and then it is also vanishing. This is the reason why we study the $\Gamma$-convergence with respect to the flat convergence, instead of weak convergence of measures. We prove that the *equicoercivity* property holds with respect to the flat convergence: sequences $\mu_n$ with uniformly bounded energy, up to a subsequence, converge with respect to the flat norm. The proof of this result represents the main difficulty in our analysis.

Our strategy is to divide the dislocations in clusters such that in each cluster the distance between the dislocations is of order $\varepsilon_n^\delta$, for some $0 < \delta < 1$. The family of clusters with *zero effective multiplicity*, namely such that the sum of the multiplicities in the cluster is equal to zero, will play the role of short dipoles; we prove that these clusters give a vanishing contribution to the flat norm. Then we prove that each cluster with non zero effective multiplicity gives a positive energetic contribution. We deduce that the number of these clusters is uniformly bounded with respect to $\varepsilon$. This will be enough to prove the equi-coercivity property, and therefore to obtain a complete $\Gamma$-convergence result for the elastic energy functionals.

## Literatur

[1] Alberti G., Baldo S., Orlandi G.: Variational convergence for functionals of Ginzburg-Landau type. *Indiana Univ. Math. J.* **54** (2005), no. 5, 1411–1472.

[2] Ariza M. P., Ortiz M.: Discrete crystal elasticity and discrete dislocations in crystals. *Arch. Rat. Mech. Anal.* **178** (2006), 149-226.

[3] Bethuel F., Brezis H., Hélein F.: *Ginzburg-Landau vortices.* Progress in Nonlinear Differential Equations and their Applications. vol. 13. Birkhäuser Boston, Boston, 1994.

[4] Cermelli P., Leoni G.: Energy and forces on dislocations. *SIAM J. Math. Anal.* **37** (2005), no. 4, 1131–1160.

[5] Jerrard, R. L., Soner, H. M.: The Jacobian and the Ginzburg-Landau energy. *Calc. Var. Partial Differential Equations* **14** (2002), no. 2, 151–191.

[6] Koslowski M., Cuitino A. M., and Ortiz M.: A phase-field theory of dislocation dynamics, strain hardening and hysteresis in ductile single crystal. *J. Mech. Phys. Solids* **50** (2002), 2597–2635.

[7] Garroni A., Müller S.: $\Gamma$-limit of a phase-field model of dislocations. *SIAM J. Math. Anal.* **36** (2005), no. 6, 1943–1964. 82B26 (49J45)

[8] Garroni A., Müller S.: A variational model for dislocations in the line tension limit. *Arch. Rat. Mech. Anal.* **181** (2006), no. 3, 535–578.

[9] Mura T.: *Micromechanics of defects in solids.* Kluwer Academic Publisher, Boston, 1987.

[10] Phillips, R.: *Crystals, defects and microstructures: modelling across scales.* Cambridge University Press, New York, 2001.

[11] Ponsiglione M.: Elastic energy stored in a crystal induced by screw dislocations: from discrete to continuous. *SIAM J. Math. Anal.* To appear.

# A variational approach to Gradient Flows and Rate Independent Problems

## Giuseppe Savaré

(joint work with Alexander Mielke, Riccarda Rossi)

Let $(X, d)$ be a complete and separable metric space, let $\mathcal{E} : [0, T] \times D \to \mathbb{R}$, $D \subset E$, be a (time dependent) lower semicontinuous functional bounded from below and differentiable with respect to time, with continuous partial derivative $\partial_t \mathcal{E}$. We also fix a convex function $\psi : [0, +\infty) \to [0, +\infty]$ with superlinear growth and $\psi(0) = 0$.

Given an initial datum $u_0 \in D$, we say that an absolutely continuous curve $u : [0, T] \to D$ is a $\psi$-Gradient Flow ($\psi$-GF) induced by $\mathcal{E}$ starting from $u_0$ if $\lim_{t \downarrow 0} u_t = u_0$, the map $t \mapsto \mathcal{E}_t(u_t)$ is absolutely continuous, and it satisfies the inequality

$$(1) \qquad \frac{d}{dt}\mathcal{E}_t(u_t) + \psi(|\dot{u}_t|) + \psi^*(|\partial\mathcal{E}_t|(u_t)) \leq \partial_t \mathcal{E}_t(u_t) \quad \text{for a.e. } t \in (0, T).$$

Here $|\dot{u}_t|$ is the *metric velocity* of $u$ and $|\partial\mathcal{E}_t|(\cdot)$ is the metric slope of $\mathcal{E}_t$ defined as

$$|\dot{u}_t| := \lim_{h \to 0} \frac{d(u_{t+h}, u_t)}{|h|}, \quad |\partial\mathcal{E}_t|(u) := \limsup_{v \to u} \frac{\left(\mathcal{E}_t(v) - \mathcal{E}_t(u)\right)^+}{d(v, u)}.$$

If

   **a:** the functionals $\mathcal{E}_t$ have locally compact sublevels,
   **b:** the metric slope is lower semicontinuous,
   **c:** the metric slope is a *strong upper gradient*, i.e. along each Lipschitz continuous curve $v : (a, b) \to D$ with $|\partial\mathcal{E}_t|(v_t) \in L^1(a, b)$, the functional $\mathcal{E}$ is absolutely continuous and it satisfies

$$\frac{d}{dt}\mathcal{E}_t(v_t) \geq \partial_t \mathcal{E}_t(v_t) - |\partial\mathcal{E}_t|(v_t)|\dot{v}_t| \quad \text{for a.e. } t \in (a, b),$$

then for every $u_0 \in D$ it is possible to prove the existence of at least one $\psi$-GF $u$ starting from $u_0$.

A gradient flow $u$ can also be characterized by the maximal slope condition

$$\frac{d}{dt}\mathcal{E}_t(u_t) = \partial_t \mathcal{E}_t(u_t) - |\partial\mathcal{E}_t|(u_t)\,|\dot{u}_t| \quad \text{for a.e. } t \in (0, T),$$

and the velocity evolution law induced by $\psi$

$$\partial\psi(|\dot{u}_t|) \ni |\partial\mathcal{E}_t|(u_t) \quad \text{or, equivalently,} \quad |\dot{u}_t| \in \partial\psi^*\big(|\partial\mathcal{E}_t|(u_t)\big), \quad \text{for a.e. } t \in (0, T).$$

We refer to [1] for the general theory of gradient flows in metric spaces in the typical case

$$\psi(r) = \psi^*(r) = \frac{1}{2}r^2, \quad \text{corresponding to} \quad |\dot{u}_t| = |\partial\mathcal{E}_t|(u_t).$$

When $X$ is a *reflexive Banach space* with the distance induced by the norm $\|\cdot\|_X$, the metric derivative of an absolutely continuous curve $u$ is simply the norm of the time derivative $u'$ of $u$ (which exists a.e.). If, moreover, the Fréchet subdifferential

$\partial \mathcal{E}_t : D(\partial \mathcal{E}_t) \subset D \to 2^{X^*}$ has a strongly-weakly closed graph, then the metric slope admits the *minimal selection* characterization

$$|\partial \mathcal{E}_t|(u) = \min \left\{ \|\xi\|_{X^*} : \xi \in \partial \mathcal{E}_t(u) \right\}.$$

In this case a $\psi$-GF is also a solution of the *doubly nonlinear evolution equation* (studied in a convex framework by [2])

$$\partial \Psi(u_t') + \partial \mathcal{E}_t(u_t) \ni 0 \quad \text{a.e. in } (0, T),$$

where $\Psi : X \to [0, +\infty]$ is the functional

$$\Psi(u) := \psi(\|u\|_X) \quad \forall\, u \in X.$$

The existence of a $\psi$-GF can be proved by passing to the limit in a variational approximation scheme. In fact, denoting by $\tau > 0$ a time step size, we can construct a sequence $(U_\tau^n)_n$, $n = 0, 1, \ldots, N$, $N\tau \geq T$, such that

(2) $\qquad U_\tau^n \quad$ minimizes the functional $\quad U \mapsto \tau \psi \left( \dfrac{d(U, U_\tau^{n-1})}{\tau} \right) + \mathcal{E}_{n\tau}(U).$

Denoting by $U_\tau$ the piecewise constant interpolant of the discrete values $U_\tau^n$ on each interval $((n-1)\tau, n\tau]$, it is possible to prove that $U_{\tau_k} \to u$ uniformly in $[0, T]$ for a suitable vanishing sequence $\tau_k \downarrow 0$.

One of the crucial arguments of the proof relies on a refined discrete energy inequality, which can be obtained by a clever variational interpolation technique introduced by E. De Giorgi [3].

When $\psi$ has a linear growth, the same discretization method (2) has been introduced by A. Mielke and his collaborators [7, 8, 5, 6] for the approximation of rate independent problems. We discuss the main technical differences between the two situations and we show how to recover a rate independent evolution starting from the $\psi_\varepsilon$-family of gradient flows associated to the functions

$$\psi_\varepsilon(r) := r + \varepsilon r^2,$$

when the "metric viscosity" parameter $\varepsilon$ goes to 0.

The lack of equicontinuity estimates for the approximating solutions $u$ can be overcome by a reparametrization technique (recently introduced in [4]), which yields in the limit a solution of the gradient flow associated to the driving function

$$\psi_0(r) = \begin{cases} r & \text{if } 0 \leq r \leq 1, \\ +\infty & \text{if } r > 1. \end{cases}$$

## Literatur

[1] L. Ambrosio, N Gigli, and G. Savaré, *Gradient flows in metric spaces and in the Wasserstein spaces of probability measures*, Lecture notes, ETH, Birkhäuser, 2005.

[2] P. Colli and A. Visintin, *On a class of doubly nonlinear evolution equations*, Comm. Partial Differential Equations (5) **15** (1990), 737–756.

[3] E. De Giorgi, A. Marino, and M. Tosques, *Problems of evolution in metric spaces and maximal decreasing curve*, Atti Accad. Naz. Lincei Rend. Cl. Sci. Fis. Mat. Natur. (8) **68** (1980), no. 3, 180–187.

[4] M. Efendiev and A. Mielke, *On the rate-independent limit of systems with dry friction and small viscosity*, J. Convex Anal. **13** (2006), 151–167.

[5] A. Mainik and A. Mielke, *Existence results for energetic models for rate-independent systems*, Calc. Var. PDEs **22** (2005), 73–99.

[6] A. Mielke, *Evolution of rate-independent systems*, in *Evolutionary equations. Vol. II*, 461–559, Handb. Differ. Equ., Elsevier/North-Holland, Amsterdam, 2005.

[7] A. Mielke and F. Theil, A mathematical model for rate–independent phase transformations with hysteresis, in "*Proceedings of the Workshop on "Models of Continuum Mechanics in Analysis and Engineering*", H.-D. Alber, R. Balean and R. Farwig (eds), (Shaker–Verlag, Aachen, 1999)", pp. 117-129.

[8] A. Mielke, F. Theil, and V. Levitas, A variational formulation of rate–independent phase transformations using an extremum principle, *Arch. Rational Mech. Anal.* **162** (2002) 137–177.

# Deterministic stick-slip dynamics in a one-dimensional random potential

TIM SULLIVAN

(joint work with Florian Theil)

In physics, engineering and other settings, it is important to understand the macroscopic behaviour of systems whose evolution is determined by microscale effects. It seems natural to consider these microscale effects to be random in nature (and, therefore, beyond the scope of classical averaging and homogenization theory) and to constitute some perturbation of a well-understood smooth structure. In the case of rate-*dependent* viscous systems, analysis of how the random microstructure determines the macroscopic behaviour can be found in the Green-Kubo relations and many further developments since their introduction in the 1950s [2] [4]. In the realm of rate-*independent* plasticity theory, there is a large literature (see, for example, [7]) surrounding ordinary differential inclusions such as

$$(1) \qquad -\nabla V(X_t) + f(t) \in \partial \psi^\gamma(\dot{X}_t); \quad X_0 = x_0;$$

which have been very successful in modelling plastic effects with their associated structures of hysteresis loops, yield surfaces and stick-slip dynamics. Stick-slip evolutions such as the movement of a dislocation line in a crystalline structure or the Barkhausen effect in a magnetic domain can be seen in this way, cf. [3]. Our interest lies in rigorously justifying such differential inclusions as scaling limits of evolutions in perturbations of the potential $V$. Here we present such a derivation for a one-dimensional example.

This derivation has been known since the 1990s in the case of a periodic perturbation: it follows easily from, for example, [1] [6] that any forced one-dimensional gradient flow $X^\varepsilon : \mathbb{R}_{\geq 0} \to \mathbb{R}$ satisfying

$$\dot{X}^\varepsilon_t = -\kappa X^\varepsilon_t - g\left(\frac{X^\varepsilon_t}{\varepsilon}\right) + f(\varepsilon t); \quad X^\varepsilon_0 = x_0;$$

for $\varepsilon, \kappa > 0$, $g \in C^0(\mathbb{R}; [\gamma^-, \gamma^+])$ periodic and surjective and $f \in \mathrm{BC}^0(\mathbb{R}_{\geq 0}; \mathbb{R})$ exhibits rate-independent stick-slip behaviour in the limit as $\varepsilon \downarrow 0$:

$$X_t^0 := \lim_{\varepsilon \downarrow 0} X_{t/\varepsilon}^\varepsilon$$

is the unique solution of the ordinary differential inclusion (1), where $\psi^\gamma : \mathbb{R} \to \mathbb{R}_{\geq 0}$ is the convex, 1-homogeneous dissipation functional induced by $g$ and given by

$$\psi^\gamma(\dot{x}) := \begin{cases} \gamma^- \dot{x}; & \dot{x} \leq 0; \\ \gamma^+ \dot{x}; & \dot{x} \geq 0. \end{cases}$$

Our result is that the same conclusion holds $\mathbb{P}$-almost surely for perturbations $g$ belonging to a wide class of stochastic processes $g : \Omega \times \mathbb{R} \to [\gamma^-, \gamma^+]$, where $(\Omega, \mathcal{F}, \mathbb{P})$ is some probability space. This result is noteworthy since $X^0$ is in principle a stochastic process dependent on the choice of "landscape parameter" $\omega \in \Omega$.

**Theorem 1** (TJS-FT, 2006–07)**.** *Let $f \in \mathrm{BC}^0(\mathbb{R}_{\geq 0}; \mathbb{R})$ and let $g : \Omega \times \mathbb{R} \to [\gamma^-, \gamma^+]$ be a stochastic process. Then $X^0$ $\mathbb{P}$-almost surely satisfies (1) if, and only if, $g$ satisfies the following "continuity and frequent attainment of bounds" conditions, collectively denoted ($\maltese$):*

*(1) The sample realizations of $g$ must be continuous $\mathbb{P}$-almost surely.*
*(2) Define a sequence of stopping distances (random variables) $D_n^\pm : \Omega \to [0, +\infty]$ as follows: let $D_0^+(\omega)$ be the least $x \geq 0$ such that $g(\omega, x) = \gamma^+$; let $D_{n+1}^+(\omega)$ be the least increase upon $\sum_{i=0}^n D_i^+(\omega)$ such that the process $g(\omega, \cdot)$ attains both values $\gamma^\pm$ in the interval*

$$\left( \sum_{i=0}^n D_i^+(\omega), \sum_{i=0}^{n+1} D_i^+(\omega) \right].$$

*Define $D_n^-$ for $x \leq 0$ similarly. Intuitively, each $D_n^\pm$ is the first return distance of $g$ from $\gamma^+$ back to $\gamma^+$ via the opposite extreme $\gamma^-$. It is then required that:*
*(a) For each $n \geq 0$, $D_n^\pm < +\infty$ $\mathbb{P}$-almost surely.*
*(b) The series $\sum_{n \geq 0} D_n^\pm = +\infty$ $\mathbb{P}$-almost surely.*
*(c) The ratio $D_{n+1}^\pm / \sum_{i=0}^n D_i^\pm \to 0$ as $n \to \infty$ $\mathbb{P}$-almost surely.*

*A fortiori, the law $(X^0)_*(\mathbb{P})$ induced on $C^0(\mathbb{R}_{\geq 0}; \mathbb{R})$ is a Dirac measure centred on the unique deterministic solution to (1).*

Note that a continuous, periodic, surjective function $g : \mathbb{R} \to [\gamma^-, \gamma^+]$ certainly satisfies ($\maltese$) (and so Theorem 1 generalizes [1]), and that a simple prototype for a stochastic process satisfying ($\maltese$) is given by a two-sided, doubly reflected Wiener process $g : \Omega \times \mathbb{R} \to [\gamma^-, \gamma^+]$.

The key step in the proof of Theorem 1 is the identification of the interval

$$\mathcal{A}^\gamma(f(t)) := \left[ \frac{f(t) - \gamma^+}{\kappa}, \frac{f(t) - \gamma^-}{\kappa} \right] \subset \mathbb{R}$$

as a suitable limit of sets in the sense of [5]. In a general metric space $(\mathbb{M}, d)$, the *Kuratowski limit inferior* of a family of subsets $\{A_\varepsilon \subseteq \mathbb{M}\}_{\varepsilon > 0}$ is defined to be

$$\underset{\varepsilon \downarrow 0}{\mathrm{Li}}\, A_\varepsilon := \left\{ x \in \mathbb{M} \left| \limsup_{\varepsilon \downarrow 0} d_{\mathrm{H}}(x, A_\varepsilon) = 0 \right. \right\},$$

where $d_{\mathrm{H}}(x, A_\varepsilon) := \inf_{y \in A_\varepsilon} d(x, y)$ is the usual Hausdorff semi-distance.

**Lemma 2** (TJS-FT, 2006–07). *Let*

$$A_\varepsilon^{g(\omega)}(F) := \left\{ x \in \mathbb{R} \left| -\kappa x - g\left( \omega, \frac{x}{\varepsilon} \right) + F = 0 \right. \right\}$$

*be the fixed-point set for the dynamics with a given realization $\omega \in \Omega$ at scale $\varepsilon > 0$ and constant loading $f(t) \equiv F$. Then $g$ satisfies (✠) if, and only if,*

$$\underset{\varepsilon \downarrow 0}{\mathrm{Li}}\, A_\varepsilon^{g(\omega)}(F) = \mathcal{A}^\gamma(F) \text{ for } \mathbb{P}\text{-almost all } \omega \in \Omega.$$
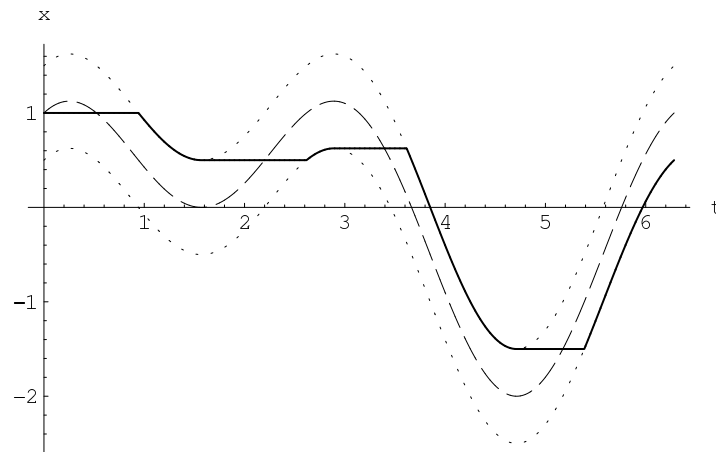


ABBILDUNG 1. The $\mathbb{P}$-almost sure trajectory of $X_t^0$ (solid) against $t$ for some continuous forcing $f(t)$ (dashed), showing the relationship with $\max \mathcal{A}^\gamma(f(t))$ and $\min \mathcal{A}^\gamma(f(t))$ (dotted).

One interpretation of Theorem 1 is that in modelling deterministic dynamics in a wiggly potential $x \mapsto \frac{\kappa}{2}x^2 + \varepsilon G\left( \omega, \frac{x}{\varepsilon} \right)$, with

$$G(\omega, x) := \int_0^x g(\omega, x')\, \mathrm{d}x',$$

it does not matter a great deal exactly which perturbation $G(\omega, \cdot)$ one chooses, since the same rate-independent limit is obtained in $\mathbb{P}$-almost all cases. In some sense, random perturbations satisfying (✠) are no worse than periodic ones.

It would be of interest to extend the above one-dimensional argument to higher- or even infinite-dimensional cases, and/or to consider the addition of a noise term representing the effect of a heat bath.

## LITERATUR

[1] R. Abeyaratne, C. Chu & R.D. James, Kinetics of materials with wiggly energies: theory and application to the evolution of twinning microstructures in a Cu-Al-Ni shape memory alloy, *Phil. Mag. A* **73** (1996), 457–497.

[2] M.S. Green, *J. Chem. Phys.* **22**(3) (1954), 398.

[3] N. Grunewald, Barkhausen effect: a stick-slip motion in a random medium, *Methods Appl. Anal.* **12**(1) (2005), 29–41.

[4] R. Kubo, Statistical-mechanical theory of irreversible processes I. General theory and simple applications to magnetic and conduction problems, *J. Phys. Soc. Jpn.* **12** (1957), 570.

[5] K. Kuratowski, *Topology, Vol. I*, New edition, revised and augmented. Translated from the French by J. Jaworowski, Academic Press, New York (1966).

[6] G. Menon, Gradient systems with wiggly energies and related averaging problems, *Arch. Ration. Mech. Anal.* **162**(3) (2002), 193–246.

[7] A. Mielke & F. Theil, On rate-independent hysteresis models, *NoDEA Nonlinear Differential Equations Appl.* **11**(2) (2004), 151–189.

# Evolutionary problems with energies with linear growth

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(joint work with Martin Kružík )

We study a rate-independent evolution of problems where the energy $W$ is a function of the deformation gradient, $W = W(Du)$, and grows linearly at infinity,

$$(1) \qquad c\,|s| - c_2 \leq W(x, s) \leq C(1 + |s|) \text{ for } x \in \bar{\Omega} \,,$$

with constants $0 < c \leq C$. Here, $\Omega \subset \mathbb{R}^n$ is a bounded domain with smooth boundary.

The aim of this note is to sketch a framework under which the existence of a rate-independent process with an energy of type (1) can be proved. Rate-independent processes are here understood in the energetic formulation, i.e., characterised by stability, energy inequality, and compatibility with initial conditions. This is made precise below.

Before moving on to the evolutionary process, we should motivate the functional analytic framework in the static context. The setting needs to be chosen such that oscillation and concentration effects are taken into account. This can be seen in the following toy model, where the task is to minimise the functional

$$\min I(u) := \int_0^1 \left[ \frac{(u'(x))^2}{1 + (u'(x))^4} + \theta^2 \, |u'(x)| + (u(x) - x)^2 \right] \mathrm{d}x,$$

with $\theta \geq 0$ among $u \in W^{1,1}(0, 1)$ with $u(0) = 0$. The second term is introduced to make the functional coercive; the third term favours solutions close to the identity. The decisive term is the first one, which becomes minimal for $u'(x) = 0$ or in the limit $u'(x) \to \pm\infty$. One would thus expect approximative solution (minimising sequences) to *oscillate* between gradient 0 and gradients which become arbitrarily large in modulus. A particular point here is that the minimising sequences thus do not oscillate between finite values for the deformation gradient (as for

the toy model $\int_0^1 \left( (u'(x))^2 - 1 \right)^2 \mathrm{d}x$ between $\pm 1$), but *concentrate* mass at $\pm\infty$. Young measures [5, 1, 3, 4] are an appropriate tool to deal with oscillations, while DiPerna-Majda measures [2] describe the limits of sequences with oscillations and concentrations.

We use DiPerna-Majda measures to describe the evolution of rate-independent processes with linear energies. Let $u \colon \Omega \to \mathbb{R}^m$ denote the deformation, where $\Omega \subset \mathbb{R}^n$ is a bounded domain with smooth boundary. We write $q := (u, \eta, \lambda)$ for a state; $u$ denotes the deformation, $\eta$ is the associated DiPerna-Majda measure, and $\lambda$ is derived from $\eta$. (To be precise, for a suitable compactification $\beta\mathbb{R}^{m\times n}$ of $\mathbb{R}^{m\times n}$ and for $\eta \cong (\widehat{\nu}, \sigma)$ via slicing, we set $\lambda(x) = \int_{\beta\mathbb{R}^{m\times n}} \frac{\Lambda}{1+|s|} \nu_x(ds) d\sigma(x)$ with $\Lambda$ bounded).

The following definitions are natural in the context of DiPerna-Majda measures (we write $\widetilde{g}(s) := \frac{g(s)}{1+|s|}$ and recall that $\beta\mathbb{R}^{m\times n}$ is a suitable compactification of $\mathbb{R}^{m\times n}$). The applied body force $f$ give rise to

$$F(q) := \int_\Omega f(x,t) \cdot u(x) \, \mathrm{d}x \quad \text{and} \quad \dot{F}(t,q) = \int_\Omega \frac{\partial f(x,t)}{\partial t} \cdot u(x) \, \mathrm{d}x;$$

the time-dependent elastic energy $E(t,q)$ is

$$(2) \qquad E(t,q) = \int_{\bar{\Omega} \times \beta\mathbb{R}^{m\times n}} \widetilde{W}(x,s) \eta(\mathrm{d}s\mathrm{d}x) - \int_\Omega f(x,t) \cdot u(x) \, \mathrm{d}x.$$

$\Gamma$ is the energy augmented by a spatial regularisation,

$$\Gamma(t,q) := E(t,q) + \int_\Omega \varrho \, |\nabla \lambda(x)|^2 \, \mathrm{d}x,$$

with $\rho > 0$.

The *dissipation distance* $\mathcal{D}$ describes the energetic loss between two states of the system characterised by $\eta_1$ and $\eta_2$. We choose $\mathcal{D}(q_1, q_2) = \int_\Omega \|\lambda_1 - \lambda_2\| \mathrm{d}x$. The *temporal dissipation* is then given by

$$\mathrm{Diss}(q, [t_1, t_2]) := \sup_{L \in \mathbb{N}} \left\{ \sum_{l=1}^{L} \mathcal{D}\left( \eta(\tau_l), \eta(\tau_{l-1}) \right) \; \big| \; t_1 = \tau_0 < \cdots < \tau_L = t_2 \right\}.$$

For given $q_0$ in the state space $Q$, the process $q \colon [0, T] \to Q$ is a *solution* if the following three conditions hold:

(1) *Stability:* For every $t \in [0, T]$, we have

$$\Gamma(t, q(t)) \leq \Gamma(t, \widetilde{q}) + D(q(t), \widetilde{q}) \text{ for every } \widetilde{q} \in Q.$$

(2) *Energy inequality:* For every $0 \leq t_1 \leq t_2 \leq T$, we have

$$\Gamma(t_1, q(t_1)) + \mathrm{Diss}(q, [t_1, t_2]) \leq \Gamma(t_2, q(t_2)) - \int_{t_1}^{t_2} \dot{F}(t, q(t)) \mathrm{d}t.$$

(3) *Initial condition:* $q(0) = q_0$ .

In this setting, the existence of a process satisfying the above conditions can be proved and suitable regularity assumptions for sufficiently small forces.

## Literatur

[1] J. M. Ball, *A version of the fundamental theorem for Young measures*, in: PDEs and continuum models of phase transitions (Nice, 1988) (M. Rascle, D. Serre, M. Slemrod, eds.), Lecture Notes in Physics **344**, Springer (1989), 207–215.

[2] R. J. DiPerna, A. J. Majda, *Oscillations and concentrations in weak solutions of the incompressible fluid equations*, Comm. Math. Phys. **108** (1987), 667–689.

[3] L. Tartar, *Compensated compactness and applications to partial differential equations*, in: Nonlinear analysis and mechanics: Heriot-Watt Symposium, Vol. IV (R. J. Knops, ed.) Pitman Res. Notes in Math. **39** (1979), 136–212.

[4] L. Tartar, *Mathematical tools for studying oscillations and concentrations: From Young measures to H-measures and their variants.* In: Multiscale problems in science and technology. Challenges to mathematical analysis and perspectives. (N. Antonič et al., eds.) Proceedings of the conference on multiscale problems in science and technology, held in Dubrovnik, Croatia, September 3–9, 2000. Springer, Berlin, 2002.

[5] L. C. Young, *Generalized curves and the existence of an attained absolute minimum in the calculus of variations*, Comptes Rendus de la Société des Sciences et des Lettres de Varsovie, Classe III **30** (1937), 212–234.

# Modeling of phase transitions in CuAlNi

## Martin Kružík

(joint work with A. Mielke, T. Roubíček)

*Shape-memory alloys* (=SMAs) belong to so-called smart materials which enjoy important applications. SMAs exhibit specific, *hysteretic* stress/strain/temperature response and a so-called *shape-memory effect.* The mechanism behind it is quite simple: atoms tend to be arranged in several crystalographical configuration having different symmetry groups: higher symmetrical one (referred to as the *austenite* phase, typically cubic) has higher thermal capacity while lower symmetrical one (called the *martensite* phase, typically tetragonal, orthorhombic, or monoclinic) has lower thermal capacity and may exist, by symmetry, in several variants (typically 3, 6, or 12, respectively). We refer e.g. to [2] for a thorough survey. Here we consider only on isothermal stress/strain-response modelling.

We consider a bounded Lipshitz domain $\Omega \subset \mathbb{R}^3$ as a reference configuration (canonically the stress-free austenite). Standardly, the *displacement* $u : \Omega \to \mathbb{R}^3$ and the *deformation* $y : \Omega \to \mathbb{R}^3$ are related by $y(x)=x+u(x)$, $x \in \Omega$. Hence the *deformation gradient* is $F=\nabla y=\mathbb{I}+\nabla u$, where $\mathbb{I} \in \mathbb{R}^{3\times3}$ denotes the identity matrix. Mechanical response is phenomenologically desribed by a specific *stored energy* $\widehat{\varphi} = \widehat{\varphi}(F)$, assumed to have a $p$-polynomial growth/coercivity structure. The *frame-indifference*, i.e. $\widehat{\varphi}(F) = \widehat{\varphi}(RF)$ for any $R \in$ SO(3), the group of orientation-preserving rotations, requires that $\widehat{\varphi}(\cdot)$ in fact depends only on the (right) Cauchy-Green stretch tensor $C := F^{\mathrm{T}}F$. We abbreviate

$$(1) \qquad \varphi(\cdot) := \widehat{\varphi}(\mathbb{I} + \cdot)\,.$$

The overall free energy related to a displacement profile $u$ is $\Phi(u) := \int_\Omega \varphi(\nabla u)\mathrm{d}x$. Considering a (time-varying) elastic support $w(t,x)$ on a part $\Gamma$ of the boundary $\partial\Omega$, we expand it to the stored energy $G(t,u) = \Phi(u) + \frac{1}{2}\int_\Gamma (u - w(t,\cdot))^{\mathrm{T}} B(u -$

$w(t, \cdot))\mathrm{d}S$ with $B^\top = B$. Due to the multiwell character of $\varphi$, the deformation gradient usually tends to develop fast spatial oscillations if it tends to minimize the overall stored energy under prescribed boundary conditions, see [1, 2], resulting to a *microstructure* that can effectively be described by so called *gradient Young measures*, which are measurably parameterized probability measures $x \mapsto \nu_x$ on $\mathbb{R}^{3\times3}$ that can be attained by gradients in the sense $\lim_{k\to\infty} \int_\Omega g(x)v(\nabla u_k) = \int_\Omega g(x) \int_{\mathbb{R}^{3\times3}} v(A)\,\nu_x(\mathrm{d}A)\mathrm{d}x$ for some sequence $\{y_k\}_{k\in\mathbb{N}} \subset W^{1,p}(\Omega;\mathbb{R}^3)$ and all $g \in L^\infty(\Omega)$ and $v \in C_0(\mathbb{R}^{3\times3})$, see [8]; the notation $C_0$, $L^p$, $W^{1,p}$ for function spaces is standard. Let us denote the set of all such parameterized measures by $\mathcal{G}^p(\Omega;\mathbb{R}^{3\times3})$. The naturally extended (so-called *relaxed*) stored energy is then

$$(2)\ \ \bar{G}(t,u,\nu) = \int_\Omega \int_{\mathbb{R}^{3\times3}} \varphi(A)\,\nu_x(\mathrm{d}A)\mathrm{d}x + \int_\Gamma \frac{(u-w(t,\cdot))^\top B(u-w(t,\cdot))}{2}\,\mathrm{d}S.$$

The pair of "macroscopical" displacement $u$ and the gradient Young measures $\nu$ represents a quite natural *mesoscopical description* of the state of the body. The "kinematically" admissible pairs $(u,\nu)$ are in

$$Q := \left\{ (u,\nu) \in W^{1,p}(\Omega;\mathbb{R}^3) \times \mathcal{G}^p(\Omega;\mathbb{R}^{3\times3});\ \int_{\mathbb{R}^{3\times3}} A\nu_x(\mathrm{d}A) = \nabla u(x)\ \text{for a.a. } x \right\}.$$

Within microstructure evolution due to time-varying loading $w$, SMAs *dissipate energy*. For sufficiently slow loading, these processes are *activated* and quite *rate independent*, leading to a *hysteretic* stress/strain response. We assume dissipative forces having a (pseudo)potential, say $R$, and that the energy dissipated during transformation process depends (counting phenomenologically, beside possible rank-one connections, with various impurities) on the starting and the final (phase)variant, only; this (simplifying) concept has been adopted also e.g. in [9]. We implement this philosophy with help of a frame-invariant "phase indicator" smooth bounded function $\widehat{\mathcal{L}} : \mathbb{R}^{3\times3} \to \mathbb{R}^L$ with $L$ denoting number of (phase) variants. Then, with $\mathcal{L}(A) := \widehat{\mathcal{L}}(\mathbb{I}+A)$ like (1), the dissipation potential is postulated as

$$(3)\qquad R(\nu) := \int_\Omega \delta_K^*(\lambda(x))\,\mathrm{d}x \qquad \text{with} \qquad \lambda(x) = \int_{\mathbb{R}^{3\times3}} \mathcal{L}(A)\,\nu_x(\mathrm{d}A)\mathrm{d}x$$

with a convex compact $K \subset \mathbb{R}^L$ determining the *activation stresses*, $\delta_P$ its indicator function, and $\delta_K^*$ its conjugate which is, of course, homogeneous degree-1. The quantity $\lambda$ plays the role of a macroscopical *volume fraction* assigned through (3) to the microstructure described by $\nu$. We state an *energetic formulation* which requires *stability*

$$(4)\qquad \forall(\widetilde{u},\widetilde{\nu}) \in Q: \quad \bar{G}(t,u(t),\nu(t)) \leq \bar{G}(t,\widetilde{u},\widetilde{\nu}) + R(\nu(t)-\widetilde{\nu}),$$

and, for any $0 \leq s < t \leq T$, the *energy equality*

$$\bar{G}(t,u(t),\nu(t)) + \mathrm{Var}_R(\nu;s,t)$$

$$(5)\qquad = \bar{G}(s,u(s),\nu(s)) - \int_s^t \int_\Gamma (u-w)^\top B\frac{\partial w}{\partial t}\,\mathrm{d}S\mathrm{d}\tau\ ,$$

where $\text{Var}_R(\nu; s, t)$ denotes the total variation over $[s, t]$ of $\nu(\cdot)$ with respect to $R$ from (3). It can be shown that the energetic formulation posseses a solution [5], see [3] for a numerical approximation. We numecically tested the above scenario on a single crystal of CuAlNi having the *orthorhombic martensite*; c.f. [3].
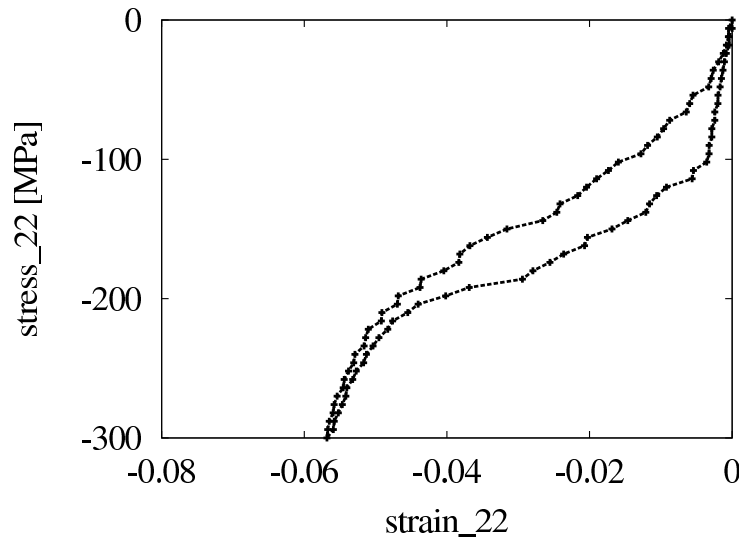


*Fig. 1. The hysteretic pseudo-elastic stress-strain response corresponding to the full loading/unloading cycle of a CuAlNi $1 - 0 - 0$ oriented single crystal.*

## LITERATUR

[1] J.M. Ball,, R.D. James, Fine phase mixtures as minimizers of energy. *Archive Rat. Mech. Anal.* **100** (1988), 13–52.

[2] K. Bhattacharya, *Microstructure of martensite. Why it forms and how it gives rise to the shape-memory effect.* Oxford Univ. Press, New York, 2003.

[3] M. Kružík, A. Mielke, T. Roubíček, Modelling of microstructure and its evolution in SMA single-crystals, in particular in CuAlNi. *Meccanica* **40** (2005), 389-418.

[4] A. Mielke, Evolution of rate-independent systems. In: *Handbook of Differential Equations:* (Eds. C. Dafermos, E. Feireisl), pp.461–559, Elsevier, Amsterdam, 2005.

[5] A. Mielke, , T. Roubíček, Rate-independent model of inelastic behaviour of shape-memory alloys. *Multiscale Modeling Simul.* **1** (2003), 571-597.

[6] A. Mielke, F. Theil, On rate-independent hysteresis models. *Nonlin. Diff. Eq. Appl.* **11** (2004) 151–189.

[7] A. Mielke, F. Theil, V.I. Levitas, A variational formulation of rate-independent phase transformations using an extremum principle. *Archive Rat. Mech. Anal.* **162** (2002), 137–177.

[8] P. Pedregal, *Parametrized Measures and Variational Principles.* Birkäuser, Basel, 1997.

[9] H. Petryk, Thermodynamic conditions for stability in materials with rate-independent dissipation. *Phil. Trans. Roy. Soc.* **A 363** (2005). 2479–2515.

[10] T. Roubíček, Models of microstructure evolution in shape memory materials. In: *Nonlin. Homogen. and its Appl.to Composites, Polycryst. and Smart Mater.* (Eds. P. Ponte Castaneda et al.), NATO Sci.Ser.**II/170**, Kluwer, Dordrecht, 2004, pp.269-304.

## dG(1) time discretisation for rate independent material simulations?

CARSTEN CARSTENSEN

The simplest and most-established model example for rate-independent time evolution is small-strain elastoplastic material behaviour with hardening [4, 5, 6]. The presentation discusses the primal and dual formulation and its time-discretisation through discontinuous Galerkin methods, written dG(k) schemes for a polynomial degree $\leq k$. After a small motivation and known numerical experiments, the presentations focusses on the mathematical justification of the dG(1) scheme.

Using standard notation on Lebesgue and Sobolev function spaces, the data on a Lipschitz domain $\Omega$ and the time interval $(0, T)$ with right-hand side $f \in L^2(0, T; \Omega)^d$, the *Primal Formulation* reads: Seek $(u, p, \xi) \in W^{1,2}(0, T; H_0^1(\Omega)^d \times L^2(\Omega; \mathbb{R}^d \times \mathbb{R}_{sym}^{d \times d} \times \mathbb{R}^m)$ with homogeneous initial values and, for almost every time $t \in (0, T)$ and for all $v \in H_0^1(\Omega)^d$ and all $(q, \zeta) \in L^2(\Omega; \mathbb{R}_{sym}^{d \times d} \times \mathbb{R}^m)$ ,

$$\int_\Omega \mathbb{C}(\varepsilon(u(t)) - p(t)) : (\varepsilon(v) - \dot{p}(t) + q) \, dx - \int_\Omega \xi(t) \cdot \mathbb{H}(\zeta - \dot{\xi}(t)) \, dx$$

$$\leq \int_\Omega f(t) \cdot v \, dx + \int_{\Gamma_D} g(t) \cdot v \, ds + \int_\Omega supp_K(q, \zeta) \, dx - \int_\Omega supp_K(\dot{p}(t), \dot{\xi}(t)) \, dx.$$

The presentation follows [3, 1] and motivates a discontinuous Galerkin method dG(1) for piecewise affine polynomials. The following typical figure displays the history of discrete stress component $\sigma_{11}(10.2729, 0.1125, t)$ at some point as a function of time in the time interval $[0, 1]$ from [3].
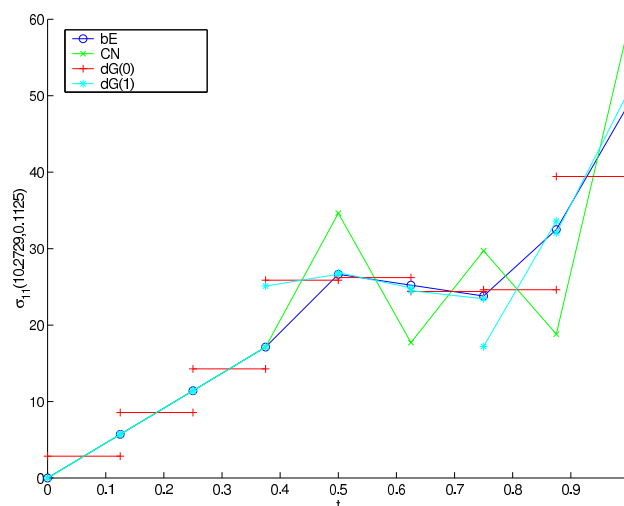


One observes some oscillations of the Crank-Nikolson scheme (CN) around the piecewise linear interpolant of the implicit Euler schme (bE). The discontinuous Galerkin schemes dG(0) and dG(1) appear closer together and the higher-order scheme appears more accurate than the lower-order one.

The convergence analysis of the dG(1) encounters a new difficulty from approximation under constraints which can be circumvented through the following lemma, posed in a general setting.

Lemma: Let K denote some convex and closed subset of some real Hilbert space H and suppose that $f \in C(a, b; K) \cap H^2(a, b; H)$ then,

$$\min_{A, B \in K, A+B=2M} ||f(a) - A||_H \le (b-a)^{3/2} ||f''||_{L^2(a,b;H)}.$$

The remaining details and proofs are subject to current research with Jochen Alberty and Simone Hock.

## LITERATUR

[1] J. Alberty: Zeitdiskretisierungsverfahren f ür elastoplastische Probleme der Kontinuums-mechanik *Ph.D. thesis*, University of Kiel, FRG. *Tenea Verlag*, 2001.

[2] J. Alberty, C. Carstensen: Numerical analysis of time-depending primal elastoplastic with hardening. *SIAM J. Numer. Anal.*, **37** 4 (2000) 1271–1294.

[3] C. Carstensen, J. Alberty: Discontinuous Galerkin Time Discretization for Elastoplasticity: Motivation, Numerical Algorithms and Applications. *Computer Methods in Applied Mechanics and Engineering*, Volume 191, Issue 43, **27** (2002), Pages 4949-4968

[4] W. Han, B.D. Reddy: Computational plasticity: the variational basis and numerical analysis. *Computational Mechanics Advances* **2** (1995) 285–400.

[5] J.C. Simo, T.J.R. Hughes: *Computational Inelasticity.* Springer-Verlag, New York, 1998.

[6] R. Temam: *Mathematical problems in plasticity.* Gauthier-Villars, Paris 1985.

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