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Variational Methods for the Modelling of Inelastic Solids

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Abstract. This workshop brought together two communities working on the same topic from different perspectives. It strengthened the exchange of ideas between experts from both mathematics and mechanics working on a wide range of questions related to the understanding and the prediction of processes in solids. Common tools in the analysis include the development of models within the broad framework of continuum mechanics, calculus of variations, nonlinear partial differential equations, nonlinear functional analysis, Gamma convergence, dimension reduction, homogenization, discretization methods and numerical simulations. The applications of these theories include but are not limited to nonlinear models in plasticity, microscopic theories at different scales, the role of pattern forming processes, effective theories, and effects in singular structures like blisters or folding patterns in thin sheets, passage from atomistic or discrete models to continuum models, interaction of scales and passage from the consideration of one specific time step to the continuous evolution of the system, including the evolution of appropriate measures of the internal structure of the system.

Mathematics Subject Classification (2010): 74Cxx, 74Bxx, 74Dxx, 74Rxx.

Introduction by the Organisers

The workshop *Variational Methods for the Modelling of Inelastic Solids*, organized by Georg Dolzmann (Regensburg), Adriana Garroni (Roma), Klaus Hackl (Bochum) and Michael Ortiz (Pasadena/Bonn) was well attended with over 50 participants with broad geographic representation including Austria, Germany, France, Italy, the Netherlands, Switzerland and the United States. The workshop

featured 23 presentations (eight presented by female participants, nine from the engineering community) and ample time for scientific discussions.

The presentations by Svendsen and Reese offered a detailed discussion of modeling in continuum mechanics, the lecture by Müller presented a completely new approach to elasticity based on data driven models and Ariza discussed models for hydrogen transport and storage, a crucial topic for the design of fuel cells. Effective behaviour and homogenization was featured by Francfort and Reina and topics related to microstructures and upscaling by Govindjee, Kochmann and Rüland. Results in the framework of plasticity were presented by Luckhaus, Mora, Schweizer, and Weinberg and for the formulation and the analysis of fracture by Negri and Truskinovsky, while the challenging area of evolution was addressed by Davoli, Friedrich and Mielke. Finally stochastic aspects were introduced by Dal Maso. Special emphasis was given to the junior attendants including the Oberwolfach Leibniz Graduate Students (OLGS) and therfore one afternoon was dedicated to the presentations by Kreutz (spin systems), Frenzel (slip-stick motion), Waimann (cyclic loading), all of them OLGSs, and Ginster (strain gradient plasticity).

All participants were unanimous in their assessment that this meeting offered the most stimulating platform for the interaction between mathematics and mechanics in this field of outstanding importance in recent years. Many discussions will be continued and deepened within the departments of the participants and it is expected that long-lasting collaborations will emerge.

Acknowledgement: The MFO and the workshop organizers would like to thank the National Science Foundation for supporting the participation of junior researchers in the workshop by the grant DMS-1641185, "US Junior Oberwolfach Fellows".

Workshop: Variational Methods for the Modelling of Inelastic Solids

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Abstracts

2D periodic homogenization in linear elasticity redux

Gilles A. Francfort
(joint work with Marc Briane)

Homogenization in linear elliptic problems usually assumes coercivity of the accompanying Dirichlet form. In contrast with the scalar case, coercivity in linear elasticity is not ensured through mere (strong) ellipticity, that is when

$$\mathbb{L}(y)a \otimes b \cdot a \otimes b \geq \alpha > 0, a, b \in \mathbb{R}^2, |a| = |b| = 1.$$

Here, $\mathbb{L}(y)$ denotes the elasticity tensor; it is assumed to be periodic and endowed with the usual elastic symmetries $\mathbb{L}_{ijkh} = \mathbb{L}_{khij} = \mathbb{L}_{jikh}$.
The estimates that render homogenization meaningful break down unless stronger assumptions, like very strong ellipticity, that is

$$\mathbb{L}(y)M \cdot M \geq \alpha > 0, M \text{ symmetric } 2 \times 2 \text{ matrix},$$

are imposed.

It was shown through various prior works [3, 1, 2] that a homogenization process could still be performed, very strong ellipticity notwithstanding, for a class of two-phase mixtures. That process was to be understood as a Γ-convergence result for the weak topology on bounded sets of $H^1_0(\Omega; \mathbb{R}^2)$.

Strikingly, it demonstrated that, in the case of a specific layered mixture of a very strongly elliptic isotropic first phase with a strongly, but not very strongly elliptic isotropic, second phase, strict strong ellipticity could be lost in the process, that is that there existed a direction e (perpendicular to the layering) such that $\mathbb{L}^0 e \otimes e \cdot e \otimes e = 0$, with $\mathbb{L}^0$ the homogenized elastic tensor. This had been first discovered through a classical, but formal, homogenization argument in [4, 5].

The obvious criticism of this result is that compactness is *a priori* assumed in any Γ-convergence process. But, in the absence of uniform coercivity, H^1_0-bounds on, say almost minimizers of any variational problem involving $\mathbb{L}(x/\varepsilon)$ as elasticity tensor could not be secured, thereby rendering the whole procedure vacuous.

A possible remedy consists in adding to the energy density

$$\int_\Omega \mathbb{L}(x/\varepsilon)\nabla v \cdot \nabla v \, dx$$

a zeroth order term of the form

$$\int_\Omega |v|^2 \, dx$$

that produces L^2-bounds in any kind of minimization process. But then, Γ-convergence has to be revisited for the weak topology on bounded sets of $L^2(\Omega; \mathbb{R}^2)$.

This is our first task in this study. The resulting Γ-limit is shown to be that obtained in the H^1_0-setting, with the exception of the pathological situation first exhibited in [4] for which case the target fields that guarantee a finite Γ-limit

can live in a larger space than $H^1_0(\Omega;\mathbb{R}^2)$. It is so because the component of the field which is transverse to the layering may lose H^1-regularity when computing its partial derivative in that same transverse direction. As a consequence, the Dirichlet boundary condition on that transverse component, say v_2, relaxes from $v_2 = 0$ to $v_2\nu_1 = 0$ where ν is the exterior normal.

The advocated L^2-setting is the right setting for the investigation of elastodynamics in such mixtures. We then demonstrate that a weak convergence result holds true for the (unique) solution u^ε to the system

$$\begin{aligned} \rho(x/\varepsilon)\frac{\partial^2 u^\varepsilon}{\partial t^2} - \operatorname{div}(\mathbb{L}(x/\varepsilon)\nabla u^\varepsilon) = 0 \quad & \text{in } \Omega\times[0,\infty) \\ u^\varepsilon = 0 \quad & \text{on } \partial\Omega\times[0,\infty) \\ u^\varepsilon(0) = f, \quad \frac{\partial u^\varepsilon}{\partial t}(0) = g \quad & \text{in } \Omega. \end{aligned}$$

where $\rho(y)$ is the mass density associated with the two-phase mixture. The limit of u^ε is the (unique) solution to the same system with $\mathbb{L}^0$ replacing $\mathbb{L}(x/\varepsilon)$.

The setting of particular interest is that in introduced in [4] for which strict strong ellipticity is lost. In that case, the solution to the "homogenized problem" *a priori* lives in the larger space already mentioned. Because of the relaxation of the boundary condition, we can exhibit domains for which the homogenized laminate allows for plane wave propagation in the direction of lamination on a bounded domain with Dirichlet boundary conditions, a possibility which does not exist for the associated two-phase microstructure at a fixed scale.

Equally striking is the realization that such a material blocks longitudinal waves in the direction of lamination, thereby acting as some kind of two-dimensional aether in the sense of e.g. Cauchy.

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Variational phase-field chemo-mechanics for multicomponent, multiphase inelastic solids at finite deformation

Bob Svendsen
(joint work with Pratheek Shanthraj, Dierk Raabe)

The purpose of this work is the development of a framework for the formulation of geometrically non-linear chemomechanical models for a mixture of $m \geqslant 2$ chemical components diffusing among $p \geqslant 2$ transforming (generally inelastic) solid phases. To this end, basic balance and constitutive relations from non-equilibrium thermodynamics and continuum mixture theory are combined with a phase-field-based description of multicomponent solid phases and their interfaces. Solid phase modeling is based in particular on a chemomechanical free energy and stress relaxation via the evolution of phase-specific concentration fields, order-parameter fields (e.g., related to chemical ordering or defects), and local internal variables. At the mixture level, contrasts in phase composition and phase local deformation are treated as mixture internal variables. In this context, one "thick" and two "thin" phase interface models are considered. In the equilibrium limit, phase contrasts in composition and local deformation are determined via (bulk) energy minimization. On the chemical side, the equilibrium limit of the current model formulation reduces to a m-component, p-phase, generalization of the two-phase binary alloy interface equilibrium conditions of [1]. On the mechanical side, the equilibrium limit of the "thick" interface model represents a generalization of Reuss-Sachs conditions from mechanical homogenization theory. Analogously, those of the "thin" interface models represent generalizations of interface equilibrium conditions consistent with laminate and sharp-interface theory [2, 3]. Finally, variational formulation of the initial boundary-value problem is based on conditions for the existence of a dissipation potential [4] and corresponding rate-variational potential [5]. For more details, the interested reader is referred to [6].

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The equilibrium measure for a nonlocal dislocation energy

Maria Giovanna Mora
(joint work with Luca Rondi, Lucia Scardia)

In this talk we discussed the minimisation problem for the nonlocal energy

$$I(\mu) = \iint_{\mathbb{R}^2\times\mathbb{R}^2} V(x-y)\,d\mu(x)\,d\mu(y) + \int_{\mathbb{R}^2} |x|^2\,d\mu(x) \tag{1}$$

defined on probability measures $\mu \in \mathcal{P}(\mathbb{R}^2)$, where V is the interaction potential given by

$$V(x) = -\log|x| + \frac{x_1^2}{|x|^2}, \qquad x = (x_1, x_2), \tag{2}$$

and the second term in the energy acts as a confinement for the measure.

The energy (1) arises as the Γ-limit of the discrete interaction energy of a system of n positive edge dislocations with Burgers vector $\mathbf{e_1}$, as n tends to infinity. More precisely, I is the Γ-limit of w_n/n^2, where

$$w_n(x^1,\dots,x^n) = \sum_{i\neq j} V(x^i - x^j) + n\sum_i |x^i|^2, \qquad \{x^i\} \subset \mathbb{R}^2, \tag{3}$$

with respect to the weak* convergence of the empirical measures $\frac{1}{n}\sum_i \delta_{x^i}$. Therefore, I is the leading order or *mean-field* behaviour of the Hamiltonian w_n, and the minimisers of I represent the mean-field description of the minimisers of w_n, namely the equilibrium dislocation patterns at the mesoscale. Although such minimisers have not been characterised analytically so far - neither in the discrete nor in the continuum case - they are conjectured to be vertical wall-like structures.

In this talk we gave a positive answer to the conjecture. We proved (see [3]) that the minimiser of I exists, is unique, and is given by a *one-dimensional, vertical* measure, namely the semi-circle law on the vertical axis

$$m_1 := \frac{1}{\pi}\delta_0 \otimes \sqrt{2-x_2^2}\,\mathcal{H}^1 \llcorner (-\sqrt{2},\sqrt{2}).$$

This is the first example of an anisotropic kernel for which the minimiser can be explicitly computed. Even in the radially symmetric case, the explicit characterisation of the equilibrium measure has been done only for the Coulomb potential in any dimension and for the logarithmic potential in dimension one.

In two dimensions the Coulomb potential, namely $V = -\log|\cdot|$, arises in a variety of contexts, such as, e.g., Fekete sets, orthogonal polynomials, random matrices, Ginzburg-Landau vortices, Coulomb gases. For the same confinement term as in (1), the minimiser is given by the circle law $m_0 := \frac{1}{\pi}\chi_{B_1(0)}$ (see [4] and the references therein). Although the radial component of the potential in (2) is exactly the Coulomb kernel, the presence of the additional anisotropic term has thus a dramatic effect on the structure of the equilibrium measure.

For the logarithmic potential in one dimension, corresponding to the so-called Log-gases energy (see, e.g., [2]), Wigner proved in [5] that the semi-circle law is

the unique minimiser. We note that the functional I in (1) coincides with the Log-gases energy on measures with support on the vertical axis, since the anisotropic term vanishes on those measures. Therefore if one could prove that the minimiser of I is supported on the vertical axis, then the minimality of the semi-circle law would follow directly.

This is however not the strategy we used. Our approach consists of two steps: We first prove the strict convexity of I on the class of measures with compact support and finite interaction energy. Strict convexity implies uniqueness of the minimiser and the equivalence between minimality and the Euler-Lagrange conditions for I. As a second step, we show that the semi-circle law satisfies the Euler-Lagrange conditions and hence is the unique minimiser of I.

For the proof of these two steps we could not rely on the machinery developed in the classical case of purely logarithmic potentials with external fields, which is heavily based on $-\log|\cdot|$ being radially symmetric, and on it being the fundamental solution of the Laplace operator, since V is neither.

The strict convexity of I is a consequence of the following key result.

Theorem 1. *Let $\mu_0, \mu_1 \in \mathcal{P}(\mathbb{R}^2)$ be measures with compact support and finite interaction energy, that is, $\int_{\mathbb{R}^2}(V * \mu_i)\, d\mu_i < +\infty$ for $i = 0, 1$. Then*

$$\int_{\mathbb{R}^2} V * (\mu_1 - \mu_0)\, d(\mu_1 - \mu_0) \geq 0, \tag{4}$$

and the integral above is zero if and only if $\mu_0 = \mu_1$.

The proof of Theorem 1 is based on the intuition that, if we could rewrite the convolution in (4) in Fourier space, then heuristically we would have that

$$\int_{\mathbb{R}^2} V * (\mu_1 - \mu_0)\, d(\mu_1 - \mu_0) = \int_{\mathbb{R}^2} \hat{V}|\hat{\mu}_1 - \hat{\mu}_0|^2 d\xi, \tag{5}$$

and hence proving that $\hat{V} > 0$ would imply the theorem.

As a first step, then, we compute the Fourier transform of V, which is a tempered distribution. Unfortunately, the Fourier transform $\hat{V}$ is not a positive distribution, but we can show that $\hat{V} > 0$ for positive test functions that are zero at $\xi = 0$. The key remark is that this is enough to conclude, since $\mu_1 - \mu_0$ is a neutral measure and thus the test function $|\hat{\mu}_1 - \hat{\mu}_0|^2$ in (5) is zero at $\xi = 0$. This heuristic argument can in fact be made rigorous, and this is the heart of the proof of Theorem 1.

Our main result is the following.

Theorem 2. *The measure*

$$m_1 = \frac{1}{\pi}\delta_0 \otimes \sqrt{2 - x_2^2}\, \mathcal{H}^1 \llcorner (-\sqrt{2}, \sqrt{2})$$

satisfies the conditions

$$(V * m_1)(x) + \frac{|x|^2}{2} = \frac{1}{2} + \frac{1}{2}\log 2 \qquad \textit{for every } x \in \operatorname{supp} m_1, \tag{6}$$

$$(V * m_1)(x) + \frac{|x|^2}{2} \geq \frac{1}{2} + \frac{1}{2}\log 2 \qquad \textit{for every } x \in \mathbb{R}^2, \tag{7}$$

and hence is the unique minimiser of I.

The proof of Theorem 2 consists of two parts: In the first part we show that (6)–(7) are the Euler-Lagrange conditions for I relative to m_1, and that the Euler-Lagrange conditions uniquely characterise the minimiser of I. This is standard and can be done as in the purely logarithmic case. In the second part of the proof we show that m_1 satisfies (6)–(7). Since on $\operatorname{supp} m_1$ the potential V reduces to the logarithm in one dimension, (6) follows from the minimality of the semi-circle law for the Log-gases energy.

Proving that m_1 satisfies also (7) is instead extremely challenging. Indeed, we note that one of the two Euler-Lagrange conditions must fail for any measure other than the minimiser. This suggests that in order to prove (7) we need to estimate the function $V * m_1$ in $\mathbb{R}^2$ with great precision and accuracy. We achieve this by using complex analysis tools.

The previous analysis can be extended to the nonlocal energy

$$I_\alpha(\mu) = \iint_{\mathbb{R}^2\times\mathbb{R}^2} V_\alpha(x-y)\, d\mu(x)\, d\mu(y) + \int_{\mathbb{R}^2} |x|^2\, d\mu(x)$$

defined for $\mu \in \mathcal{P}(\mathbb{R}^2)$, where the interaction potential V_α is now given by

$$V_\alpha(x) = -\log|x| + \alpha\frac{x_1^2}{|x|^2}, \qquad x = (x_1, x_2), \tag{8}$$

and $\alpha \in \mathbb{R}$. Here the parameter α has the role of *tuning* the strength of the anisotropy, making it more or less prominent.

In [1] we prove that the values $\alpha = \pm 1$ are *critical* values of the parameter, at which an abrupt change in the dimension of the support of the minimiser occurs. Indeed, for $\alpha \in (-1, 1)$ we prove that the unique minimiser of I_α is the normalised characteristic function of the region surrounded by an ellipse of semi-axes $\sqrt{1-\alpha}$ and $\sqrt{1+\alpha}$. On the other hand, we show that for every $\alpha \geq 1$ the only minimiser of I_α is the semi-circle law m_1 on the vertical axis, while for $\alpha \leq -1$ it is the semi-circle law on the horizontal axis.

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Dynamic perfect plasticity as convex minimization

Elisa Davoli
(joint work with Ulisse Stefanelli)

In this talk we have discussed a new approximation result obtained in [3] for solutions to the problem of *dynamic perfect plasticity* for the classical *Prandtl-Reuss* model

$$\rho\ddot{u} - \nabla \cdot \sigma = 0, \tag{1}$$

$$\sigma = \mathbb{C}(Eu - p), \tag{2}$$

$$\partial H(\dot{p}) \ni \sigma_D \tag{3}$$

describing the plastic behavior of metals. In the expression above, $u(t) : \Omega \to \mathbb{R}^3$ is the (time-dependent) displacement of a body with reference configuration $\Omega \subset \mathbb{R}^3$ and density $\rho > 0$, and $\sigma(t) : \Omega \to \mathbb{M}^{3\times 3}_{\mathrm{sym}}$ is its stress. Equation (1) describes conservation of momenta. The constitutive relation (2) relates the stress $\sigma(t)$ to the *linearized strain* $Eu(t) := (\nabla u(t) + \nabla u(t)^\top)/2 : \Omega \to \mathbb{M}^{3\times 3}_{\mathrm{sym}}$ and the (deviatoric) *plastic strain* $p(t) : \Omega \to \mathbb{M}^{3\times 3}_D$ (deviatoric tensors) via the fourth-order *elasticity tensor* $\mathbb{C}$. Finally, the differential inclusion (3) expresses the plastic-flow rule: $H : \mathbb{M}^{3\times 3}_D \to [0, +\infty)$ is a positively 1-homogeneous, convex *dissipation* function, σ_D stands for the deviatoric part of the stress, and the symbol ∂ is the subdifferential in the sense of Convex Analysis. The system is driven by imposing a nonhomogeneous time-dependent boundary displacement.

Our main result consists in recovering weak solutions to the dynamic perfect plasticity system (1)-(3) by minimizing a sequence of parameter-dependent convex functionals over entire trajectories, and by passing to the limit as the parameter tends to zero. In particular, we consider the *Weighted-Inertia-Dissipation-Energy (WIDE)* functional of the form

$$I_\varepsilon(u,p) = \int_0^T \int_\Omega \exp\left(-\frac{t}{\varepsilon}\right)\left(\frac{\rho\varepsilon^2}{2}|\ddot{u}|^2 + \varepsilon H(\dot{p}) + \frac{1}{2}(Eu-p) : \mathbb{C}(Eu-p)\right) dx\, dt, \tag{4}$$

defined on suitable admissible classes of entire trajectories $t \in [0,T] \mapsto (u(t), p(t)) : \Omega \to \mathbb{R}^3 \times \mathbb{M}^{3\times 3}_D$ fulfilling given boundary-displacement and initial conditions (on u and p, respectively). The name of the functional reflects the fact that it is given by the sum of the inertial term $\rho|\ddot{u}|^2/2$, the dissipative term $H(\dot{p})$, and the energy term $(Eu-p) : \mathbb{C}(Eu-p)/2$, weighted by different powers of ε, as well as by the function $\exp(-t/\varepsilon)$.

For all $\varepsilon > 0$ one can prove that (a suitable relaxation of) the convex functional I_ε admits minimizers $(u^\varepsilon, p^\varepsilon)$ which indeed approximate solutions to the dynamic perfect plasticity system (1)-(3). In particular, by computing the corresponding Euler-Lagrange equations one finds that the minimizers $(u^\varepsilon, p^\varepsilon)$ weakly solve the

elliptic-in-time approximating relations

$$\varepsilon^2 \dddot{\rho} \ddddot{u}^\varepsilon - 2\varepsilon^2 \ddot{\rho} \dddot{u}^\varepsilon + \rho \ddot{u}^\varepsilon - \nabla \cdot \sigma^\varepsilon = 0, \tag{5}$$

$$\sigma^\varepsilon = \mathbb{C}(Eu^\varepsilon - p^\varepsilon), \tag{6}$$

$$-\varepsilon(\partial H(\dot{p}^\varepsilon))^{\cdot} + \partial H(\dot{p}^\varepsilon) \ni \sigma_D^\varepsilon, \tag{7}$$

complemented by Neumann conditions at the final time T.

The dynamic perfect plasticity system (1)-(3) is formally recovered by taking $\varepsilon \to 0$ in system (5)-(7). The main result presented in the talk consists in making this intuition rigorous, resulting in a new approximation theory for dynamic perfect plasticity.

Note that existence results for (1)-(3) are indeed quite classical. In the dynamic case $\rho > 0$ both the first existence results due to Anzellotti and Luckhaus [1] and their recent revisiting by Babadjian and Mora [2] are based on viscosity techniques. With respect to the available existence theories our approach is new, for it does not rely on viscous approximation but rather on a global variational method.

We briefly outline the main steps of the proof. First, by time discretization we prove a uniform energy estimate for minimizers of the WIDE functionals selected via time-discrete to continuum Γ-convergence. This uniform upper bound allows to deduce compactness and convergence of the sequence of ε-dependent weak solutions to (5)-(7) to weak solutions to (1)-(3). A key point in our argument is to show that the limit stress and plastic strain satisfy (3). This indeed does not follow directly by the uniform energy estimate but is rather obtained by proving a delicate ε-dependent energy equality. The proof of this last result follows closely the strategy of [6, Theorem 2.5 (c)]. The main additional difficulties in our setting are due to the linear growth of the dissipation function.

The WIDE approach in the dynamic case $\rho > 0$ has been the object of a long-standing conjecture by De Giorgi on semilinear waves [4]. The conjecture was solved in the positive in [7] for finite-time intervals and then by Serra and Tilli in [5] for the whole time semiline, that is in its original formulation. De Giorgi himself pointed out in [4] the interest of extending the method to other dynamic problems. The result presented in this talk delivers the first realization of De Giorgi's suggestion in the context of Continuum Mechanics.

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Energy-minimizing patterns via numerical relaxation

Dennis M. Kochmann
(joint work with A. Vidyasagar)

We predict microstructural patterns as energy minimizers in mechanical problems involving non-quasiconvex energy landscapes such as, e.g., during phase transformations, deformation twinning, and finite-strain crystal plasticity. The quasistatic equilibrium deformation mapping $\boldsymbol{\varphi} : \Omega \to \mathbb{R}^d$ for a body Ω is found by minimization of the total potential energy,

$$\mathcal{I}[\boldsymbol{\varphi}] = \int_\Omega W(\nabla\boldsymbol{\varphi})\,\mathrm{d}V - \ell(\boldsymbol{\varphi}), \tag{1}$$

where W denotes the Helmholtz free energy density and $\ell(\boldsymbol{\varphi})$ a linear potential of external forces. If W lacks quasiconvexity [1], then solutions are to be found as infimizing sequences; i.e., fine-scale patterns form as energy minimizers which may be interpreted as microstructural patterns on a lower spatial scale. By assuming a separation of scales between fine-scale patterns and the macroscopic boundary value problem, the solution to the macro-problem is found by replacing the energy density W by its quasiconvex hull

$$QW(\nabla\boldsymbol{\varphi}) = \inf\left\{ \frac{1}{|\omega|}\int_\omega W(\nabla\boldsymbol{\varphi} + \nabla\boldsymbol{\phi})\,\mathrm{d}V \;\middle|\; \boldsymbol{\phi} \,:\, \boldsymbol{\phi} = \mathbf{0} \text{ on } \partial\omega \right\} \tag{2}$$

for a representative volume element (RVE) ω. The small-scale fluctuation field $\boldsymbol{\phi}$ describes the microstructural patterns at the RVE-level. The quasiconvex hull and the associated microstructures are generally hard to calculate due to the nonlocal nature of (2). Prior approaches primarily relied upon (i) analytical energy relaxation, see e.g. [2, 3], or on (ii) RVE-level finite element simulations [4].

Here, we use a numerical approach to compute periodic energy-minimizing structures inside an RVE ω_h, i.e., we numerically approximate (2) by

$$NW(\nabla\boldsymbol{\varphi}) = \inf\left\{ \frac{1}{|\omega_h|}\int_{\omega_h} W(\nabla\boldsymbol{\varphi} + \nabla\boldsymbol{\phi}_h)\,\mathrm{d}V \;\middle|\; \boldsymbol{\phi}_h \,:\, \boldsymbol{\phi}_h^+ = \boldsymbol{\phi}_h^- \text{ on } \partial\omega \right\}, \tag{3}$$

where $\boldsymbol{\phi}_h$ is a discrete perturbation field (in our spectral approach represented by a truncated Fourier series, admitting high resolution and introducing a relative length scale). We employ a stabilized Fourier spectral scheme for periodic homogenization at the RVE-level, which is based on higher-order finite-difference approximations of spatial derivatives [5, 6]. This formulation approximates sharp

by diffuse interfaces and introduces a relative length scale. Previously, analytical prediction of such patterns was restricted to relatively simple problems, while numerical calculations limited problems to small 2D samples with insufficient resolution for capturing complex microstructural patterns due to computational expenses. Here, we demonstrate an alternative for microstructural pattern prediction in complex 3D problems based on the improved Fourier spectral scheme.

As a first example, we consider a hyperelastic St. Venant-Kirchhoff solid with

$$W(\boldsymbol{F}) = \frac{1}{8}(\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F} - \mathbf{I}) \cdot \mathbb{C}\,(\mathbf{F}^{\mathrm{T}}\mathbf{F} - \mathbf{I}). \tag{4}$$

When assuming isotropic elastic moduli and loading the body in uniaxial compression, the resulting energy lacks convexity and microstructural patterns form as energy-minimizers. As a second example, we study the classical problem of single-slip single-crystal plasticity at finite strains [7]. Figure 1 shows calculated relaxed energies and example microstructural patterns obtained numerically.

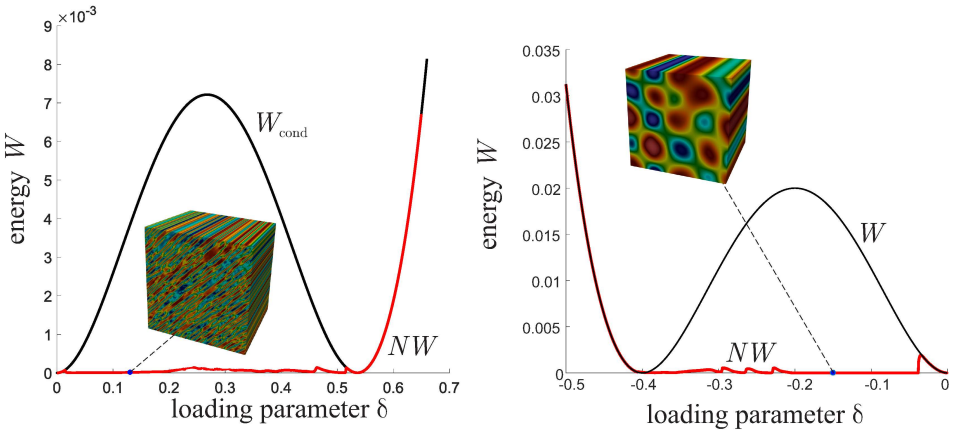

FIGURE 1. Left: single-slip crystal plasticity for simple shear without finite-difference (FD) approximation (comparing condensed and numerically relaxed energies); right: St. Venant-Kirchhoff solid in uniaxial compression with FD approximation.

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Data-driven problems in elasticity

Stefan Müller
(joint work with Sergio Conti, Michael Ortiz)

This talk is based on [1]. We consider a new class of problems in elasticity, called data-driven problems, which are defined on the phase space of pairs of strain-stress field. The problem consists of minimizing the distance between a given material data $\mathcal{D}$ set and the subspace $\mathcal{E}$ of pairs of strain-stress fields which are compatible and in equilibrium.

To define a suitable abstract setting we consider systems whose state is characterized by points z in a reflexive Banach space (Z, d). The compatibility and equilibrium constraints are encoded in a subset $\mathcal{E} \subset Z$. The behaviour of the material is encoded in the material data set $\mathcal{D} \subset Z$ The data driven problem is

$$\inf_{z\in\mathcal{E}} d(z, \mathcal{D}). \tag{1}$$

It is clear that the range of data-driven problems is larger than that of classical problems since the local material data sets, even if they define a curve in phase space, need not be a graph. In the setting of geometrically linear elasticity classical solutions correspond to the data set

$$\mathcal{D} = \{(\varepsilon, \sigma) \in L^2(\Omega, \mathbb{R}^{d\times d}_{\rm sym}) \times L^2(\Omega, \mathbb{R}^{d\times d}_{\rm sym}) : (\varepsilon(x), \sigma(x)) \in \mathcal{D}_{\rm loc} \text{ for a.e. } x \in \Omega\} \tag{2}$$

where $\mathcal{D}_{\rm loc}$ ia a graph

$$\mathcal{D}_{\rm loc} = \{(\varepsilon, , \hat{\sigma}(\varepsilon)) : \varepsilon \in \mathbb{R}^{d\times d}_{\rm sym}\}.$$

We show that for uniformly monotone $\hat{\sigma}$ the solution of the data-driven problem exists and agrees with the classical solution.

For general data sets we develop a suitable notion of relaxation which ensures existence of solutions. We also develop criteria which ensure that the data-driven solutions for an approximating sequence of sets $\mathcal{D}^h_{\rm loc}$ converge to the data-driven solution for a suitable limit set $\mathcal{D}_{\rm loc}$. We explicitely compute the relaxation for the two-well problem (with equal elastic moduli) and we show that the relaxed set is much larger than the set obtained by relaxation of the energy.

The point of view that the nonlinear partial differential equations of continuum mechanics are most naturally written as a set of linear partial differential equations (universal balance laws) and nonlinear pointwise relations between the quantities in the balance laws (material-dependent constitutive relations) has been emphasized by Luc Tartar since the 1970s; see, for example, [4] and [5]. Our notion of relaxation can also be couched in terms of A-quasiconvexity, see [2], p. 14 and pp. 100-112, as well as [3].

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Continuum mechanical framework for anisotropic inelastic material behaviour

Stefanie Reese

(joint work with Tim Brepols, Bob Svendsen, Stephan Wulfinghoff)

Introduction. The prediction of material degradation (damage) and failure is a very important task in the evaluation of engineering designs and processes. Most continuum mechanical models formulated for this purpose are based on a scalar internal damage variable usually called D (see [9],[14]). Exploiting the famous effective stress concept [7], one arrives at the following relation between the true (or effective) stress tensor $\tilde{\boldsymbol{\sigma}}$ and the continuum mechanical stress tensor $\boldsymbol{\sigma}$:

$$\boldsymbol{\sigma} = (1 - D)\, \tilde{\boldsymbol{\sigma}}. \tag{1}$$

It means that - independently of the actual loading of a system - every effective stress component is influenced in the same way. Obviously, this is a very simple outcome of a damage model and not completely convincing.

For this reason, one seeks for a more complex mapping between the two stress tensors which might be formulated in terms of either a second order tensor or a fourth order tensor. The latter approach is for instance discussed in [5] and [2], the former e.g. in [10] or [1].

The main advantage of using a second order tensor (which is here preferred) lies in the still feasible complexity. On the other hand, it is difficult to find a suitable Helmholtz free energy function. In order to tackle the latter problem, we consider the second order damage tensor - from now on denoted by $\mathbf{D}$ - as directly related to a structural tensor $\mathbf{H} := \mathbf{I} - \mathbf{D}$, where $\mathbf{I}$ is the identity tensor. See for the concept of structural tensors the references [3],[8].

Helmholtz free energy. The Helmholtz free energy (per reference volume) ψ is then given as isotropic function of the elastic strain $\mathbf{E}_e := (\mathbf{C}_e - \mathbf{I})/2$ ($\mathbf{C}_e$ elastic right Cauchy-Green tensor) and the structural tensor. As such, ψ becomes a function of ten invariants $I_i = \operatorname{tr} \mathbf{C}_e^i$, $I_{i+3} = \operatorname{tr} \mathbf{H}^i$ $(i = 1, 2, 3)$, $I_7 = \operatorname{tr} (\mathbf{C}_e\, \mathbf{H})$,

$I_8 = \mathrm{tr}\,(\mathbf{C}_e^2\,\mathbf{H})$, $I_9 = \mathrm{tr}\,(\mathbf{H}\,\mathbf{C}_e^2)$, $I_{10} = \mathrm{tr}\,(\mathbf{C}_e^2\,\mathbf{H}^2)$ and further scalar variables, e.g. quantities which represent isotropic and damage hardening.

Clausius-Duhem inequality. To reduce the formulation further, it is important to state the relationships

$$\mathbf{C}_e = \mathbf{F}_p^{-T}\,\mathbf{C}\,\mathbf{F}_p^{-1}, \quad \mathbf{H} = \mathbf{F}_p\,\mathbf{H}_r\,\mathbf{F}_p^T, \tag{2}$$

where $\mathbf{C}$ is the right Cauchy-Green tensor and $\mathbf{H}_r$ a tensor of the reference configuration being the "reference" counterpart to $\mathbf{H}$. In the latter relations the multiplicative decomposition of the deformation gradient $\mathbf{F} = \mathbf{F}_e\,\mathbf{F}_p$ into elastic ($\mathbf{F}_e$) and plastic ($\mathbf{F}_p$) parts has been exploited.

Using (2), it is possible to represent all invariants I_j $(j = 1, ..., 10)$ in terms of $\mathbf{C}_p$ and $\mathbf{H}_r$. Exploiting the Clausius-Duhem inequality for isothermal processes, we arrive at the statement

$$\boldsymbol{\Sigma}_r \cdot \frac{1}{2}\,\dot{\mathbf{C}}_p - \mathbf{Y}_r \cdot \frac{1}{2}\,\dot{\mathbf{H}}_r + q\,\dot{\xi} \geq 0, \tag{3}$$

where the stress tensors $\boldsymbol{Sigma}_r$, $\mathbf{Y}_r$ and the stress-like quantity q are given by

$$\boldsymbol{\Sigma}_r = 2\,\mathbf{F}_p^{-1}\,(\frac{\partial \psi}{\partial \mathbf{C}_e}\,\mathbf{C}_e - \mathbf{H}\,\frac{\partial \psi}{\partial \mathbf{H}})\,\mathbf{F}_p^{-T} = -2\,\frac{\partial \psi}{\partial \mathbf{C}_p}, \tag{4}$$

$$\mathbf{Y}_r = 2\,\mathbf{F}_p^T\,\frac{\partial \psi}{\partial \mathbf{H}}\,\mathbf{F}_p = 2\,\frac{\partial \psi}{\partial \mathbf{H}_r} \quad \text{and} \quad q = -\frac{\partial \psi}{\partial \xi}, \tag{5}$$

respectively. It is a very important result that all tensors showing up in (3) are symmetric. See for more information about this subtle point the work of [12].

Internal variables and evolution equations. Consequently, we have to formulate evolution equations for the internal variables $\mathbf{C}_p$, $\mathbf{H}_r$ and ξ. This is a very interesting point of the formulation, because this includes the fact that the plastic deformation gradient $\mathbf{F}_p = \mathbf{R}_p\,\mathbf{U}_p$ does not have to be computed. In other words, its rotational part $\mathbf{R}_p$ and consequently also the plastic spin remain unknown.

Example 1. Kinematic hardening. The continuum mechanical framework laid down here is very broad and in no way restricted to damage. Let us first look at Armstrong-Frederick type kinematic hardening (see [6], [13]). We have in this case an additive split of the Helmholtz free energy $\psi = \psi_{\mathrm{el}}\,(\mathbf{C}_e) + \psi_{\mathrm{kin}}\,(\mathbf{C}_{p_{el}}) + \psi_{\mathrm{iso}}\,(\xi)$ into three parts, where the second one depends on the tensor $\mathbf{C}_{p_{el}} = \mathbf{F}_{p_{el}}^T\,\mathbf{F}_{p_{el}}$ with $\mathbf{F}_{p_{el}}$ being defined by the multiplicative split of $\mathbf{F}_p = \mathbf{F}_{p_{el}}\,\mathbf{F}_{p_{in}}$ into elastic and inelastic parts. We can finally state $\mathbf{H} = \mathbf{B}_{p_{el}}$ and come to the evolution equations

$$\frac{1}{2}\,\dot{\mathbf{C}}_p = \dot{\lambda}_p\,(\frac{\partial \Phi_p}{\partial \boldsymbol{\Xi}})^T\,\mathbf{C}_p, \quad \frac{1}{2}\,(\mathbf{C}_{p_{in}}^{-1})^{\cdot} = -\dot{\lambda}_p\,\frac{b}{c}\mathbf{C}_{p_{in}}^{-1}\,(\mathbf{Y}_r\,\mathbf{C}_{p_{in}}^{-1})^D, \quad \dot{\xi} = \dot{\lambda}_p\,\sqrt{\frac{2}{3}}, \tag{6}$$

where the plastic potential Φ_p is given by

$$\Phi_p = ||(\underbrace{\mathbf{C}_p\,\boldsymbol{\Sigma}_r}_{=:\,\boldsymbol{\Xi}})^D|| - \sqrt{\frac{2}{3}}\,(\sigma_{\mathrm{y}} - q) \tag{7}$$

and the Kuhn-Tucker conditions $\Phi_p \leq 0$, $\dot{\lambda}_p \geq 0$ and $\dot{\lambda}_p \, \Phi_p = 0$ have to be fulfilled.

Example 2. Anisotropic plasticity of fibre-reinforced materials. A formulation for fibre-reinforced flexible membranes [11] can be also put into this framework. Important is in this context that two structural tensors have to be introduced which represent the dyadic product of the direction $\mathbf{N}_1$ and $\mathbf{N}_2$, respectively.

Example 3. Plasticity-coupled anisotropic damage. Here, the challenge lies in the fact that two processes - plastification and damage - run in parallel. In order to cope with this problem, two potentials are introduced. Besides Φ_p (7) which is now formulated in terms of the effective stresses $\tilde{\boldsymbol{Sigma}}_r$ and $\tilde{q}$, a so-called damage potential

$$\Phi_d = (\mathbf{Y}_r \cdot \mathbf{A}\,[\mathbf{Y}_r])^{2\,a} - (\gamma - q_d) \tag{8}$$

is introduced, where $\mathbf{A} := \mathbf{B} \otimes \mathbf{B}$ with $\mathbf{B} := f_d^{1/(4\,a)}\,\mathbf{X}/\mathrm{tr}\,\mathbf{X}$ is the so-called fourth order damage interaction tensor, γ the damage threshold and q_d the stress thermodynamically conjugate to the damage hardening variable ξ_d. The quantity f_d denotes a function of $\mathbf{D}$. The second order tensor $\mathbf{X}$ is a "joker" which can be a stress or strain tensor or a quantity suitable to incorporate tension-compression asymmetry. The scalar a is a material parameter. The format (8) has the advantage that it correctly reduces to the isotropic damage model of [4].

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Microstructures in Shape-Memory Alloys: Rigidity, Flexibility and Some Numerical Experiments

Angkana Rüland
(joint work with Jamie M. Taylor, Christian Zillinger, Barbara Zwicknagl)

Introduction

Shape-memory alloys are materials which undergo a first order diffusionless solid-solid phase transformation upon cooling below a certain critical temperature. Here the material transforms from a highly symmetric high temperature phase (*austenite*) to a low temperature phase (*martensite*), which is typically characterized by less symmetric (microscopic) lattice structures. This loss of symmetry gives rise to multiple variants of the low temperature phase. Mathematically, this together with the underlying assumption of frame indifference, leads to *nonlinear* and *non-quasiconvex* structures and to the presence of a variety of interesting microstructures.

Shape-memory alloys and their microstructures have been very successfully modelled by the phenomenological theory of elasticity [1]. Since this still leads to complex mathematical variational structures, in this talk, which is based on the articles [5], [6] and [7], I focused on the study of exactly stress-free material patterns. At a fixed temperature θ below the critical temperature, this typically leads to a differential inclusion – the *m-well problem*–

$$\begin{aligned} &\nabla u \in K(\theta) \text{ in } \Omega, \\ &\nabla u = M \text{ in } \mathbb{R}^n \setminus \overline{\Omega}. \end{aligned} \tag{1}$$

Here the vector-valued mapping $u : \mathbb{R}^n \to \mathbb{R}^n$ is the material deformation, $M \in \mathbb{R}^{n\times n}$ is an imposed boundary condition and $K(\theta) \subset \mathbb{R}^{n\times n}$ is typically of the form

$$K(\theta) = \bigcup_{j=1}^{m} SO(n)\alpha_j(\theta)U_j.$$

The matrices $U_j \in \mathbb{R}^{n\times n}$ correspond to the different *variants of martensite* and $\alpha_j(\theta) : \mathbb{R}^n \to (0,\infty)$ models the thermal expansion of the martensite. In the study of differential inclusions of the form (1), an interesting dichotomy arises. For instance for the compatible two-well problem (in which case $m = 2$) with two rank-one connections the following behaviour is known:

- **Flexibility:** On the one hand, if no regularity assumption is imposed on ∇u, a multitude of solutions to the corresponding version of (1) exist [2], [3]. These are obtained by convex integration schemes and by definition satisfy $\nabla u \in L^\infty(\Omega)$.
- **Rigidity:** On the other hand, if surface energy constraints are imposed, i.e. if $\nabla u \in BV(\Omega) \cap L^\infty(\Omega)$, then the problem becomes very rigid and only very few solutions exist. Up to boundary effects, these are all one dimensional simple laminate structures [4].

In this talk, I addressed this dichotomy and presented first higher order regularity results on the flexible regime, which were obtained in collaboration with J. M. Taylor, Ch. Zillinger and B. Zwicknagl [5], [6], [7]. More precisely, for the model setting of the geometrically linearized hexagonal-to-rhombic phase transformation I discussed first higher regularity results within the flexible regime, showing that under (low) Sobolev regularity for ∇u the wild, convex integration solutions persist. The structure of these were illustrated by numerical simulations.

Results

In the talk, I first presented the main result of [5] showing that in the context of the geometrically linearized hexagonal-to-rhombic phase transformation higher regularity convex integration solutions exist.

Theorem 1. *Let $\Omega \subset \mathbb{R}^2$ be a bounded Lipschitz domain. Let $K = \{e^{(1)}, e^{(2)}, e^{(3)}\}$ be the exactly stress-free states for a hexagonal-to-rhombic material, and let $e(M) = \frac{1}{2}(M + M^t) \in intconv(K)$. Then there exists $\theta_0 \in (0,1)$ depending on $\frac{dist(e(M),\partial conv(K))}{dist(e(M),K)}$ and a deformation $u : \mathbb{R}^2 \to \mathbb{R}^2$ with $u \in W^{1,\infty}_{loc}(\mathbb{R}^2)$*

$$\nabla u = M \text{ a.e. in } \mathbb{R}^2 \setminus \Omega,$$
$$e(\nabla u) \in K \text{ a.e. in } \Omega,$$

and for all $s \in (0,1), p \in (1,\infty)$ with $0 < sp < \theta_0$

$$\nabla u \in W^{s,p}_{loc}(\mathbb{R}^2) \cap L^\infty(\mathbb{R}^2).$$

The derivation of this result relies on carefully tracking the dependences of the iterative convex integration scheme using an interpolation result for Besov spaces.

While the proof of Theorem 1 exploited both the two-dimensional and geometrically linearized setting, it is also possible to derive a method which also deals with more general phase transformations, e.g. the geometrically linearized three-dimensional cubic-to-orthorhombic phase transformation. In order to explain this, I briefly introduced the convex-integration scheme from [6]. These ideas also allow

one to obtain uniform dependences on the regularity exponents $\theta_0 = sp$, independent of the position of the boundary datum M in the convex hull of K. I illustrated the convex integration constructions by presenting first numerical simulations of these [7]. Here the difference between the two schemes from [5] and [6] was emphasized.

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Effective Dynamic Behavior of Heterogeneous Structures

Celia Reina

(joint work with Chenchen Liu)

The dynamic response of heterogeneous media is receiving increased interest due to the development of composites/metamaterials with unique dynamic properties. These include structures that exhibit subwavelength bandgaps, frequency dependent density and/or stiffness, or dynamically-induced anisotropies.

In this talk we present a computational homogenization strategy to understand the real time dynamic evolution of these structures in the context of their applications, i.e., finite size domains with specific boundary conditions and potentially non-linear and history dependent constitutive relations for the microconstituents. The proposed approach [1] represents a variational coarse-graining procedure that seamlessly extends the classical FE^2 method to the dynamic setting, while being applicable to both discrete and continuum systems. This is achieved by recasting the finite element time-incremental dynamic problem as an equivalent static problem, to which static homogenization strategies are applied. The procedure is exercised of various composite structures, demonstrating its capability to capture the dispersive nature of the media under dynamic excitation.

We further present in this talk bio-inspired hierarchical metamaterial designs with ultrabroradband properties [2]. The designs are the result of a detailed analysis of the effect of hierarchy on the effective response of the infinite mass-spring models with resonant units. The resulting designs are validated over more realistic finite continuum samples using finite element simulations.

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Quasistatic crack growth in 2d-linearized elasticity

Manuel Friedrich

(joint work with Francesco Solombrino)

In variational fracture mechanics displacements and crack paths are determined from an energy minimization principle: the fundamental idea is that the formation of cracks may be seen as the result of the competition between the elastic energy of the body and the energy needed to produce a new crack. The rigorous mathematical formulation of the problem goes back to the seminal work by Francfort and Marigo [5]. A function $t \to (u(t), \Gamma(t))$, associating to each time t a deformation $u(t)$ of the reference configuration and a crack set $\Gamma(t)$, is called a quasistatic evolution if the following conditions are satisfied:

- (a) irreversibility: $\Gamma(s)$ is contained in $\Gamma(t)$ for $0 \leq s < t$.
- (b) static equilibrium: for every t the pair $(u(t), \Gamma(t))$ minimizes the energy at time t among all admissible competitors.
- (c) nondissipativity: the derivative of the internal energy equals the power of the applied forces.

Establishing a rigorous mathematical framework for the existence of such evolutions has proved to be quite a hard task. First breakthrough results in this direction are due to Dal Maso and Toader [3] and Chambolle [1] tackling in a planar setting the case of anti-plane shear and linearized elasticity, respectively. In their setting, existence can be proved under the additional restriction that the admissible cracks have at most a fixed number of connected components. Later a different and more powerful approach has been proposed by Francfort and Larsen [4] to avoid all restriction on the geometry of the jump set. It allows to treat a free discontinuity problem in the framework of SBV functions in arbitrary dimension.

The existence of time-continuous evolutions is proved by following the natural idea of starting with time-discretized evolutions, and then letting the time-step go to zero. In general, the fundamental problem consists in proving that the static equilibrium property (b) is conserved in the passage to the time-continuous solutions. The main tool of the approach in [4] is a geometrical construction,

usually called *Jump Transfer Lemma*, which relies on the coarea formula in BV and enables a suitable 'transfer' of the jump set of any competitor.

The goal of the paper [6] is to prove a two-dimensional existence result for a variational model of crack growth for brittle materials in the framework of generalized special functions of bounded deformation (see [2]). Specifically, we consider a Griffith-energy of the form

$$\mathcal{E}(u,\Gamma) := \int_{\Omega\setminus\Gamma} Q(e(u))\,\mathrm{d}x + \mathcal{H}^1(\Gamma)$$

for $u \in GSBD^2(\Omega)$, where Q is a quadratic form acting on the symmetrized gradient $e(u)$. The major difficulty lies in the fact that, in showing the stability of the static equilibrium condition, the strategy of [4] cannot be reproduced straightforwardly as the coarea formula is not available in the space $GSBD$. Nevertheless, by means of a Korn-type inequality

$$\|\nabla u\|_{L^1(\Omega)} \leq C\|e(u)\|_{L^2(\Omega)} + C\|u\|_{L^\infty(\Omega)}(\mathcal{H}^{d-1}(J_u) + 1)$$

for $u \in SBD^2(\Omega) \cap L^\infty(\Omega)$ and subsequent refined versions of this inequality, we are able to adapt the Jump Transfer Lemma to the $GSBD$ setting. This is the main technical tool which allows to prove the aforementioned existence result of a quasistatic evolution in the geometrically linear setting.

In this paper, we also discuss a general compactness theorem for this framework and prove existence of the evolution without imposing a-priori bounds on the displacements or applied body forces.

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Global existence for finite-strain viscoplasticity

Alexander Mielke
(joint work with Riccarda Rossi (Brescia) and Giuseppe Savaré (Pavia))

1. Introduction

This talk is based on our joint work [MRS18].

We consider the deformation $\varphi : \Omega \to \mathbb{R}^d$ of a bounded body $\Omega \subset \mathbb{R}^d$ and decompose the deformation gradient into an elastic and a plastic part, namely

$$\nabla\varphi = F_{\mathrm{el}}F_{\mathrm{pl}} = F_{\mathrm{el}}P. \tag{1}$$

While the elastic part contributes to energy storage and is governed by an equilibrium equation, the plastic tensor P evolves by a plastic flow rule. The multiplicative decomposition (1) leads to geometric nonlinearities in the energy functional $\mathcal{I} = \mathcal{I}(t, \varphi, P)$ driving the evolution of the elastoplastic process. These nonlinearities are compatible with polyconvexity of the energy density, and we will exploit the existence theory for polyconvex materials.

A fundamental step towards the analysis of the evolution of finite-strain elastoplastic materials was made in [OrS99]: therein it was pointed out that evolutionary elastoplastic models can be discretized by time-incremental problems that can be written as minimization problems for the sum of the dissipated and of the stored energy. This observation forms the basis of the existence theory in [MiM06, MaM09, HHM12], where the flow rule for the plastic tensor was considered to be rate-independent.

Viscoplasticity is a rate-dependent process which manifests itself in the superlinear growth of the dissipation potential $\mathcal{R}(P, \cdot)$. Because of the nonlinear and nonsmooth relation between plastic stress and plastic flow rate one cannot use the well-established variational theory for gradient flows (see [Amb95]), but the notion of generalized gradient systems [Mie15] is applicable in principle. Following the footsteps of [MRS13] one can define a suitable solution concept relying on the so-called energy-dissipation principle, which encodes the variational structure in terms of a balance between the change of energy, the work of the external forces, and the dissipation written is a special dual form.

2. Modeling of viscoplasticity

The evolution is governed by two principles:

Energy storage: via a time-dependent Gibbs' free energy $\mathcal{I}(t, \varphi, P)$ and
Energy dissipation: via a dissipation potential $\mathcal{R}(P, \dot{P})$.

We assume that inertial effects can be ignored and that viscoelasticity is not relevant as it has much smaller time scales (quasistatic approximation) such that the equations of interest take the abstract variational form

$$\varphi(t) \in \mathrm{Argmin}\{\, \mathcal{I}(t, \widetilde{\varphi}, P(t)) \,:\, \widetilde{\varphi} \in \mathcal{F} \,\}. \tag{2a}$$

$$0 \in \partial_{\dot{P}}\mathcal{R}(P, \dot{P}) + \mathrm{D}_P\mathcal{I}(t, \varphi, P). \tag{2b}$$

Here $\mathcal{F}$ is the fixed set of admissible deformations, which is given in terms of Dirichlet boundary conditions, (2a) provides the balance of linear momentum, and (2b) contains the plastic flow rule. The term $\mathrm{D}_P\mathcal{I}$ contains the plastic backstress and the convex subdifferential $\partial_{\dot P}\widehat{\mathcal{R}}$ contains the viscoplastic stresses.

The stored energy $\mathcal{I}$ and the dissipation potential $\mathcal{R}$ take the form

$$\begin{aligned}\mathcal{I}(t,\varphi,P) &= \int_\Omega W(x,\nabla\varphi(x),P(x),\nabla P(x))\,\mathrm{d}x - \langle \ell(t),\varphi\rangle\\ \text{and } \mathcal{R}(P,\dot P) &= \int_\Omega R(x,P(x),\dot P(x))\,\mathrm{d}x,\end{aligned} \tag{3}$$

where ℓ is a sufficiently smooth time-dependent loading.

The energy density W and the pointwise dissipation potential R feature geometric nonlinearities arising from frame indifference, non-self-interpenetration, and the Lie group structure of finite strains like the multiplicative decomposition (1):

$$W(x,F,P,A) = W_{\mathrm{el}}(x,F\,P^{-1}) + H(x,P,A), \quad R(x,P,\dot P) = \widehat{R}(x,\dot P\,P^{-1}), \tag{4}$$

where W_{el} satisfies polyconvexity, spatial frame indifference, and local injectivity, i.e. $W_{\mathrm{el}}(x,F_{\mathrm{el}}) = \infty$ for $\det F_{\mathrm{el}} \le 0$.

The multiplicative structures in W_{el} and $\widehat{R}$ give rise to strong geometric nonlinearities, which is when writing the PDE system induced by (2) explicitly:

$$\varphi(t) \in \operatorname{argmin}\left\{ \int_\Omega W(x,\nabla\widetilde{\varphi}(x)P^{-1}(t,x))\,\mathrm{d}x - \langle \ell(t),\widetilde{\varphi}\rangle \;:\; \widetilde{\varphi}\in\mathcal{F}\right\}, \tag{5a}$$

$$\partial R(x,\dot P) = B(\nabla\varphi,P) - \mathrm{D}_P H(P,\nabla P) + \operatorname{div}\big(\mathrm{D}_{\nabla P}H(P,\nabla P)\big), \tag{5b}$$

where the plastic backstress is $B(F,P) = (FP^{-1})^\top \mathrm{D}_{F_{\mathrm{el}}}W(FP^{-1})P^{-\top}$. Our global solutions will be weak solutions to this PDE system.

3. Variational approaches: rate-independent versus rate-dependent evolution

Variational approaches and formulations are ideal for treating material models involving finite-strain elasticity and finite-strain plasticity. The reason is that the direct methods from the calculus of variations rely on the flexible concept of weak lower semicontinuity, which allows us to circumvent the much too strong convexity methods that are available for small-strain theories. A first global existence result for finite-strain elastoplasticity was obtained in [MaM09], where solvability of (5) was in terms of energetic solutions for purely rate-independent systems.

Our system is induced by a generalized gradient system $(X,\mathcal{E},\mathcal{R})$ with the reduced energy functional $\mathcal{E}$ given by $\mathcal{E}(t,P) := \inf\{\mathcal{I}(t,\varphi,P) \;:\; \varphi\in\mathcal{F}\}$. Then, (5) can be rewritten as the abstract subdifferential inclusion

$$0 \;\in\; \partial\mathcal{R}(P(t),\dot P(t)) + \mathfrak{F}(t,P(t)) \quad \text{in } X^* \text{ for a.a. } t\in(0,T), \tag{6}$$

with state space $X = L^p(\Omega;\mathbb{R}^{d\times d})$, and the multivalued marginal subdifferential $\mathfrak{F}:[0,T]\times X \rightrightarrows X^*$ of $\mathcal{E}$ (cf. [MRS13]) is defined via

$$\mathfrak{F}(t,P) := \{\mathrm{D}_P\mathcal{I}(t,\varphi,P) \;:\; \varphi \text{ is a minimizer for (5a)}\}.$$

Denoting by $\mathcal{R}^*(P,\cdot)$ the Fenchel-Moreau conjugate of $\mathcal{R}(P,\cdot)$ and De Giorgi's energy-dissipation principle we define the so-called EDI solutions for (5) by asking the following form of the **energy-dissipation inequality**:

$$\text{(EDI)}\qquad \begin{cases} \text{For } s=0 \text{ and a.a. } s\in(0,T] \text{ and all } t\in(s,T] \text{ we have} \\ \mathcal{E}(t,P(t)) + \displaystyle\int_s^t \Big(\mathcal{R}(P(r),\dot P(r)) + \mathcal{R}^*(P(r),-\Xi(r))\Big)\,\mathrm{d}r \\ \qquad \le \mathcal{E}(s,P(s)) + \displaystyle\int_s^t \partial_r\mathcal{E}(r,P(r))\,\mathrm{d}r\,, \quad \text{where } \Xi(r)\in\mathfrak{F}(r,P(r)). \end{cases}$$

4. The main results

Based on the semi-implicit time-incremental minimization scheme ($\tau = T/N$)

$$P_\tau^n \;\in\; \operatorname*{Argmin}_{P\in X}\Big(\tau\mathcal{R}\big(P_\tau^{n-1},\tfrac{1}{\tau}(P-P_\tau^{n-1})\big) + \mathcal{E}(n\tau,P)\Big) \tag{7}$$

be obtain two piecewise constant, affine, and variational integrands $\overline{P}_\tau$, $\underline{P}_\tau$, $\widetilde{P}_\tau$, and $\widetilde{P}_\tau$, respectively as well as $\widetilde{x}i_\tau$ with $\widetilde{\xi}_\tau(t)\in\mathfrak{F}(t,\widetilde{P}_\tau(t))$. For this construction suitable coercivity assumptions are imposed that allow for good existence results for the incremental steps.

Then, these approximations satisfy the discrete energy-dissipation inequality ($0\le s=k\tau<t=n\tau\le T$)

$$\mathcal{E}(t,\overline{P}_\tau(t)) + \int_s^t \big(\mathcal{R}(\underline{P}_\tau,\dot{\widehat{P}}_\tau) + \mathcal{R}^*(\underline{P}_\tau,-\widetilde{\xi})\big)\,\mathrm{d}r = \mathcal{E}(s,\overline{P}_\tau(s)) - \int_s^t \langle\dot\ell,\overline{P}_\tau\rangle\,\mathrm{d}r.$$

After choosing suitable subsequences, it is then relatively standard to pass to the limit in this inequality, but it is absolutely non-trivial to establish the closedness of the subdifferential $\mathcal{F}$. In particular one has to show that $P_n\rightharpoonup P$, $\varphi_n\rightharpoonup\varphi$ in $\mathrm{W}^{1,q_{\mathrm{F}}}$, and $\varphi_n\in\operatorname{Argmin}\mathcal{I}(t,\cdot,P_n)$ imply that $B(\nabla\varphi_n,P_n)\rightharpoonup B(\nabla\varphi,P)$ in L^1. For this, one can use the techniques developed in [FrM06], which were stimulated by [DFT05].

Altogether global existence of EDI solutions for (5) can be established under natural assumptions for viscoplastic materials at finite strains, see [MRS18].

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Gradient flows and quasi-static evolutions for phase-field fracture

Matteo Negri

(joint work with Stefano Almi, Sandro Belz, Dorothee Knees)

We consider two evolutions for a separately quadratic phase-field energy in brittle fracture. Both are obtained by time discretization and by suitable alternate minimization schemes, taking, in this way, full advantage of the separate quadratic structure of the energy. In both the evolutions irreversibility is imposed by monotonicity (in time) of the phase-field variable.

In the first case we consider a system which combines a unilateral L^2-gradient flow for the phase field variable with the equilibrium equation for the displacement field. First we consider a time-discrete approximation, in which the incremental problem is a one-step alternate minimizing movement: minimization in the displacement is followed by constrained minimization in the phase field. Second, we consider an infinite-step unconstrained alternate minimization scheme with a posteriori truncation: minimization in the displacement is followed by unconstrained minimization in the phase field, which in turn is followed by truncation with respect to the previous (in time) configuration. Third, we take into account a finite element multi-step version. We show that numerically the multi-step scheme provides good results in a large range of time increments. Numerically the scheme is very efficient since it relies on the solution of two linear systems. Next, we characterize the time continuous limit in terms of DeGiorgi's energy identity, without relying on chain rule and thus on compactness in time-Sobolev spaces. Truncation allows indeed only for estimates in time-Lebesgue spaces. Moreover, we study the vanishing viscosity limit, at least in the case of the one step scheme. To this end, we first parametrize the evolutions by arc-length and prove that the lengths are uniformly finite. This delicate technical step is obtained by means of a suitable discrete Gronwall argument, which in turns provides also the local regularity in time-Sobolev spaces. Then we can pass to the limit, which is characterized again in terms of a quasi-static BV-evolution. In this case we first show the energy balance and then deduce, by means of the chain rule, the corresponding PDEs. We can show that in the regime of stable propagation the limit evolution is in equilibrium,

in both the variables, while in the regime of unstable propagation is characterized by a system of PDEs which is nothing but the original time-continuous system in the parametrization variable.

For the second evolution we employ instead a constrained alternate minimization scheme in which the time-update configuration is found by an iterative procedure, either finite or infinite. Irreversibility is imposed at each step of the constrained minimization for the phase-field. In this case the updated configuration is always an equilibrium point for the energy. This algorithm can be recast both as a separate gradient flow, with respect to a suitable family of intrinsic norms, and as a "quasi-Newton" method. Both the representations highlight the underlying family of intrinsic norms for the evolution. After re-parametrizing the evolution by means of an arc-length parameter we can conveniently pass to the limit, characterized in terms of a (parametrized) BV-evolution. In particular we show that in the regime of stable (or steady state) propagation the limit evolution satisfies equilibrium for the displacement variable and a suitable form of Griffith's criterion for the phase-field variable, written in terms of a phase-field energy release rate. We further show that the irreversibility constraint, given by the monotonicity of the phase-field variable, is thermodynamically consistent, since the associated dissipated energy is non-decreasing in time. Further we characterize the unstable regime of propagation in terms of gradient flows (in the parametrization variable) with respect to the intrinsic norms. The fact that the limit evolution is "simultaneous" in the two variable, even if the algorithm is not, is justified by continuous dependence.

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On phase-field models with application to fracture at linearized and finite strains

Kerstin Weinberg

The basic idea of phase-field simulations of fracture is to mark the material's state by an order parameter $s : [0, T] \times \mathcal{B} \to [0, 1]$, evolving over the domain of the body $\mathcal{B} \subset \mathbb{R}^3$ during a time span $[0, T]$, with $s = 0$ indicating the intact solid and $s = 1$ the broken state. While cracks are actually sharp two-dimensional hypersurfaces, the use of a continuous order parameter field -or phase field- regularizes the sharp material discontinuities with smooth transitions between broken and unbroken regions. Generally, the evolution of the phase-field follows a partial differential

equation

$$\dot{s} = -MY, \tag{1}$$

where parameter M describes a kinematic mobility (or, taking the inverse, a viscous regularization) and the dimensionless function $Y : [0,T] \times \mathcal{B} \to \mathbb{R}^+$ summarizes all generalized driving forces of crack growth.

Most phase-field fracture simulations use a modified Ambrosio-Tortorelli functional [AT90] of rate-independent damage to model the crack driving force, and formulate Y in a variational form, i.e. $Y = \delta_s \bar{\Psi}$ with $\bar{\Psi}$ being a normalized energy density, [WDS$^+$16]. In practise, modifications allow to account for the anisotropy of fracture, i.e., the fact that cracks only increases under tensile loadings but not under compression. The application of (1) to fracture evolution also requires additional developments to properly account for the no-healing irreversibility constraint of crack evolution. Other modifications consider the evolution problem at finite strains using energy densities, which are polyconvex with respect to the gradient of the deformation $\varphi : [0,T] \times \mathcal{B}_0 \to \mathbb{R}^3$, cf. [HW14, HGO$^+$17].

In brittle fracture the energy density Ψ of the body is solely elastic. To meet the anisotropy constraint, this energy is split in fracture sensitive and fracture insensitive parts,

$$\Psi(\nabla\varphi, s) = \Psi^+(\nabla\varphi, s) + \Psi^-(\nabla\varphi) \tag{2}$$

where only the first term shows dependence on fracture and is used to drive the crack. Elastic energy densities are subjected to convexity constrains and cannot be linear in $\nabla\varphi$, [Bal77]. Thus, the split (2) practically never fulfills the identity $\Psi^+ = \Psi - \Psi^-$. Instead an energy part $\Psi^+(\nabla\varphi, s)$ is postulated to be the crack driving force. It may base, e.g., on positive principal strains. The energy-splits are becoming even more arbitrarily when non-linear elastic energy contribution are involved.

We discuss different decomposition models in linearized and in finite elasticity and present recent results on the mathematical analysis for a phase-field model at finite strains, cf. [TBW17], where we formulate the phase-field with polyconvex energy densities in terms of the modified invariants of the right Cauchy-Green strain tensor. Additionally we discuss finite element simulations of conchoidal fracture in a brittle specimen. The main challenge of conchoidal fracture simulations is, that it requires the ability of a numerical method to predict crack nucleation and fracture without stress concentration at a notch, kerb or at an initial crack.

The elastic specimen is here made of a non-linear Yeoh material, fixed at the bottom and subjected to an upward deformation by prescribed incremental displacement steps. The crack initiates in the center of the block, followed by a brutal and complete crack growth, see Fig. 1. Please note that the characteristic rippled surface of conchoidal fracture can nicely be observed. More details and further investigations can be found in [BKKW17].

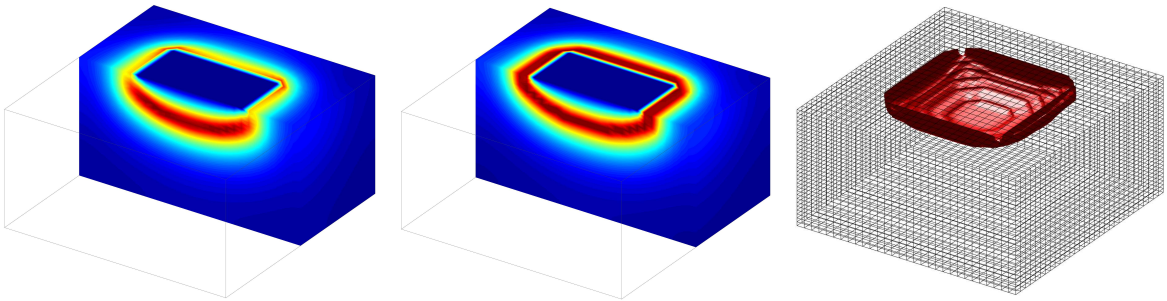

FIGURE 1. Crack initiation, final state and crack surface in conchoidal fracture computed with a mesh of $30 \times 30 \times 30$ elements.

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Fracture in disordered solids: a simple model of critical behavior

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(joint work with Hudson Borja da Rocha)

Power law distributed avalanches accompany fracture phenomena in disordered elastic solids. Such scale free behavior is of interest from the fundamental point of view because it results from the intricate interplay between disorder and long range interactions. The observed scaling in such processes has been previously linked to spinodal points associated with first order phase transitions and to critical points associated with second order phase transitions. The mystery is complicated by the fact that athermal fracture can be modeled in two ways: as incremental energy minimization phenomenon (zero temperature limit) and as incremental marginal

equilibration phenomenon (zero viscosity limit). We use the simplest mean field model of fracture under controlled displacement to show that both spinodal and critical associations are relevant. To study the effect of the displacement control (hard device loading) we augmented the classical fiber bundle model by adding seemingly innocent internal (series to fibers) and external (series to the bundle) springs. We show that by changing the effective rigidity in such model one can simulate a broad class of mechanical responses. Most importantly, such system displays an out-of-equilibrium phase transition between brittle and quasi-brittle (ductile) responses, where the former is characterized by a power law distribution of avalanches, while the latter exhibits predominantly Gaussian statistics of avalanches. The realization of a particular scenario depends on the two parameters representing disorder and rigidity. In brittle systems with either high rigidity or low disorder the super-critical scaling is robust belonging to the spinodal universality class. The boundary of the brittle domain is critical with different (non-spinodal) exponents. For ductile systems with either high disorder or low rigidity the scaling is absent. We show that if dynamics is energy minimizing, as in the case of zero temperature equilibrium systems, the spinodal scaling is lost while the critical systems remain in the same universality class as their non-equilibrium analogs. When rigidity is conditioned by the system size, spinodal avalanaches remain robust while critical scaling emerges only as a finite size effect. We argue that the robust criticality, as in the case of earthquakes and collapse of compressed porous materials, can only result from self tuning of the system towards the border separating brittle and ductile behaviors.

Variational upscaling in inelastic materials

Sanjay Govindjee
(joint work with Klaus Hackl, Miklos Zoller)

The homogenization of elastic composites has a well known variational structure, where the constitutive response for the average stress is given in terms of essential macroscopic quantities like average macroscopic strain through the derivative of an energy functional derived via the relaxation of the pointwise elastic energy. The relaxation allows for local pointwise fluctuations in the displacement field in order to lower the systems energy. For systems that are not elastic it would be interesting to have a similar variational structure.

If we define the state of the system to be in terms of state variables x that can be controlled and internal state variables z, we can postulate a free energy density for the system as $\Psi(\nabla x, x, z)$, where ∇ is the gradient operator. For materials that can be modeled by Biot's principle[1], we can also postulate a dissipation (density) potential $\Delta(z, \dot{z})$, where superposed dots indicate time differentiation. The equilibrium relations for the system can be found be minimizing the integral of the free energy density over the system subject to boundary constraints. The evolution of the internal state can be found by minimizing $\dot{\Psi} + \Delta$ with respect to $\dot{z}$ – a.k.a. Biot's principle [1, 2, 3].

Homgenization of this model can be achieved by splitting the space $X = X_{ess} \oplus X_{mar}$ for the state variables and the space $Z = Z_{ess} \oplus Z_{mar}$ for the internal state variables into essential and marginals components. In this arrangement, the essential components are the macroscopic components of interest. The homogenized model can then be determined via minimizing the integrals of the free energy density and the integral of the dissipation potential with respect to the state and internal state variables under the constraint that the projection of the pointwise state and internal state be equal to an element of $X_{ess} \times Z_{ess}$. This results in macroscopic potentials $\Psi_M(x_{ess}, z_{ess})$ and $\Delta_M(z_{ess}, \dot{z}_{ess})$. Stress-strain equations for the homogenized system follow as gradients of Ψ_M with respect to the essential state variables (typically macroscopic strain). The evolution of the essential internal state follows by the application of Biot's principle to $\dot{\Psi}_M + \Delta_M$, where minimization is now with respect to $\dot{z}_{ess}$.

Successful application of this structure has been made to finite deformation viscoelasticity within the framework of Miehe's microsphere model, including comparisons to experimental data. The structure described has also been successfully applied to one- and two-dimensional problems in elasto-perfectly-plastic composites, where reference solutions, used to check the homogenized results, have been constructed using converged finite element simulations.

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Small angle grain boundaries and Cosserath structures

Stephan Luckhaus

(joint work with Gianluca Lauteri)

The physical problem is to describe dislocation structures in metals after the annealing in the (industrial) hardening process. Here we give an explanation via energy bounds (from below) in terms of the total curl of a (strain) matrix field. More precisely, we use the following model of the energy (free energy) of a strain field A with dislocations

$$E_\epsilon(A) = \mathrm{Vol}(\{x|\ \mathrm{dist}(x, \mathrm{spt}(\mathrm{curl}A)) < \epsilon\}) + \int \mathrm{dist}(A, SO(n))^2.$$

The estimates we want to prove are

$$\epsilon \left| \int \psi \mathrm{curl} A \right| < c|\psi|_{C_0^1(\Omega)} \left[E_\epsilon(A)^{1+\delta} + \left| \ln \left(\frac{E_\epsilon(A)}{\mathrm{diam}(\Omega)^{\frac{1}{d-1}} \epsilon} \right) \right|^{-\beta} \int_\Omega \mathrm{dist}(A, SO(n))^2 \right],$$

where δ is small positive, $\|A\|_\infty$ is bounded, β is in general $\frac{1}{2}$, if the winding number

$$\int_\gamma A\dot{\gamma} \notin (0, \tau\epsilon)\ \forall\gamma \cap \mathrm{spt}(\mathrm{curl}A) = \emptyset,\ \tau = O(1)$$

is quantized, then $\beta = 1$.

These estimates from below are of the same order as the Reid-Shockley formula for the energy of a small angle grain boundary. As an immediate consequence we have: If A_ϵ are such that $E_\epsilon(A_\epsilon) < \text{const}\ \epsilon$, then wlog

$$A_\epsilon \overset{L^1}{\to} A,\ A = \sum_{\mathbb{N}} \chi_i R_i,\ R_i \in SO(n),\ \chi_i = \chi_{M_i},\ \|\nabla\chi_{M_i}\|_{L^1} < \infty,$$

i.e. A_ϵ is close to a piecewise constant field of rotations – a Cosserath structure, as we call it.

The case of $n = 2$ is published on arXiv [1]. The proof of $n = 3$ is so far restricted to the non-quantized version and has still to be checked again.

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A variational material model for the cyclic behavior of polycrystalline shape memory alloys

Johanna Waimann

(joint work with Philipp Junker, Klaus Hackl)

The material behavior of shape memory alloys is characterized by a transformation between an austenitic and several martensitic phases. Cyclic loading is accompanied by a formation of dislocations which stabilize an amount of the martensitic phases. This irreversible process results in the effect of functional fatigue which is characterized by a decrease of the stress plateaus and an increasing remaining strain in the stress/strain diagram as presented in Figure 1 for a cycled tension test, see e.g. [3] and [4].

The irreversible processes during cycling are considered by coupling the reversible transformation with a stabilization of martensite. The microstructural evolutions are described by use of a reversible volume fraction of the individual phases $\boldsymbol{\lambda}$ and corresponding irreversible martensitic volume fractions $\boldsymbol{\rho}$. The polycrystalline structure is taken into account by an evolving set of Euler angles $\boldsymbol{\alpha} = \{\varphi, \vartheta, \omega\}$ which describes the averaged orientation of the transforming grains, see [2]. The evolution equations for the internal variables $\boldsymbol{\lambda}$, $\boldsymbol{\rho}$ and $\boldsymbol{\alpha}$ are derived by use of the principle of the minimum of the dissipation potential, see [1]. It is

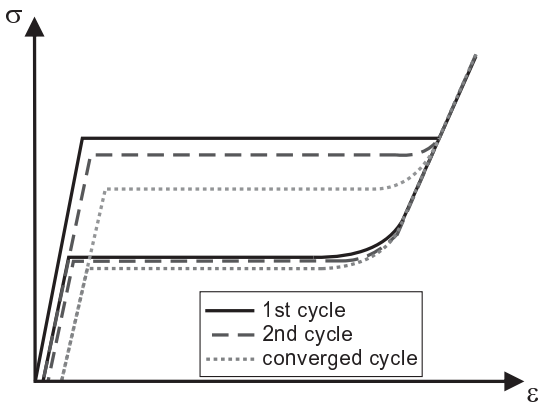

FIGURE 1. Schematic stress/strain diagram of a cycled tension test, see [4].

based on the idea of minimizing a Lagrange functional with respect to the internal variables' rates and thus, reads for the examined problem

$$\mathcal{L} = \dot{\Psi}\left(\boldsymbol{\varepsilon}, \theta, \boldsymbol{\alpha}, \boldsymbol{\lambda}, \boldsymbol{\rho}\right) + \mathcal{D}\left(\boldsymbol{\lambda}, \boldsymbol{\rho}, \dot{\boldsymbol{\alpha}}, \dot{\boldsymbol{\lambda}}, \dot{\boldsymbol{\rho}}\right) + \text{cons} \quad \rightarrow \underset{\dot{\boldsymbol{\alpha}}, \dot{\boldsymbol{\rho}}, \dot{\boldsymbol{\lambda}}}{\text{stat}} \quad . \tag{1}$$

The first part in (1) is the rate of the Helmholtz free energy which is described in terms of the strain $\boldsymbol{\varepsilon}$, the temperature θ and the internal variables. By use of a Reuss-bound, it has the form

$$\Psi = \frac{1}{2}\left(\boldsymbol{\varepsilon} - \boldsymbol{Q}^{\mathrm{T}} \cdot \bar{\boldsymbol{\eta}} \cdot \boldsymbol{Q} - \boldsymbol{Q}^{\mathrm{T}} \cdot \bar{\boldsymbol{\upsilon}} \cdot \boldsymbol{Q}\right) : \bar{\mathbb{E}} : \left(\boldsymbol{\varepsilon} - \boldsymbol{Q}^{\mathrm{T}} \cdot \bar{\boldsymbol{\eta}} \cdot \boldsymbol{Q} - \boldsymbol{Q}^{\mathrm{T}} \cdot \bar{\boldsymbol{\upsilon}} \cdot \boldsymbol{Q}\right) + \bar{c} \tag{2}$$

with the rotation tensor $\boldsymbol{Q} = \boldsymbol{Q}(\boldsymbol{\alpha})$ and the effective values for the reversible and irreversible transformation strains, $\bar{\boldsymbol{\eta}}$ and $\bar{\boldsymbol{\upsilon}}$, the stiffness $\bar{\mathbb{E}}$ and the caloric energy $\bar{c}$. The effective quantities are calculated by

(3)

$$\bar{\boldsymbol{\eta}} = \sum_{i=0}^{n} \lambda_i \boldsymbol{\eta}_i, \; \bar{\boldsymbol{\upsilon}} = \sum_{i=0}^{n} \rho_i \boldsymbol{\eta}_i, \; \bar{\mathbb{E}} = \left[\sum_{i=0}^{n} \left(\lambda_i + \rho_i\right) \left(\mathbb{E}_i\right)^{-1}\right]^{-1}, \; \bar{c} = \sum_{i=0}^{n} \left(\lambda_i + \rho_i\right) c_i \; .$$

The second part in the Lagrangean (1) is the dissipation function $\mathcal{D}$. It describes the energy which dissipates due to the microstructural change. We choose a rate-independent coupled ansatz for the reversible and irreversible phase transformation and a rate-dependent form for the evolution of the Euler angles:

$$\mathcal{D} = r_{\mathrm{T}} \sqrt{\sum_{i=0}^{n} \left(f \dot{\lambda}_i\right)^2 + \sum_{i=0}^{n} \left(g \dot{\rho}_i\right)^2} + \frac{\sqrt{2}\, r_{\mathrm{R}}}{2} \left(\dot{\varphi}^2 + \dot{\vartheta}^2 + 2\dot{\varphi}\dot{\omega}\cos\vartheta + \dot{\omega}^2\right) \tag{4}$$

with the dissipation parameter r_{T} and the viscous parameter r_{R}. The factor g accounts for the different amount of energy which is necessary to form irreversible martensite instead of reversible phases. The factor f can be calculated by

$$f = \begin{cases} \left(1.0 - f_1 \sum_{i=0}^{n} \rho_i\right) & \mathrm{A} \rightarrow \mathrm{M} \\ \left(1.0 + f_2 \sum_{i=0}^{n} \rho_i\right) & \mathrm{M} \rightarrow \mathrm{A} \end{cases} \tag{5}$$

and favors the transformation from austenite to martensite and delays the reverse transformation with increasing $\boldsymbol{\rho}$ as experimentally observed.

The third part in the Lagrange function (1) cons considers constraints – namely the non-negativity of the volume fractions, mass conservation, the irreversibility of $\boldsymbol{\rho}$ and a maximum value for the total irreversible volume fraction $\rho_{\max}$. The minimization of the Lagrange function directly results in evolution equations for the internal variables. A more detailed description of the material model as well as an experimentally based calibration of the model parameters can be found in [5].

Subsequently, the material model is implemented within a finite-element framework. In Figure 2 the force/displacement diagram of a cyclic loaded plate with a hole is presented which shows the experimentally observed decrease of the plateau stresses and formation of a remaining strain during cycling. The contour plot of

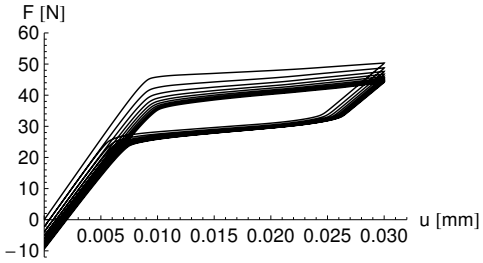

FIGURE 2. Force/displacement diagram of a cyclic loaded plate with a hole.

the austenitic volume fraction λ_0 in Figure 3 for the maximum load in the last load cycle shows a localized arc-like martensitic structure. Consequently, the total irreversible martensite $\bar{\rho}$ forms in the same areas as presented in Figure 4 after cycling. The simulations on the finite-element level show the model's ability to predict the effect of functional fatigue.

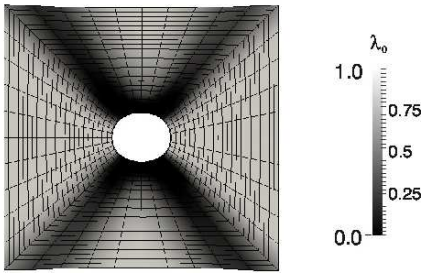

FIGURE 3. Austenitic volume fraction at maximum load in the last load cycle.

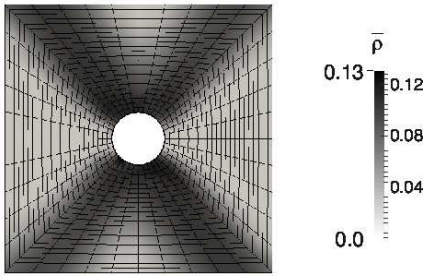

FIGURE 4. Total irreversible martensitic volume fraction after cycling.

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Some results on ferromagnetic spin systems and related results

Leonard Kreutz

(joint work with Andrea Braides, Antonin Chambolle)

The optimization of the design of structures can sometimes be viewed as a minimization or maximization problem of a cost or compliance subjected to design constraints. A typical example is shape optimization for given loads of conducting or elastic structures composed of a prescribed amounts of a certain number of materials. In that case the existence of an optimal shape is not guaranteed, and a relaxed formulation must be introduced that takes into account the possibility of fine mixtures. The homogenization method can be regarded as subdividing the problem into the description of all possible materials obtained as mixtures, and subsequently optimize in the enlarged class of homogenized materials that satisfy the corresponding relaxed design constraint.

In this talk we consider the problem of describing the overall properties of mixtures of two types of nearest-neighbour interactions; i.e., of characterizing the continuum limits of Ising systems of the form

$$\sum_{<i,j>} c_{i,j}(u_i - u_j)^2,$$

where $u_i \in \{-1, +1\}$, $< i, j >$ denotes all nearest neighbours in a square lattice and the 'bonds' $c_{i,j}$ are periodic coefficients, that may take only two positive values α and β with

$$\alpha < \beta.$$

The identification of the continuum limit is done by a discrete-to-continuum convergence method using the tool of Γ-convergence. A representation theorem shows that the limiting energy can be represented by an integral functional of the form

$$\int_{\partial^*\{u=1\}} \varphi(x, \nu_u(x)) \mathrm{d}\mathcal{H}^1$$

defined on the 'magnetization' parameter $u \in BV_{\mathrm{loc}}(\mathbb{R}^2\{-1,+1\})$, which is a continuum counterpart of the spin variable.

Under the assumption that the bonds are periodic we give a precise description of all the homogenized surface energy densities that may obtained in this way, using the volume fraction θ of β-bonds. This set is denoted by $\mathcal{H}(\theta)$. We show that, with fixed θ, all possible such φ are the (even positively homogeneous of degree one) convex functions such that

$$\alpha(|\nu_1| + |\nu_2|) \leq \varphi(\nu) \leq c_1|\nu_1| + c_2|\nu_2|, \text{ for all } \nu \in \mathbb{S}^1$$

for some c_1 and c_2, where the coefficients c_1 and c_1 satisfy

$$\alpha \leq c_1, c_2 \leq \beta, \quad c_1 + c_2 = 2(\beta\theta + (1-\theta)\alpha).$$

On the other hand we show that the homogenized energy density of a spin system with bonds, that have a fixed period, is always of crystalline type, i.e. it is the support function of a convex polyhedron, whose number of extreme points depends on the period of the bonds.

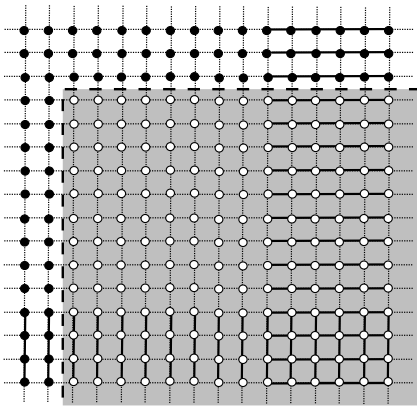

FIGURE 1. A periodicity cell giving the lower bound

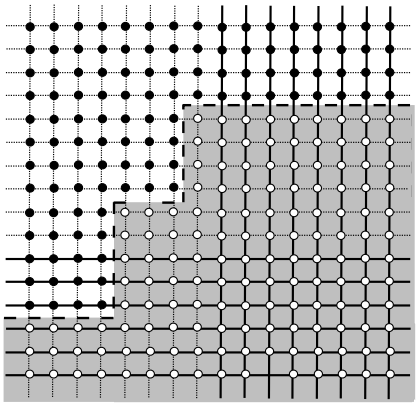

FIGURE 2. A periodicity cell giving the upper bound

We describe the 'extreme' geometries as shown in Fig. 1 and Fig. 2, where α-connections are represented as dotted lines, β-connections are represented as solid lines, and the nodes with the value $+1$ or -1 as white circles or black circles, respectively. In Fig. 1 there are pictured the periodicity cell of a mixture giving as a result the lower bound $\alpha(|\nu_1| + |\nu_2|)$ and an interface with minimal energy. Fig. 2 represents the periodicity cell of a mixture giving a upper bound of the form $c_1|\nu_1| + c_2|\nu_2|$. Note that the interface pictured in that figure crosses exactly a number of bonds proportional to the percentage θ_v of β-bonds in the horizontal direction.

It must be noted that, contrary to the elastic case, the bounds (i.e., the sets of possible φ) are increasing with θ, and in particular they always contain the minimal surface tension $\alpha(|\nu_1| + |\nu_2|)$, which can be achieved with an arbitrarily small amount of α-bonds.

We then prove a localization principle, similar to the one for quadratic gradient energies in the Sobolev space setting stated by Dal Maso and Kohn. In our case, this amounts to proving that all φ that we may obtain are exactly those such that, upon suitably choosing their representative,

$$\varphi(x, \cdot) \in \mathcal{H}(\theta(x))$$

for almost all x.

Finally we show that the results presented before can be applied to weak membrane energies of the form

$$\sum_{<i,j>} \varepsilon^2 W_\varepsilon^{i,j} \left(\frac{|u_i - u_j|}{\varepsilon} \right),$$

where $\varepsilon \to 0$ is the lattice spacing, $W_\varepsilon^{i,j}(z) = z^2 \wedge (\varepsilon^{-1} c_{i,j})$ and $u : \varepsilon\mathbb{Z}^2 \to \mathbb{R}$. We prove that the Γ-limit of the above functionals is of the form

$$\int f(x, \nabla u) \mathrm{d}x + \int_{S(u)} \varphi(x, \nu_u(x)) \mathrm{d}\mathcal{H}^1,$$

defined for functions $u \in GSBV^2_{\mathrm{loc}}(\mathbb{R}^2)$ and f is a function described by an asymptotic cell formula of suitable elastic energies, while φ coincides with the surface energy density for the spin systems above.

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Slip-stick motion via a wiggly energy model and relaxed EDP-convergence

Thomas Frenzel
(joint work with Patrick Dondl, Alexander Mielke)

We study the convergence of solutions to an evolution equation $\dot{u}_\varepsilon = \mathcal{A}_\varepsilon(u_\varepsilon)$ in the context of gradient flows, i.e, the gradient system $(\mathbb{X}, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)$ induces the flow for $\mathcal{A}_\varepsilon(u) = \partial\mathcal{R}_\varepsilon^*\big(-\mathrm{D}\mathcal{E}_\varepsilon(t,u)\big)$ where $\mathbb{X}$ is the state space, $\mathcal{E}_\varepsilon : [0,T]\times\mathbb{X} \longrightarrow \mathbb{R}\cup\{\infty\}$ is the energy and $\mathcal{R}_\varepsilon : \mathbb{X}\times\mathbb{X} \longrightarrow [0,\infty]$ is the dissipation potential.

In the limit as $\varepsilon \searrow 0$ we want to derive the limiting gradient system $(\mathbb{X}, \mathcal{E}_0, \mathcal{R}_{\mathrm{eff}})$ such that u_0, the limit of u_ε, is the solution to the gradient flow induced by the limiting gradient system. There exists already a body of literature [1, 2, 3] that investigates how to pass to the limit $(\mathbb{X}, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon) \rightsquigarrow (\mathbb{X}, \mathcal{E}_0, \mathcal{R}_{\mathrm{eff}})$.

We introduce the notion of relaxed EDP-convergence that determines $\mathcal{R}_{\mathrm{eff}}$ uniquely. We study the wiggly energy model proposed by [4] and give an explicit relation between $\mathcal{R}_\varepsilon$ and $\mathcal{R}_{\mathrm{eff}}$. The equation is given by

$$\nu\dot{u}(t) = -u + \ell(t) - \kappa'\Big(\frac{u}{\varepsilon}\Big), \quad u(0) = u_0 \tag{1}$$

where $u(t) \in \mathbb{R}$. The energy and dissipation potential are given by

$$\mathcal{E}_\varepsilon(t,u) = \frac{1}{2}u^2 - \ell(t)u + \varepsilon\kappa\Big(\frac{u}{\varepsilon}\Big) \qquad \text{and} \qquad \mathcal{R}(v) = \frac{\nu}{2}v^2$$

The notion of relaxed EDP-convergence is based on a reformulation of (1) as the energy dissipation balance (EDB)

$$\mathcal{E}_\varepsilon\big(T, u(T)\big) + \mathfrak{D}_\varepsilon\big(u(\cdot)\big) \le \mathcal{E}_\varepsilon(0,u_0) + \int_0^T \partial_t\mathcal{E}_\varepsilon(t,u)\,\mathrm{d}t \tag{EDB$_\varepsilon$}$$

where the total dissipation functional is given by

$$\mathfrak{D}_\varepsilon\big(u(\cdot)\big) = \int_0^T \mathcal{R}(\dot{u}) + \mathcal{R}^*\big(-\mathrm{D}\mathcal{E}_\varepsilon(t,u)\big)\,\mathrm{d}t.$$

In order to pass to the limit, we compute the Γ-limits of $\mathcal{E}_\varepsilon$ in the static state space $\mathbb{R}$ and of $\mathfrak{D}_\varepsilon$ in the dynamic space $\mathrm{H}^1(0,T;\mathbb{R})$. However, it is a result of [5], that $\mathfrak{D}_0 := \Gamma\text{-}\lim \mathfrak{D}_\varepsilon$ is not of the (Ψ,Ψ^*)-form, i.e.,

$$\mathfrak{D}_0\big(u(\cdot)\big) \neq \int_0^T \Psi(\dot{u}) + \Psi^*\big(-\mathrm{D}\mathcal{E}_0(t,u)\big)\,\mathrm{d}t$$

for any Ψ.

However, we have relaxed EDP-convergence and hence, we obtain a uniquely determined $\mathcal{R}_{\mathrm{eff}}$ such that the limit evolution is described by the gradient system $(\mathbb{R}, \mathcal{E}_0, \mathcal{R}_{\mathrm{eff}})$. This means for $\Phi_\varepsilon(u) := \mathcal{E}_\varepsilon(t,u) + \ell(t)u$ we have Γ-convergence of

$$\mathfrak{J}_\varepsilon(u,\xi) = \int_0^T \mathcal{R}(\dot{u}) + \mathcal{R}^*\big(-\mathrm{D}\Phi_\varepsilon(u) + \xi\big)\,\mathrm{d}t$$

with respect to weak convergence of u_ε in $\mathrm{W}^{1,2}(0,T;\mathbb{R})$ and, in duality, strong convergence of ξ_ε in $\mathrm{L}^2(0,T;\mathbb{R})$ with a Γ-limit of the form

$$\mathfrak{J}_0(u,\xi) = \int_0^T \mathcal{N}(u,\dot{u},\xi)\ \mathrm{d}t$$

and $\mathcal{N}$ satisfies (2).

Indeed, for the wiggly energy model we have for $\mathcal{M}(v,\eta) = \mathcal{N}\big(u,v,\eta+\mathrm{D}\Phi_0(u)\big)$

$$\mathcal{M}(v,\eta) := \inf_{z\in \mathrm{W}^{1,2}_v} \left\{ \int_0^1 \left[\mathcal{R}(|v|\dot{z}(s)) + \mathcal{R}^*\big(\eta - \kappa'(z(s))\big)\right]\ \mathrm{d}s \right\}$$

where $\mathrm{W}^{1,2}_v = \big\{v \in \mathrm{W}^{1,2}(0,1) :\ z(1) = z(0)+\mathrm{sign}(v)\big\}$. We still have, as for the pair (Ψ,Ψ^*), that $\mathcal{M}(v,\eta) \geq \eta v$ which implies by virtue of the limiting (EDB_0) that the limit evolution satisfies

$$\big(\dot{u}(t), -\mathrm{D}\mathcal{E}_0(t,u(t))\big) \in \mathrm{C}_{\mathcal{M}} := \{(v,\xi)\in\mathbb{R}\times\mathbb{R} :\ \mathcal{M}(v,\eta) = \eta v\}.$$

Characterizing the contact set $\mathrm{C}_{\mathcal{M}}$ we find the kinetic relation

$$(v,\eta)\in \mathrm{C}_{\mathcal{M}} \Longleftrightarrow v = \begin{cases} 0 & \text{if } \eta \in \mathrm{Range}(\kappa') \\ \left(\int_0^1 \Big(\partial\mathcal{R}^*\big(\eta-\kappa'(z)\big)\Big)^{-1}\mathrm{d}z\right)^{-1} & \text{if } \eta \notin \mathrm{Range}(\kappa') \end{cases}$$

which defines the effective dual dissipation potential via the relation

$$\mathrm{C}_{\mathcal{M}} = \{(v,\xi) : v \in \partial\mathcal{R}_{\mathrm{eff}}(\xi)\}. \tag{2}$$

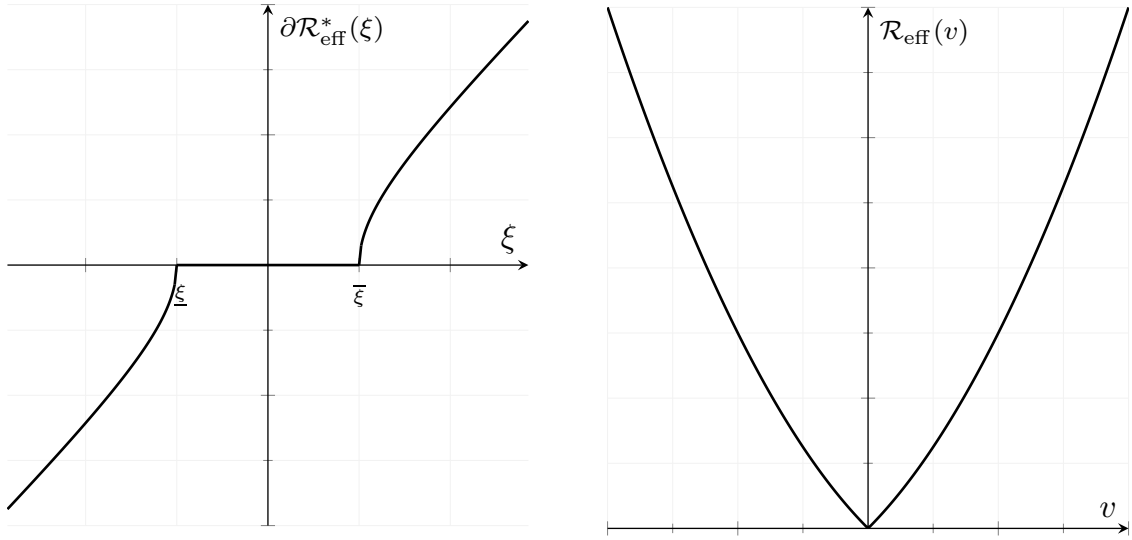

FIGURE 1. Kinetic relation defining the (subdifferential of the) effective dual dissipation potential (left) and the effective primal dissipation potential (right).

Hence the wiggly energy model leads to an effective dissipation potential that is not given as a (Γ-) limit of the dissipation potential for the ε-model. However,

the notion of relaxed EDP-convergence gives an explicit relation between $\mathcal{R}$ and $\mathcal{R}_{\text{eff}}$ and determine the latter uniquely.

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Strain-Gradient Plasticity as the Γ-limit of an Energy for Edge Dislocations without the Assumption of Well-Separateness

Janusz Ginster

Crystal plasticity is the effect of a crystal undergoing an irreversible change of shape in response to applied forces. At the atomic scale, dislocations — which are local defects of the crystalline structure — are considered to play a main role in this effect. We focus on the case of a body with an infinite cylindrical symmetry and straight parallel dislocation lines of edge type. By considering an orthogonal plane and the corresponding in-plane strains, we reduce the problem to a two-dimensional situation in which the dislocations only appear as point defects in a two-dimensional domain. We are then interested in understanding the behavior of the stored elastic energy in this plane.

We use a semi-discrete model to describe the dislocations and the strains, i.e. the set of admissible dislocation densities in the slice $\Omega \subset \mathbb{R}^2$ is given by

$$X = \left\{ \mu \in \mathcal{M}(\Omega;\mathbb{R}^2) : \mu = \sum_{k=1}^{M} b_k \delta_{x_k}, M \in \mathbb{N}, b_k \in \mathbb{S}, x_k \in \Omega \right\}. \tag{1}$$

where $\mathbb{S}$ is a discrete lattice of (renormalized) Burgers vectors. In the continuum theory of dislocations the elastic strain $\beta : \Omega \to \mathbb{R}^{2\times 2}$ satisfies the equation $\operatorname{curl} \beta = \mu$ for an admissible dislocation measure. It is well-known that this constraint is not compatible with a finite elastic energy which grows quadratically in the strains. Hence, we regularize the constraint and define the set of admissible strains as

follows

$$\mathcal{AS}_\varepsilon(\mu) = \Big\{ \beta \in L^2(\Omega;\mathbb{R}^{2\times 2}) : \beta = 0 \text{ in } B_\varepsilon(\mathrm{supp}(\mu)),\ \mathrm{curl}\,\beta = 0 \text{ in } \Omega \setminus B_\varepsilon(\mu),$$
$$\text{and for every smoothly bounded open set } A \subseteq \Omega \text{ such that}$$
$$\partial A \subseteq \Omega \setminus B_\varepsilon(\mathrm{supp}(\mu)) \text{ it holds } \int_{\partial A} \beta \cdot \tau \, d\mathcal{H}^1 = \mu(A) \Big\}.$$

The stored elastic energy is then defined to be

$$F_\varepsilon(\mu,\beta) = \begin{cases} \int_\Omega \frac{1}{2}\mathcal{C}\beta : \beta \, dx + |\mu|(\Omega) & \text{if } \mu \in X(\Omega) \text{ and } \beta \in \mathcal{AS}_\varepsilon(\mu), \\ +\infty & \text{else.} \end{cases}$$

Here, $\mathcal{C} \in \mathbb{R}^{2\times 2\times 2\times 2}$ is an elastic tensor, i.e. it is positive definite on symmetric matrices. The term $|\mu|(\Omega)$ accounts for the energy stored inside the dislocation cores. Similar models have been considered in [1, 2, 5, 6, 7, 8]. The main difference to existing literature is that we do *not* assume the well-separateness of dislocations, i.e. we do not assume that two different dislocations are separated on a scale which is much larger than ε.

Heuristically, the two major contributions to the energy are the self-energy of the dislocations and the elastic interactions of the dislocations. The self-energy is concentrated in discs around the dislocations which shrink to zero as $\varepsilon \to 0$ but are asymptotically much larger than ε. We consider the regime in which both contributions are of the same order. This is the case for $\sim |\log\varepsilon|$ dislocations. The energy is of order $|\log\varepsilon|^2$. Other regimes have been considered in [5, 8].
We prove a Γ-convergence result for the rescaled energy $\frac{1}{|\log\varepsilon|^2}F_\varepsilon$. The toplogy will be the following. We say that $(\mu_\varepsilon,\beta_\varepsilon) \subseteq \mathcal{M}(\Omega;\mathbb{R}^2)\times L^2(\Omega;\mathbb{R}^{2\times 2})$ convergences to (μ,β) if

$$\frac{\beta_\varepsilon}{|\log\varepsilon|} \rightharpoonup \beta \text{ in } L^2(\Omega;\mathbb{R}^{2\times 2}) \text{ and } \frac{\mu_\varepsilon}{|\log\varepsilon|} \to \mu \text{ in } \left(W_0^{1,\infty}(\Omega;\mathbb{R}^2)\right)^*.$$

Note that the convergence for the dislocation measures allows for annihilation of large clusters of dipoles in the limit.
We show that as a Γ-limit we find a strain gradient plasticity model, see, for example, [3] and references therein.

Theorem 1. *It holds*

$$F_\varepsilon \xrightarrow{\Gamma} F,$$

where $F : \mathcal{M}(\Omega;\mathbb{R}^2)\times L^2(\Omega;\mathbb{R}^{2\times 2}) \to [0,\infty]$ *is defined by*

$$F(\mu,\beta) = \begin{cases} \int_\Omega \frac{1}{2}\mathcal{C}\beta : \beta \, dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu| & \text{if } \mu \in \mathcal{M}(\Omega;\mathbb{R}^2) \cap H^{-1}(\Omega;\mathbb{R}^2), \\ & \beta \in L^2(\Omega;\mathbb{R}^{2\times 2}), \text{ and } \mathrm{curl}\,\beta = \mu, \\ +\infty & \text{else.} \end{cases}$$

The function φ *is* 1*-homogeneous and subadditive. It can be given via a relaxed cell formula.*

In order to prove a complementing compactness result for the rescaled strains $\frac{\beta_\varepsilon}{|\log\varepsilon|}$, we use Korn's inequality for incompatible fields which was proved in [5],

$$\int_\Omega \left|\frac{\beta_\varepsilon - W_\varepsilon}{|\log\varepsilon|}\right|^2 dx \le C\left(\int_\Omega \left|\frac{(\beta_\varepsilon)_{sym}}{|\log\varepsilon|}\right|^2 dx + \frac{1}{|\log\varepsilon|^2}|\operatorname{curl}\beta_\varepsilon|(\Omega)^2\right)$$

for some $W_\varepsilon \in Skew(2)$. The first term on the right hand side can easily be bounded by the rescaled energy. If one additionally assumes the well-separateness of dislocations, one can also control the second term on the right hand side using the self-energy of the dislocations. In our case this is not possible as we cannot compute the self-energy for the different dislocations individually since the different dislocations are not assumed to be separated on the relevant scale. Instead, one might hope to find good clusters of dislocations such that

$$|\log\varepsilon| \sum_{\text{clusters } C} |\mu(C)| \le F_\varepsilon(\mu,\beta). \tag{2}$$

In a second step, the strains could then be modified in a way such that the above inequality can be used for its curl.

We find good clusters of dislocations which satisfy the inequality (2) by using a modified version of the ball-construction technique, which was developed in the context of the Ginzburg-Landau energy, see [4, 9], and already successfully applied in the subcritical regime with only finitely many dislocations, see [2]. The main difficulty in our situation is that during the construction we need to avoid thin structures on which a massive loss of rigidity could prevent uniform lower bounds. We show how a combination of a modified discrete ball-construction and combinatorical arguments bounding the numbers of bad clusters lead to uniform lower bounds.

The resulting compactness result is

Theorem 2. *Let $\Omega \subseteq \mathbb{R}^2$ a connected, bounded Lipschitz domain. Let $(\mu_\varepsilon,\beta_\varepsilon) \in X \times \mathcal{AS}_\varepsilon(\mu_\varepsilon)$ such that $\sup_\varepsilon \frac{1}{|\log\varepsilon|^2}F_\varepsilon(\mu_\varepsilon,\beta_\varepsilon) < \infty$. Then there exist $\beta \in L^2(\Omega;\mathbb{R}^{2\times 2})$, $\mu \in \mathcal{M}(\Omega;\mathbb{R}^2) \cap H^{-1}(\Omega;\mathbb{R}^2)$, and $W_\varepsilon \in Skew(2)$ such that for a subsequence it holds*

1. *$\frac{\mu_\varepsilon}{|\log\varepsilon|} \to \mu$ in $\left(W_0^{1,\infty}(\Omega;\mathbb{R}^2)\right)^*$ and $\frac{(\beta_\varepsilon)_{sym}}{|\log\varepsilon|} \rightharpoonup \beta_{sym}$ in $L^2(\Omega;\mathbb{R}^{2\times 2})$,*
2. *for all $1 > \gamma > 0$ and $U \subset\subset \Omega$ we have $\frac{\beta_\varepsilon - W_\varepsilon}{|\log\varepsilon|}\mathbf{1}_{\Omega\setminus B_{\varepsilon^\gamma}(\mu_\varepsilon)} \rightharpoonup \beta$ in $L^2(U;\mathbb{R}^{2\times 2})$,*
3. *$\operatorname{curl}\beta = \mu$.*

Moreover,

$$\liminf_{\varepsilon\to 0} F_\varepsilon(\mu_\varepsilon,\beta_\varepsilon) \ge \int_\Omega \mathcal{C}\beta : \beta\, dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu|.$$

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Gamma-convergence and stochastic homogenisation of free-discontinuity problems

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(joint work with Filippo Cagnetti, Lucia Scardia, and Caterina Ida Zeppieri)

In [2] we consider a sequence of free-discontinuity functionals of the form

$$\mathcal{E}_k(u,A) := \int_{A\setminus J_u} f_k(x,\nabla u)dx + \int_{A\cap J_u} g_k(x,[u],\nu_u)d\mathcal{H}^{n-1},$$

where $A \subset \mathbb{R}^n$ is a bounded open set, $u\colon A \to \mathbb{R}^m$ is a function, J_u is its jump set, $[u] := u^+ - u^-$ is the amplitude of the jump of u, and ν_u is a unit normal to J_u.

Under suitable assumptions on the sequences (f_k) and (g_k), we prove that there exist a subsequence, not relabelled, and a functional $\mathcal{E}$ of the form

$$\mathcal{E}(u,A) := \int_{A\setminus J_u} f(x,\nabla u)dx + \int_{A\cap J_u} g(x,[u],\nu_u)d\mathcal{H}^{n-1},$$

such that $\mathcal{E}_k(\cdot,A)$ Γ-converges to $\mathcal{E}(\cdot,A)$ for every bounded open set $A \subset \mathbb{R}^n$.

Moreover, we prove that the integrands $f(x,\xi)$ and $g(x,\zeta,\nu)$ of the limit functional can be obtained by considering the minimum values of the functionals

$$\frac{1}{\rho^n}\int_{Q_\rho(x)} f_k(y,\nabla u)dy \qquad \text{and} \qquad \frac{1}{\rho^{n-1}}\int_{Q^\nu_\rho(x)\cap J_u} g_k(y,[u],\nu_u)d\mathcal{H}^{n-1}$$

with simple boundary conditions on suitable cubes centred at x with side length ρ. For the former the boundary condition is $u(y) = \xi y$ for $y \in \partial Q_\rho(x)$, while for the latter it is $u(y) = 0$ on $\partial^- Q^\nu_\rho(x)$ and $u(y) = \zeta$ on $\partial^+ Q^\nu_\rho(x)$, where

$$\partial^\pm Q^\nu_\rho(x) := \{y \in \partial Q^\nu_\rho(x) : \pm(y-x)\cdot\nu > 0\}.$$

The values of $f(x,\xi)$ and $g(x,\zeta,\nu)$ are obtained by taking the limit first as $k \to +\infty$ and then as $\rho \to 0+$.

After a change of variables, this allows us to use the subadditive ergodic theorem [1] in order to prove the almost sure Γ-convergence, as $\varepsilon \to 0+$, of the sequence

$$\mathcal{E}_\varepsilon(u,A) := \int_{A\setminus J_u} f(\frac{x}{\varepsilon}, \nabla u)dx + \int_{A\cap J_u} g(\frac{x}{\varepsilon}, [u], \nu_u)d\mathcal{H}^{n-1},$$

where f and g are stationary random integrands (see [3]).

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Deformation-diffusion coupled computational model for hydrogen diffusion in nanomaterials

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(joint work with Xingsheng Sun, Michael Ortiz, Kevin G. Wang)

Understanding the transport of hydrogen within metallic nanomaterials is crucial for the advancement of energy storage and the mitigation of hydrogen embrittlement. Using nanosized palladium particles as a model, recent experimental studies have revealed several highly nonlinear phenomena that occur over long time periods. The time scale of these phenomena is beyond the capability of established atomistic models such as molecular dynamics. In this work, we present a new approach, referred to as diffusive molecular dynamics (DMD), to the simulation of long-term diffusive mass transport at the atomic scale. DMD is a class of recently developed computational models for the simulation of long-term diffusive mass transport at atomistic length scales. Compared to previous atomistic models, e. g., transition state theory based accelerated molecular dynamics, DMD allows the use of larger time-step sizes, but has a higher computational complexity at each time-step due to the need to solve a nonlinear optimization problem at every time-step.

The basic assumption underlying DMD is that the time scale of diffusion is much larger than that of microscopic state transitions. Therefore, at an intermediate time scale, the microscopic state variables — such as the instantaneous position and occupancy of a lattice site — can be considered as random variables. More recently, Li et al. [1] have extended DMD to handle diffusive mass transport by vacancy exchange and have applied it to study nanoindentation and sintering processes [1] and dislocation reaction mechanisms [2]. Venturini et al. [3, 4] have developed a general framework for diffusive molecular processes, including heat and mass transport. A recent theoretical review of DMD can be found in [5].

Following [3], in the present work we couple an empirical diffusion model, or *master equation*, driving the evolution of the mean value of atomic site occupancies, with a non-equilibrium statistical thermodynamics model that determines the mean value of atomic positions and atomic fractions by minimizing a grand-canonical free entropy. In terms of numerical implementation, our approach involves the numerical integration of the *master equation*, and the numerical solution of a highly nonlinear optimization problem at every time-step. By working with atomic fractions, the characteristic time-step size of our DMD simulations can be much larger than those based on either AMD and KMC methods, since we do not explicitly track the individual atom/vacancy hops. As a consequence, the time-step size in our calculations is not restricted by the frequency of those events. Instead, it is only limited by the diffusive time scale, e. g., by the speed of the propagation of a phase boundary, which can be as slow as 1 nm/s [6].

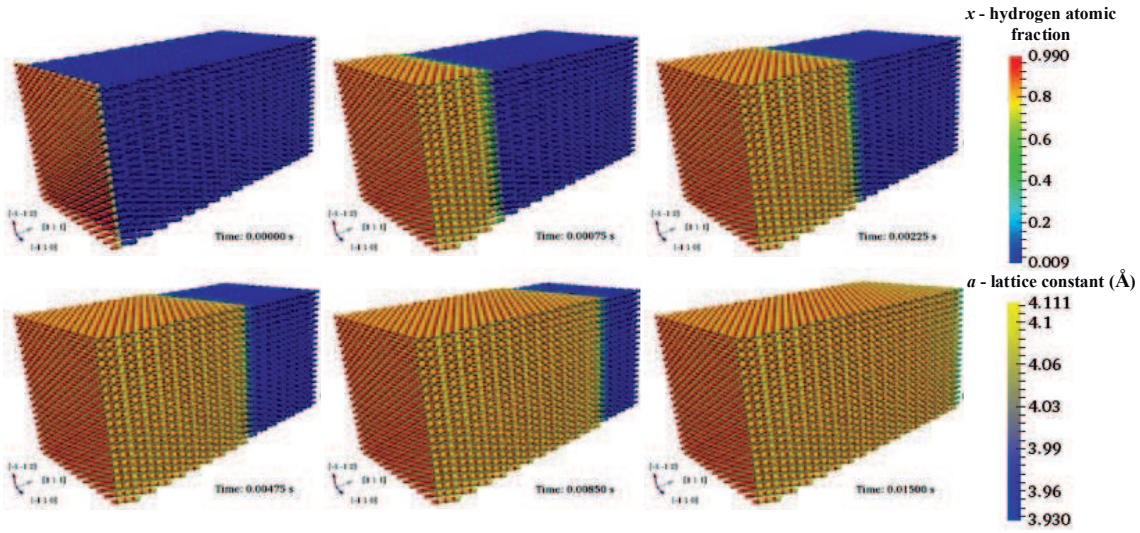

FIGURE 1. Deformation-diffusion coupled process of H absorption in Pd.

To assess the proposed DMD model, we take the palladium-hydrogen (Pd-H) system as an example, and simulate the diffusion of H atoms in Pd nanoparticles. The Pd-H system has broad impacts in several application areas, including hydrogen storage, purification filters, isotope separation, and fuel cells [7, 8]. At room temperature, Pd-H exhibits two distinct phases: the dilute α phase with low hydrogen concentration (up to $PdH_{0.015}$), and the β phase with high hydrogen concentration ($PdH_{0.6}$ and above). In both phases, the Pd sublattice maintains the face-centered cubic (FCC) structure, while the H atoms occupy the octahedral interstitial sites. Attendant to the α/β phase transformation, there is a lattice expansion within 10.4% increase in volume [9]. We adopt the EAM potential developed by Zhou and Zimmerman [10], which is capable of capturing the above fundamental features (Figures 1 and 2).

The ability of DMD to predict the propagation of atomically-sharp phase boundaries over a time window of more than 30 s with full atomistic realism is particularly

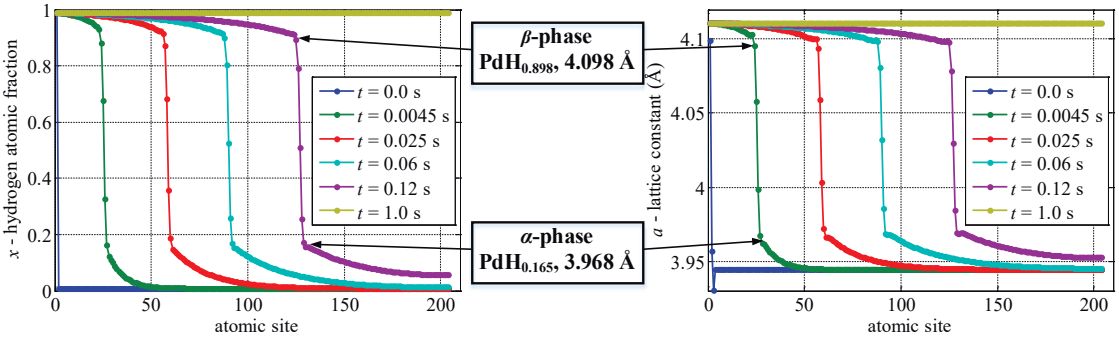

FIGURE 2. H absorption in 460 Pd nanofilms by the proposed model. (a) H atomic fraction. (b) Lattice constant.

noteworthy. We also note that the scope of DMD is not limited to metal hydrides and a broad range of multi-species systems of practical interest suggest themselves as worthwhile foci for future studies.

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Visco-plasticity with $|\mathrm{curl}(p)|^2$-term in the energy

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(joint work with Matthias Röger)

We present an existence result for a geometrically linear model of visco-plasticity. Denoting the deformation by u and decomposing the gradient into an elastic and a plastic part as $\nabla u = e + p$, the relevant energies are

$$\mathcal{W}_e(\nabla u, p) = \int_\Omega Q(\mathrm{sym}(\nabla u - p))\,, \tag{1}$$

$$\mathcal{W}_p(p) = \int_\Omega |\mathrm{curl}\, p|^2 + \delta |\nabla p|^2\,, \tag{2}$$

where Q is a convex, but not necessarily quadratic energy density function, $\delta \geq 0$ is a real parameter. The inclusion of the integral of $|\mathrm{curl}\, p|^2$ is motivated by the fact that $\mathrm{curl}\, p$ is a measure for the density of dislocation lines. Instead, the full gradient of p has no clear physical motivation, we are thus particularly interested in the case $\delta = 0$. We write the elastic energy density in the form $W_e(F,p) = Q(\mathrm{sym}(F-p))$ and the total energy as $\mathcal{W}(\nabla u, p) = \mathcal{W}_e(\nabla u, p) + \mathcal{W}_p(p)$. The two energies are accompanied by a dissipation rate functional $\mathcal{R}$ with convex dual $\mathcal{R}^*$.

In its strong form, the plastic evolution problem reads

$$-\nabla \cdot \sigma = f\,, \tag{3}$$

$$\sigma = \mathrm{sym}\ \nabla_F W_e(\nabla u, p)\,, \tag{4}$$

$$-\Sigma \in \partial_p \mathcal{W}(\nabla u, p)\,, \tag{5}$$

$$\partial_t p \in \partial \mathcal{R}^*(\Sigma)\,. \tag{6}$$

We note that the first two equations may also be written in a more compact form as $f \in \partial_u \mathcal{W}(\nabla u, p)$. The last two equations can be formulated as a Biot-law: $\partial \mathcal{R}(\partial_t p) = -\partial_p \mathcal{W}(\nabla u, p)$. We note that the back-stress variable Σ contains the contribution $\mathrm{curl}\,\mathrm{curl}\, p$.

The two main results of our contribution [1] concern the existence of solutions. The proof uses the standard approach: We consider a time-discrete version of the system. Existence for the time-discrete version is shown with the direct method of the calculus of variations. A priori estimates are obtained in energy spaces by a testing procedure in the time-discrete system. The most interesting step is the last one: One verifies that the weak limit of approximate solutions is a solution of the nonlinear system.

In order to show that a weak limit is a solution, it is important to introduce a weak solution concept. We use, essentially, the following: We demand that u, p and Σ are functions in space time with the properties $u \in L^2(0,T; H^1_D(\Omega;\mathbb{R}^3))$, $\Sigma \in L^2(0,T; L^2(\Omega;\mathbb{R}^{3\times 3}))$, $p, \partial_t p \in L^2(0,T; L^2(\Omega;\mathbb{R}^{3\times 3}))$. We demand the pointwise in time energy minimization

$$\int_\Omega W_e(\nabla u(t), p(t)) - \int_\Omega f(t)\cdot u(t) \leq \int_\Omega W_e(\nabla \varphi, p(t)) - \int_\Omega f(t)\cdot \varphi \tag{7}$$

for all $\varphi \in H^1_D(\Omega;\mathbb{R}^3)$, the back-stress equation

$$\mathcal{W}(\nabla u, p) + \mathcal{W}^*(\nabla u, -\Sigma) = \langle -\Sigma, p\rangle \ , \tag{8}$$

and the energy inequality

$$\begin{aligned}\Big[\mathcal{W}(\nabla u(s), p(s)) - \int_\Omega f(s)\cdot u(s)\Big]_{s=0}^t + \int_0^t \{\mathcal{R}(\partial_t p(s)) + \mathcal{R}^*(\Sigma(s))\}\, ds \\ \leq -\int_0^t \langle \partial_t f(s), u(s)\rangle\, ds\,.\end{aligned} \tag{9}$$

Indeed, we use an even more condensed system in [1]: Given p and f, we denote the minimal energy that can be acchieved by a deformation by

$$\mathcal{E}_1(p;f) := \inf\Big\{\mathcal{W}_e(\nabla\varphi, p) - \langle f,\varphi\rangle \Big| \ \varphi \in H^1_D(\Omega;\mathbb{R}^3)\Big\}\ , \tag{10}$$

$$\mathcal{E}(p;f) := \mathcal{E}_1(p;f) + \mathcal{W}_p(p)\,. \tag{11}$$

If we always assume that $u(t)$ is the deformation that realizes $\mathcal{E}(p;f)$ and denote the set of such deformations as $M(p,f)$, then the system of equations can be reduced to

$$\mathcal{E}\big(p;f\big) + \mathcal{E}^*\big(-\Sigma;f\big) = \langle -\Sigma, p\rangle \ . \tag{12}$$

and

$$\begin{aligned}\big[\mathcal{E}\big(p(s);f(s)\big)\big]_{s=0}^t + \int_0^t \{\mathcal{R}(\partial_t p(s)) + \mathcal{R}^*(\Sigma(s))\}\, ds \\ \leq -\int_0^t \inf_{\tilde u\in M(p(s),f(s))} \langle \partial_t f(s), \tilde u\rangle\, ds\,.\end{aligned} \tag{13}$$

The main result can be formulated as a stability property of this system. Loosely stated: If $\bar p^N$, $\hat p^N$, and $\bar\Sigma^N$ are approximate solutions (equation (12) is only satisfied up to a small error), and p, Σ are weak limits in energy norms of these functions, then (p,Σ) is a solution to (12) and (13).

The proof in the case $\delta > 0$ is quite standard, since compactness of the sequence $\hat p^N$ can be concluded from space- and time-regularity; we have indeed the strong convergence $\hat p^N \to p$ in $L^2(0,T;L^2(\Omega;\mathbb{R}^{3\times 3}))$. In consequence, by an abstract result on interpolations, one also has $\bar p^N \to p$. In this case, the limit in relation (12) can be formed directly because of weak lower semi-continuity of the left hand side and the convergence of the right hand side. In a second step one shows that, when $\bar u^N$ are minimizers for the approximate solutions, then the weak limit u of $\bar u^N$ is a minimizer for the limits. Exploiting also here the strong convergence of $\bar p^N$, the proof of this property is direct. Finally, taking limits in (13) is easy by weak lower semi-continuity. In this last step we exploit the reconstruction of minimizers from the second step to deal with the two sets of minimizers $\tilde u^N \in M(\bar p^N, f)$ and $\tilde u \in M(\bar p, f)$.

In the case $\delta = 0$, one does not have the strong convergence $\hat p^N \to p$. The proof must be based on the div-curl lemma and a Helmholtz decomposition. More precisely, the limit in relation (12) can be performed as before with the div-curl

lemma with the observation that the curl of $\bar{p}^N$ and the divergence of $\bar{\Sigma}^N$ are controlled. Forming the limit in (13) is done as before once the reconstruction property is shown. The reconstruction step is based on a Helmholtz decomposition from [2], which allows to construct, given an arbitrary comparison function φ, a sequence of comparison functions φ^N such that

$$\varphi^N \rightharpoonup \varphi \text{ in } L^2(0,T;H^1(\Omega;\mathbb{R}^3))\,, \tag{14}$$

$$\nabla\varphi^N - \bar{p}^N \to \nabla\varphi - p \text{ in } L^2(0,T;L^2(\Omega;\mathbb{R}^{3\times 3}))\,. \tag{15}$$

The energy depends only on the difference $\nabla\varphi^N - \bar{p}^N$, the strong convergence of this difference therefore allows to conclude the fact that u is an energy minimizer for p.

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