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Mini-Workshop: Scales in Plasticity

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Abstract. This mini-workshop was devoted to the current state of our understanding of dislocations (essentially slips of lines of atoms in a crystalline solid) and of their impact on the macroscopic behavior of those solids.

Mathematics Subject Classification (2010): Primary: 74 C15+C20, 49 J40+S05. Secondary: 35 J50, 74 K35+H35.

Introduction by the Organisers

The mini-workshop successfully brought together researchers with different expertise (experimentalists, engineers, theoretical mechanicians, applied mathematicians) working on plasticity. The main focus was on bridging the gap between the mesoscopic theory of what we would like to call the dislocation configuration and the macroscopic, mainly rate independent theory of plastic deformations. At the mesoscopic level, dislocations are viewed atomistically while the surrounding material is treated macroscopically as a purely elastic medium.

The range of topics that were discussed was extremely broad. In particular, the following topics were discussed:

- experimental results with accompanying detailed phenomenological laws;
- upscaling of dislocation walls;
- line tension models and iterated Gamma-convergence;
- differential geometric aspects of dislocations and disclinations;
- rate dependent dynamics of dislocations;
- gradient plasticity models and generalizations;
- dimensional reduction in small strain elasto-plasticity;

- plates with incompatible strains;
- structured deformations, among other themes.

Further, two discussion sessions were organized to confront viewpoints.

The input by the experimentalists in the group was extremely important. One of the outcomes of the discussion sessions was that there is still a large gap in our understanding of the "free energy" of neutral dislocation configurations, i.e., those with net Burgers vector zero. Another problem that emerged is the relationship between macroscopic hardening laws and the mesoscopic interaction of dislocations moving on a glide plane with the farthest dislocations transversal to the plane.
In a different direction, the presentations in the workshop showed the variety of expertise in the application of energetic methods (Γ-convergence and energy descent flows) in the context of linear elasticity with defects, as well as in that of nonlinear elasticity with defects.

In the nonlinear elastic context, the workshop brought forth the need to develop the connection between the PDE approach to nonlinear elasticity and the differential geometric description of the elastic strain field à la Kondo and Kröner.

The topic of large scale dislocation dynamics simulation was unfortunately not represented at this workshop. This should be another topic for a future workshop or mini-workshop on plasticity.

Generally speaking, the participants felt that the mini-workshop format with less than twenty researchers was particularly successful in promoting discussions and new interactions. The week was pleasantly enhanced by the magnificent weather that was kind enough to stay with us even during the traditional walk to Saint Roman.

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-1049268, "US Junior Oberwolfach Fellows".

Mini-Workshop: Scales in Plasticity

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Abstracts

Structured deformations, elasticity with disarrangements, and plasticity

David R. Owen

In this two-part talk, I summarize the background on the multiscale geometry of structured deformation that is needed in order to broaden sufficiently the field theory of finite elasticity so as to incorporate the effects both of non-smooth, submacroscopic geometrical changes (disarrangements) and of smooth submacroscopic geometrical changes. One of the key features of a structured deformation (g, G) is the ability to approximate the smooth, injective macroscopic deformation g and the continuous tensor field G (with $0 < \det G \leq \det \nabla g$) by a sequence of piecewise-smooth, injective deformations f_n that converge to g and whose classical gradients ∇f_n converge to G. A corollary to this Approximation Theorem shows that the difference $M = \nabla g - G = \nabla \lim_{n\to\infty} f_n - \lim_{n\to\infty} \nabla f_n$ is a volume density of jumps in the approximating deformations f_n, and this yields an additive decomposition $\nabla g = G + M$ in which both terms have definite geometrical meanings and definite transformation properties under changes in observer and changes in reference configuration. We are then justified in calling M the (volumetric) disarrangement density and G the deformation without disarrangements. Since G is invertible, this yields immediately two multiplicative representations $\nabla g = GM_r = M_l G$ in which each factor along with its transformation properties is precisely identified . The additive and multiplicative decompositions are purely geometrical and all are valid for finite deformations, and the latter provide a connection with the geometrical starting point of theories of plasticity. Further connections with the geometry of plastic deformation are noted through the identification of analogues in structured deformations of the Burgers vector and of the dislocation density common to theories of bodies with continuous distributions of dislocations.

The geometrical refinements associated with structured deformations in turn provide refinements for the stress field in any body, independent of its constitutive properties. In particular, the stress S in the reference configuration is shown to decompose additively and multiplicatively. The additive decomposition $(\det K)S = S_\backslash + S_d$ (with $K = (\nabla g^{-1})G$) provides both a stress field $S_\backslash$ away from disarrangement sites and a stress field S_d at disarrangement sites while, at the same time, the field $S_\backslash$ has the dual role of the stress in a "virgin configuration" of the body. The multiplicative decomposition $(\det K)S = S_\backslash K^T$ and the additive decomposition yield the consistency relation $S_\backslash M^T + S_d(\nabla g)^T = 0$ that, for a given structured deformation, connects the two stress fields $S_\backslash$ and S_d. This consistency relation is universal (it applies to any material) and has a certain uniqueness property. Moreover, the additive decompositions of ∇g and of $(\det K)S$ together yield a four-term additive decomposition of the stress-power $(\det K)S \cdot (\nabla g\ )^{\cdot}$ in which the sum of the two "mixed terms" $S_\backslash \cdot \dot{M} + S_d \cdot \dot{G}$

is identified as a source of internal dissipation that emerges from the multiscale geometry.

This background is then used to provide the constitutive assumptions that prescribe an elastic body capable of undergoing disarrangements and then to record the complete field relations that govern the isothermal, dynamical evolution of such a body under prescribed boundary tractions and placements. The requirements that both the free energy response function $(G, M) \longmapsto \Psi_{\text{edis}}(G, M)$ and the internal dissipation be frame-indifferent imply that the Cauchy stress is symmetric, and these field relations reduce to those of classical, finite elasticity when the deformations of the body are restricted to be classical deformations $(g, \nabla g)$, i.e., when $G = \nabla g$ so that no disarrangements occur. A broadened version of elasticity with disarrangements is presented that allows for the presence of strain-gradients through the enriched geometry of "second-order structured deformations", and this is shown to lead to the assumption that the free-energy response is of the form $(G, M, \nabla G) \longmapsto \Psi(G, M, \nabla G)$. In this version, the field ∇G is shown to be a disarrangement density that accounts for jumps in the gradients ∇f_n of approximating deformations. A restricted version of elasticity with disarrangements is considered in which the disarrangements are purely dissipative, in the sense that Ψ_{edis} no longer depends upon M.

Elasticity with purely dissipative disarrangements is then used to define the notion of "disarrangement phase" and to provide a basis for modelling granular bodies, i.e., bodies composed of much smaller elastic bodies for which mutual short-range forces across common boundaries are weak (cohesionless granular media). Examples of disarrangement phases include both compact phases (no disarrangements) and loose phases (stress-free, minimum energy phases). The former are available for every macroscopic deformation g, while the latter are available only when the macroscopic volume change $\det \nabla g$ is sufficiently large. The availability of both loose and compact phases in a granular body leads to the study of moving interfaces that separate these two phases, a phenomenon readily visible when one shovels a thin layer of powdered snow or bends a paper-back book.

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Energy Scaling of Prestrained Thin Plates and Monge-Ampère Anomalies

Mohammad Reza Pakzad
(joint work with Marta Lewicka)

Consider the thin plate

$$\Omega^h := \Omega \times (-h/2 \times h/2), \quad \Omega \subset \mathbb{R}^2,$$

where Ω is simply-connected. We assume the existence of a smooth enough prestrain tensor field $A^h : \Omega^h \to \mathbb{R}^{3\times 3}$, $\det A^h > 0$, with the perturbation scaling $A^h - \mathrm{Id} \sim h^\gamma$ for the range $0 < \gamma < 2$ on Ω^h. In this framework, we consider a fully nonlinear elastic variational model for the deformations

$$u \in W^{1,2}(\Omega^h, \mathbb{R}^3),$$

with the elastic energy:

$$E^h(u) := \frac{1}{h} \int_{\Omega^h} W((\nabla u)(A^h)^{-1}),$$

where the elastic energy density W satisfies standard properties of normalization, frame invariance and non-degeneracy [1]. This model could be justified through the standard multiplicative decomposition ansatz $\nabla u = F_e A^h$, where A^h represents growth, plasticity or any other similar phenomenon; or derived through the observation that the prestrain A^h induces a natural Riemannian metric $G^h := (A^h)^T A^h$ on Ω^h. From this latter perspective, by minimizing the energy E^h, we seek orientation preserving deformations u closest possible to the ideal isometric immersions of the Riemannian manifold (Ω^h, G^h) into $\mathbb{R}^3$. We do not consider any boundary conditions or body forces.

The main question is: "How does the infimum of the energy E^h scale in the thickness variable h?" In a first step, it can be shown that

$$\inf E^h > 0$$

iff the Riemann curvature tensor of G^h does not identically vanish [4]. It is further proven that

$$\inf E^h \sim h^{\gamma+2}$$

iff there exists $v \in W^{2,2}(\Omega)$ solving the Monge-Ampère equation

$$\det \nabla^2 v = f, \tag{1}$$

where $f : \Omega \to \mathbb{R}$ is calculated through the first moment of the prestrain perturbation by

$$f := \lim_{h\to 0} \frac{1}{h^{\gamma+1}} \int_{-h/2}^{h/2} \mathrm{curl}\,\mathrm{curl}(A^h - \mathrm{Id})\mathrm{d}x_3 \not\equiv 0.$$

In this regime, the Γ-limit of $\frac{1}{h^{\gamma+2}}E^h$ is given by the small slope biharmonic model $I(v) := \int_\Omega Q_2(\nabla^2 v - B)$, subject to the Monge-Ampère constraint $\det \nabla^2 v = f$, where the positive quadratic form Q_2 and B are respectively dependent on W and the asymptotic behavior of the first moments of A^h [3].

Focusing on the question of the existence of weak and very weak solutions for the Monge-Ampère equation, we reformulate (1) as

$$\mathcal{D}et\, \nabla^2 v := -\frac{1}{2}\mathrm{curl}\,\mathrm{curl}(\nabla v \otimes \nabla v) = f. \tag{2}$$

We show that for all $0 < \alpha < 1/7$, $f \in L^2(\Omega)$ and $v_0 \in C^0(\bar{\Omega})$, there exists a sequence $v_n \in C^{1,\alpha}(\bar{\Omega})$, uniformly converging to v_0, and solving $\mathcal{D}et\, \nabla^2 v = f$ [5]. This result has been obtained through convex integration methods à la Nash and Kuiper and shows the total degeneracy of the very weak Monge-Ampère operator $\mathcal{D}et\, \nabla^2$ in this regime. A direct consequence is that under minimal regularity assumptions on A^h:

$$\inf E^h \ll h^{1/2}.$$

Moreover, it implies that the Γ-limit of $\frac{1}{h^\beta}E^h$ for $0 \leq \beta < 1/2$ is a degenerate model and points to the appearance of wrinkling patterns in these energy regimes.

It is established that a very weak solution $v : \Omega \to \mathbb{R}$ of (2) displays rigidity features, if $v \in C^{1,\alpha}$, $\alpha > 2/3$ [5], or if $v \in W^{2,2}$ [6, 2]. Therefore, in these better regularity regimes the equation displays a structure which is absent in the flexible one discussed above. Not much is known for solutions $v \in W^{2,p}$ if $1 \leq p < 2$. The best one can hope from the Nash-Kuiper iteration method is to obtain $C^{1,\alpha}$ solutions in the regime $\alpha < 1/3$, which would lead to the estimate

$$\inf E^h \ll h.$$

A major open problem is to understand the qualitative behavior of the solutions to (2) in the regime $1/3 < \alpha < 2/3$. In the same vein, the asymptotic behavior of the minimizers or approximate minimizers of prestrained variational energy E^h is not yet well understood in the energy regimes:

$$h^{\gamma+2} \ll \inf E^h \ll h.$$

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Engineering Approach to Plasticity: Work Hardening

Günter Gottstein

Crystalline Solids, in particular metallic materials, deform by crystallographic glide, i.e. by simple shear on discrete slip planes and in discrete slip directions. The mechanical properties of such materials are technically defined in a tension test, where a cylindrical sample is extended at constant rate while concurrently the force is measured that is necessary to maintain the rate of deformation. If the force is divided by the initial cross section of the sample, we obtain the engineering stress σ. The engineering strain ϵ is defined by the elongation divided by the initial length of the specimen. If the engineering stress is plotted versus the engineering strain, we obtain the so-called flow curve or hardening curve of a material. While the flow curves of different materials are different in detail, they all show an increase of the stress with strain. This phenomenon is referred to as strain hardening. The underlying physical mechanisms can be best investigated on single crystals, where the crystallography of deformation is defined and where the stress strain curve can be converted to a shear stress τ-shear strain γ curve in the activated glide system. A typical shear stress-shear strain curve can be subdivided in 4 regimes, the elastic regime, stage I (easy glide), stage II (linear athermal hardening), and stage II (dynamic recovery). Of importance for strain hardening are stages II and III (stage I does not occur in single crystals oriented for multiple slip or in polycrystals and is an idiosyncrasy of single slip). A simple introduction can be found in [1].

Most commercial alloys, except ferritic steels, have a face centered cubic crystal structure, where the slip planes are $\{111\}$ planes and the slip directions are parallel to $\langle 110\rangle$. Hence, there are 12 different slip systems in fcc crystals. The mechanism of crystallographic slip is the motion of dislocations in the crystal. Their Burgers vector (glide vector) b is parallel to the glide direction. The flow stress of a material is equivalent to the glide resistance that a dislocation experiences during its motion on the glide plane. Typically a dislocation moves a distance L of about 100 times the average spacing of the dislocations in the crystal before it is arrested. Even a well annealed metal crystal has a dislocation density of typically $\rho \approx 10^{10} m^{-2}$, i.e. a dislocation spacing of $\rho^{-\frac{1}{2}} \approx 10^{-5} m$ or $10 \mu m$. A strongly deformed crystal can obtain a maximum dislocation density of the order of $10^{16} m^{-2}$. The glide resistance of a dislocation is the sum of two contributions, the long range stress field τ_p of parallel dislocations (i.e. of the same slip system but at other locations) and the short range stress field τs of dislocations intersecting the glide plane, which have to be cut for a continuous motion of the dislocation, i.e. $\tau = \tau_p + \tau_s$. The passing stress τ_p is an athermal stress (depends on temperature like the shear

modulus μ) and cannot be thermally activated. The cutting stress τ_s is a short range stress and can be overcome by thermal activation. Both stress components scale with μb and the spacing of the respective dislocations, i.e. $\tau_p \sim \mu b\sqrt{\rho_p}$ and $\tau_s \sim \mu b\sqrt{\rho_s}$, where ρ_p and ρ_s are the parallel and intersecting dislocation densities. The experimentally confirmed principle of similitude states that all dislocation densities develop proportional to the total dislocation density ρ, which yields according to Taylor [2]

$$\tau = \alpha\mu b\sqrt{\rho} \tag{1}$$

with $\alpha \approx 0.5$. Kocks and Mecking [3] consider the total dislocation density ρ as only state parameter of plastic deformation, which is a reasonable assumption for stages II and III. To predict the flow curve, it is necessary to know the evolution of the dislocation density with strain. In a strain increment $\mathrm{d}\epsilon$ the total dislocation density changes by storage of moving dislocations $\mathrm{d}\rho^+ = (bL)^{-1}\mathrm{d}\gamma \sim \sqrt{\rho}\,(L - \text{slip length of dislocation})$ and annihilation of stored dislocations $\mathrm{d}\rho^- = -L_R\rho\mathrm{d}\gamma$, where L_R is the annihilated dislocation density per strain increment with

$$\mathrm{d}\rho = \mathrm{d}\rho^+ + \mathrm{d}\rho^-, \tag{2}$$

$$\frac{\mathrm{d}\rho}{\mathrm{d}\epsilon} = A_1\sqrt{\rho} - B_1\rho = A_2\tau - B_2\tau^2. \tag{3}$$

For $L_R = 0$, $\frac{\mathrm{d}\tau}{\mathrm{d}\gamma} = \text{const.}$ (stage II, linear and athermal hardening). For $L_R > 0$, the hardening rate $\frac{\mathrm{d}\tau}{\mathrm{d}\gamma}$ decreases with increasing strain (stage III, dynamic recovery). With constants $A_{1,2}$ and $B_{1,2}$, equation 3 integrates to

$$\tau = \tau_s - (\tau_s - \tau_0)\exp\left(-\frac{\gamma}{\gamma_c}\right), \tag{4}$$

where τ_s is the steady state flow stress, τ_0 is the yield stress (critical resolved shear stress for plastic deformation) and γ_c a characteristic shear strain. Equation 4 is also known as *Voce-equation*. It follows that the strain hardening rate decreases linearly with stress

$$\frac{\mathrm{d}\tau}{\mathrm{d}\gamma} = A_3 - B_3\gamma, \tag{5}$$

$\mathrm{d}\tau/\mathrm{d}\gamma$ vs. τ is also referred to as Kocks-Mecking plot. For polycrystals one uses the relations

$$M\tau = \sigma \text{ and } \mathrm{d}\epsilon = \frac{\mathrm{d}\gamma}{M} \tag{6}$$

to obtain a prediction of the flow curve $\sigma(\epsilon)$ (M is the so-called Taylor factor). For tensile deformation of a polycrystal with random crystallographic texture $M = 3.06$. The Voce equation is usually a good fit to the measured stress-strain curves.

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Rate-independent versus viscous evolution of dislocation microstructures in finite crystal plasticity

Klaus Hackl

(joint work with Christina Günther, Philipp Junker, Dennis Kochmann)

1. Introduction

For nonconvex energy densities, no homogeneous deformation can be found as a minimizer. The former homogeneous material forms patterns which reduce the energy of the crystal instead. We outline numerical schemes for a viscous evolution and a rate-independent evolution of laminates as the minimizing microstructures.

2. Variational framework

This material model is derived in a variational setting. Thus, a Lagrangian is introduced which consists of the time derivative of the specific Helmholtz free energy density $\Psi(\nabla\mathbf{u}, \mathbf{z})$ and the dissipation potential $\Delta(\mathbf{z}, \dot{\mathbf{z}})$ [2],

$$L(\nabla\mathbf{u}, \mathbf{z}, \dot{\mathbf{z}}) = \frac{\mathrm{d}}{\mathrm{d}t}\Psi(\nabla\mathbf{u}, \mathbf{z}) + \Delta(\mathbf{z}, \dot{\mathbf{z}}). \tag{1}$$

The actual displacement field $\mathbf{u}$ is obtained from the principle of minimum potential energy, while the evolution of the internal variables $\mathbf{z}$ is governed by the minimum of the dissipation potential [3],

$$\dot{\mathbf{z}} = \operatorname{argmin}\{L(\nabla\mathbf{u}, \mathbf{z}, \dot{\mathbf{z}}) \mid \dot{\mathbf{z}}\}. \tag{2}$$

3. Material Model

Here we consider incompressible neo Hookean material for which the derivation of the partially relaxed energy for a first order laminate can be found for example in [1]. The internal variables describing the laminate are the volume fraction λ, the plastic slips γ_i, the orientation angle of the laminate ϕ, and the hardening parameters p_i. The dissipation potential consists of a rate independent contribution, and for the viscous evolution a quadratic term in the rate of plastic slip is added. The complete dissipation potential takes the form

$$\Delta(\dot{\gamma}) = r\,|\dot{\gamma}| + \frac{s}{2}\dot{\gamma}^2, \tag{3}$$

with s being a viscous material parameter. Based on Eq. (3), the relaxed dissipation potential for a first order laminate with two domains can be determined. In the case, that the viscous parameter s equals zero, the stationarity conditions take the form

$$\frac{\partial \Psi^{\mathrm{rel}}}{\partial \lambda} \ni r\,|\gamma_1-\gamma_2|\,\mathrm{sign}\dot{\lambda} \tag{4}$$

$$\frac{\partial \Psi^{\mathrm{rel}}}{\partial \gamma_1}+\frac{\partial \Psi^{\mathrm{rel}}}{\partial p_1}\mathrm{sign}\dot{\gamma}_1 \ni r(1-\lambda)\,|\dot{\gamma}_1|\,\mathrm{sign}\dot{\gamma}_1 \tag{5}$$

$$\frac{\partial \Psi^{\mathrm{rel}}}{\partial \gamma_2}+\frac{\partial \Psi^{\mathrm{rel}}}{\partial p_2}\mathrm{sign}\dot{\gamma}_2 \ni r\lambda\,|\dot{\gamma}_2|\,\mathrm{sign}\dot{\gamma}_2. \tag{6}$$

From these, the evolution equations are obtained and a numerical scheme can be outlined [1]. Taking the viscous contribution into account, one has to introduce a smooth transition zone with the width of δ (volume ratio) between the domains. The derivation and the result are presented in [4]. The application of the principle of the minimum of the dissipation potential leads to explicit evolution equations,

$$\dot{\lambda}=-\frac{2\delta}{s\,(\gamma_1-\gamma_2)^2}\left(\left|\frac{\partial \Psi^{\mathrm{rel}}}{\partial \lambda}\right|-r\,|\gamma_1-\gamma_2|\right)_+\mathrm{sign}\frac{\partial \Psi^{\mathrm{rel}}}{\partial \lambda} \tag{7}$$

for the volume fraction of the second domain (the volume fraction of the first domain is $1-\lambda$), and

$$\dot{\gamma}_i=-\frac{1}{s\lambda_i}\left(\left|\frac{\partial \Psi^{\mathrm{rel}}}{\partial \gamma_i}\right|-r\lambda_i\right)_+\mathrm{sign}\frac{\partial \Psi^{\mathrm{rel}}}{\partial \gamma_i} \tag{8}$$

for the plastic slip in both domains. The update of the angle is found by a local minimization, thus

$$\dot{\phi}=-\frac{\delta}{2s\lambda\,(1-\lambda)\,(\gamma_1-\gamma_2)^2}\left(\left|\frac{\partial \Psi^{\mathrm{rel}}}{\partial \phi}\right|-4r\lambda\,(1-\lambda)\,|\gamma_1-\gamma_2|\right)_+\mathrm{sign}\frac{\partial \Psi^{\mathrm{rel}}}{\partial \phi}. \tag{9}$$

The updating of the hardening parameters follows the procedure presented in [1].

4. Numerical example

As a numerical example, a shear test is presented with the deformation gradient described by

$$\boldsymbol{F}=\begin{pmatrix}1+w & 0 & 0\\ 0 & \frac{1}{1+w} & 0\\ 0 & 0 & 1\end{pmatrix}. \tag{10}$$

and a slip system characterized by a slip angle of $\varphi=70°$. For the viscous evolution, the resulting evolution of the microstructure is time dependent. In order to reach a viscosity limit, the material gets relaxation time after every load update. This loading velocity can be controlled by an integer ϑ so that the loading velocity reads $\frac{\Delta w}{\vartheta \Delta t}$ and in this example $\vartheta=10$ is chosen. The evolution of the volume fraction have similar behaviors, the volume of one laminate region increases from zero to one, then the crystal only consists of this region. Also the evolution

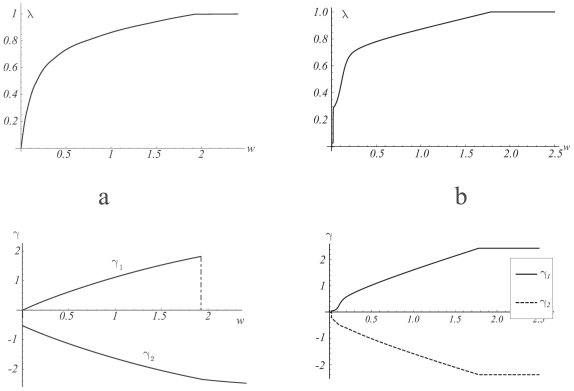

FIGURE 1. History variables, a. rate-independent, b. modified approach

of the plastic slip show a good agreement, Fig. 1. In contrast to these similarities, the stress of both approaches drastically deviate from each other, Fig. 2.

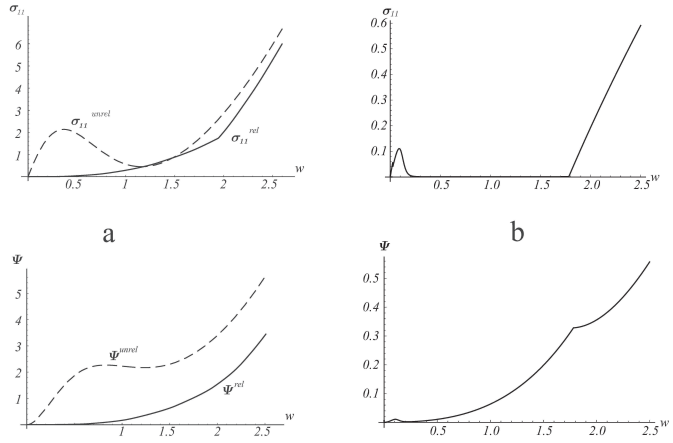

FIGURE 2. Stresses and energy, a. rate-independent, b. modified approach

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Why gradient flows of some energies good for defect equilibria are not good for dynamics, and an improvement

Amit Acharya

(joint work with Chiqun Zhang, Xiaohan Zhang, Dmitry Golovaty, Noel Walkington)

Screw dislocations appear in the microscopic structure of crystalline materials (e.g. metals) and wedge disclinations occur in nematic liquid crystals, the latter an intermediate phase of matter between liquids and solids. Mathematically, their study is challenging since they correspond to topological singularities that result in blow-up of total energies of finite bodies when utilizing most commonly used classical models of energy density; as a consequence, formulating nonlinear dynamical models (especially pde) for the representation and motion of such defects is a challenge as well. Summarizing and adapting the ideas in [1], I will discuss the development and implications of a single pde model intended to describe equilibrium states and dynamics of these defects. The model alleviates the nasty singularities mentioned above and it will also be shown that incorporating a conservation law for the topological charge of line defects allows for the correct prediction of some important features of defect dynamics that would not be possible just with the knowledge of an energy function. These include an 'intrinsic pinning' effect, i.e. a Peierls stress effect, of realistic magnitude in *translationally invariant* media as well as defect annihilation, repulsion, and dissociation. The L_2 gradient flow dynamics of the energy function involved is shown to be incapable of displaying these effects and the reason behind this deficiency is explained.

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A generalization of Korn's first inequality to incompatible tensor fields with applications in gradient plasticity

Patrizio Neff

In infinitesimal gradient plasticity with plastic spin, one seeks to determine the displacement $u\colon \Omega \subset \mathbb{R}^3 \to \mathbb{R}^3$ and the non-symmetric plastic distortion $p\colon \Omega \subset \mathbb{R}^3 \to \mathbb{R}^{3\times 3}$. A simple isotropic model connecting these two fields can be obtained by choosing an energy function

$$\int_\Omega \underbrace{\mu \,\|\operatorname{sym}(\nabla u - p)\|^2}_{\text{elastic energy}} + \underbrace{\mu \,\|\operatorname{sym} p\|^2}_{\substack{\text{lin. kinematic}\\ \text{hardening}}} + \underbrace{\mu\, L_c \,\|\operatorname{Curl} p\|^2}_{\text{dislocation energy}} \,\mathrm{dx}\,, \tag{1}$$

where $\|\,.\,\|$ is the Frobenius matrix norm, $\operatorname{sym} X = \frac{1}{2}\,(X + X^T)$ is the symmetric part of $X \in \mathbb{R}^{3\times 3}$ and $\operatorname{Curl} p$ denotes the curl applied row-wise. Here, $\operatorname{sym}(\nabla u - p)$ represents the symmetric elastic strain and $\operatorname{Curl} p$ is the dislocation density tensor. The balance of linear momentum is obtained from (1) by taking free variations with respect to u and suitably integrating by parts, which leads to

$$\operatorname{Div}\, 2\mu(\operatorname{sym}(\nabla u - p)) = 0\,, \qquad u\big|_{\partial\Omega} = u_0(t)\,. \tag{2}$$

The usual evolution equation for p, satisfying the second law of thermodynamics, can be obtained as

$$\dot p \in \partial\chi\,(2\mu\, \operatorname{sym}(\nabla u - p) + 2\mu\, \operatorname{sym} p - \operatorname{Curl}\operatorname{Curl} p)\,, \quad p\times n\big|_{\partial\Omega} = 0\,,\ p(0) = p_0\,, \tag{3}$$

where $\partial\chi$ is the subdifferential of an elastic domain in generalized stress space. Both equations (2) and (3) can be reformulated, using convex analysis, as a variational inequality of second type. The existence and uniqueness of a solution to such a formulation hinges on the coercivity of (1) in suitable Sobolev spaces, giving a precise sense to the tangential traces for p. We use the Sobolev space $H^1_0(\Omega)$ for the displacement u and the space $H(\operatorname{Curl};\mathbb{R}^{n\times n})$ for the plastic distortion.

Regarding the coercivity of the energy, the following is established in [1, 2, 3]:

$$\exists\, C^+ > 0\ \ \forall\, p \in H(\operatorname{Curl};\mathbb{R}^{n\times n})\,,\ p\times n\big|_{\partial\Omega} = 0\,:$$
$$\int_\Omega \underbrace{\|\operatorname{sym} p\|^2}_{\text{plastic strain}} + \|\operatorname{Curl} p\|^2 \,\mathrm{dx} \ \ge\ C^+ \int_\Omega \underbrace{\|p\|^2}_{\substack{\text{plastic}\\ \text{distortion}}} + \|\operatorname{Curl} p\|^2 \,\mathrm{dx}\,. \tag{4}$$

For $p = \nabla\vartheta$, $\vartheta \in H^1_0(\Omega)$ we recover a version of Korn's inequality and for a skew-symmetric tensor field $p = A$ we obtain Poincaré's inequality, since

$$\operatorname{Curl} A(x) \cong \nabla A$$

for all fields of skew-symmetric matrices A. From (4), it follows that the system (2), (3) has a unique, global-in-time solution.

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Engineering Approach to Plasticity: Work Softening

Günter Gottstein

Dislocations are crystal defects which do not occur in thermodynamic equilibrium. The dislocations stored in a deformed metal are therefore in mechanical equilibrium but thermodynamically unstable. If the temperature increases, new deformation mechanisms become available (for instance climb of dislocations owing to self-diffusion) which renders the dislocation structure unstable and therefore, reduces the dislocation density. There are two kinds of processes that reduce the dislocation density, recovery and recrystallization. Recovery encompasses all processes that lead to annihilation of dislocations or to their rearrangement in lower energy dislocation structures, e. g. low angle grain boundaries. Recrystallization occurs by the nucleation of strain free (virtually dislocation free) grains and their growth with concurrent destruction of the stored dislocation structure. If these processes occur subsequent to deformation during annealing they are referred to as static recovery and static recrystallization, in case they proceed concurrently with deformation, notably during elevated temperature deformation, they are called dynamic recovery and dynamic recrystallization. Dynamic recovery leads to the attainment of a steady state flow stress, dynamic recrystallization makes itself felt by one or more maxima of the flow curve and also the attainment of a steady state flow stress at a stress level below the maximum stress. During elevated temperature deformation stage III hardening is succeeded by two more stages, stage IV and stage V. During stage IV the hardening rate remains low but constant, whereas in stage V the hardening rate goes to zero and correspondingly, steady state flow is attained when strain hardening and dynamic recovery balance each other. Owing to these additional stages, the simple hardening model of Kocks and Mecking [1], which predicts only stages II and III of the hardening curve, cannot predict the observed hardening behavior at large strains. In order to account for stages IV and V and the observation of dynamic recovery in terms of dislocation patterning by the formation of subgrain structures (essentially low angle grain boundaries), we proposed a work hardening model, which is based on three different dislocation densities as microstructural state variables, namely mobile dislocations ρ_m,

dislocations in cell walls ρ_w, and dislocations in cell interiors ρ_i [2].

$$\tau = f(\rho_m, \rho_w, \rho_i, \dot{\epsilon}, T)$$

In stage IV the voluminous cell walls condense to subgrain boundaries which become mobile in stage V. This structural conversion will locally lead to the nucleation of dynamic recrystallization which will then spread out over the entire deformed volume. The initiation of dynamic recrystallization is associated with the transition from stage IV to stage V, which corresponds to a point of inflection on the $\mathrm{d}\tau/\mathrm{d}\gamma$ vs. τ curve [2]. This point of inflection was also predicted by Poliak and Jonas [3] as point of instability from thermodynamic reasons.
The hardening model is formulated as follows [4].

$$\begin{cases} \dot{\rho}_m & = f\left(\rho_m, \rho_w, \rho_i, \dot{\epsilon}, T\right), \\ \dot{\rho}_w & = f\left(\rho_m, \rho_w, \dot{\epsilon}, T\right), \\ \dot{\rho}_i & = f\left(\rho_m, \rho_i, \dot{\epsilon}, T\right), \\ \dot{\rho} & = \dot{\rho}^+ + \dot{\rho}^-. \end{cases}$$

The dislocation density per increment of strain increases due to the production of mobile dislocations, it decreases by various interactions among the dislocations [4]. The kinetic equation of state is given by the Orowan equation, which relates the strain rate to the dislocation velocity v [5, 6]

$$\begin{cases} \dot{\epsilon} & = \rho_m b v, \\ v & = v_0 \lambda_{i,w} \exp\left(-\frac{Q}{kT}\right) \sinh\left(\frac{\tau_{\mathrm{eff},i,w} V_{i,w}}{kT}\right), \quad V_{i,w} = bh\lambda_{i,w}, \quad \lambda_{i,w}^{-1} = \sqrt{\rho_{i,w}}. \end{cases}$$

The respective resolved shear stresses read

$$\tau_{i,w} = \tau_{\mathrm{eff},i,w} + \alpha\mu b\sqrt{\rho_{i,w}},$$

from which the external stress (flow stress) can be calculated as

$$\sigma_{\mathrm{ext}} = M\left(f_i\tau_i + f_w\tau_w\right).$$

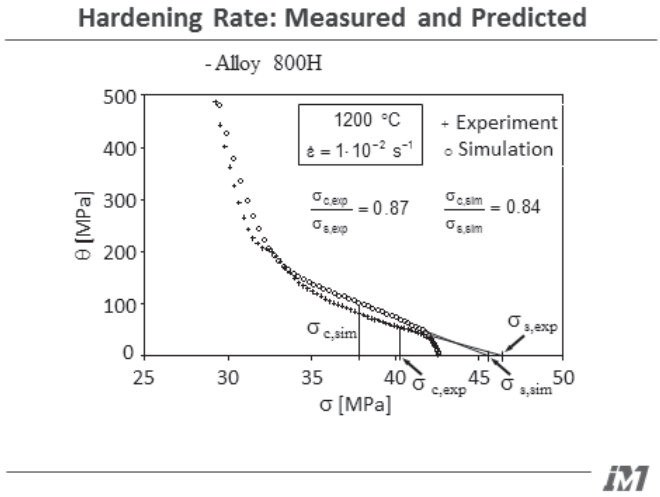
Here f_i and f_w are the volume fractions of cell interior and cell wall, respectively, Q (the activation energy for the obstacle) dislocation interaction, V (the activation volume), λ (the obstacle spacing), μ (the shear modulus), and $\alpha \approx 0.5$. Stage IV can be obtained in the model by making f_w dependent on the hardening rate $\theta = \frac{\mathrm{d}\tau}{\mathrm{d}\gamma}$

$$\sigma_{ext} = M\left(f_i\tau_i + f_w(\theta)\tau_w\right).$$

Stage V takes also the dislocation annihilation due to subboundary motion into account

$$\dot{\rho} = \frac{v_s\rho}{V},$$

where v_s is the subboundary velocity and V the swept volume. With this information the flow curve and in particular the point of inflection on the $\theta(\sigma)$ curve can be calculated [2, 7].



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Homogenization of dislocation dynamics

Lucia Scardia

(joint work with Maria Giovanna Mora and Mark Peletier)

It is well known that plastic, or permanent, deformation in metals is caused by the concerted movement of many curve-like defects in the crystal lattice, called dislocations. What is not yet known is how to use this insight to create theoretical predictions at continuum scales. It would be natural to take a sequence of systems with increasing numbers of dislocations, and derive an effective description in terms of dislocation densities. A mathematical procedure that proved to be very successful for the micro-to-macro upscaling is based on Γ-convergence, a variational convergence that is well known in the mathematical community and has been already applied to a variety of problems in materials science.

In [4] and [9] we used Gamma-convergence to derive a continuum description of the behaviour of *walls of dislocations* close to an obstacle, starting from a discrete model of the dislocation interactions. Our rigorous approach led to a family of upscaled models that we compared with other theories proposed in the literature, offering a selection criterion to identify the hidden assumptions in some of the previous derivations.

In [6] we extended these results to more general distributions of positive dislocations in the plane, still in the single-slip case with Burgers vector $b = e_1$, but removing the constraint for the dislocations to arrange into vertically periodic structures.

More precisely, for a density of dislocations given by $\mu = \frac{1}{n}\sum_{i=1}^{n} \delta_{z_i}$, with $z_i \in \Omega \subset \mathbb{R}^2$ for every i, we considered a semi-discrete dislocation energy of the form

$$F_n(\mu) = \inf_{\beta \in \mathcal{A}_n(\mu)} \left\{ \frac{1}{2} \int_{\Omega_n(\mu)} \mathbb{C}\beta : \beta \, dx \right\}, \tag{1}$$

where $\Omega_n(\mu) = \Omega \setminus \cup_i B_{\varepsilon_n}(z_i)$, with $\varepsilon_n \ll 1/n$, and the admissible class $\mathcal{A}_n(\mu)$ is defined as

$$\mathcal{A}_n(\mu) := \Big\{ \beta \in L^2(\Omega; \mathbb{R}^{2\times 2}) : \int_{\partial B_{\varepsilon_n}(z_i)} \beta \, \tau \, d\mathcal{H}^1 = \frac{e_1}{n} \text{ for every } i = 1, \dots, n \Big\}.$$

It was shown in [3] that the energy contribution in a small neighbourhood of every dislocation is of order $|\log \varepsilon_n|/n^2$ (hence the total *self* energy is of order $|\log \varepsilon_n|/n$), while every pair of dislocations contributes an interaction energy of order n^{-2} (hence the total *interaction* energy is of order 1). Therefore, depending on how ε_n scales with respect to n, one of the two energy contributions will be dominant. On the other hand, the self energy is a (possibly very large) constant and plays no role in the dislocations interactions, which is our main interest.

For this reason, instead of studying the asymptotic behaviour as $n \to \infty$ of the energy F_n in (1), we first subtracted the self energy contribution from F_n, obtaining an interaction energy $\mathcal{F}_n$. In [6] we proved that the Γ-limit of $\mathcal{F}_n$ with respect to narrow convergence is the functional $\mathcal{F}$ given by

$$\mathcal{F}(\rho) = \iint_{\Omega\times\Omega} V(x,y) d\rho(x) d\rho(y) + \min I_\rho(v), \tag{2}$$

where ρ is the limit of discrete measures μ_n. In (2) the interaction potential V is defined as

$$V(x,y) := \int_\Omega \mathcal{C}K_x(z) : K_y(z) \, dz,$$

where K_x is the canonical strain field generated by a single dislocation at x in $\mathbb{R}^2$, namely it solves

$$\begin{cases} \operatorname{div} \mathcal{C}K(\cdot; x) = 0 & \text{in } \mathbb{R}^2, \\ \operatorname{Curl} K(\cdot; x) = e_1 \delta_x & \text{in } \mathbb{R}^2. \end{cases} \tag{3}$$

The second term in (2) is a boundary term due to the boundedness of the domain Ω, and represents their interactions with $\partial\Omega$.

The continuum limit energy (2) has an expression that is common to many (also unrelated) systems of interacting particles. In particular, from (3) follows that $|V(x,y)| \sim -\log|x-y|$ for x close to y, and potentials with a logarithmic singularity have been studied extensively in the literature (see e.g. [1], [8]-[7]). Our work is an important first step towards the analysis of equilibrium dislocation configurations and patterning.

However, macroscopic plasticity is heavily dependent on dynamic properties of the dislocation curves. This motivated us to go further and try to extend our results to the dynamical case. In [6] we added to the interaction energy $\mathcal{F}_n$ a time-dependent forcing term

$$\int_\Omega f(x,t)\, d\mu(x)$$

and coupled the total microscopic energy $\widetilde{\mathcal{F}}_n(\mu) := \mathcal{F}_n(\mu) - \int_\Omega f d\mu$ with a dissipation distance of the following form:

$$d(\mu,\nu) := \begin{cases} \inf_{\gamma\in\Gamma(\mu,\nu)} \iint_{\Omega\times\Omega} |x-y|\, d\gamma(x,y) & \text{if } (\pi_2)_\#\mu = (\pi_2)_\#\nu, \\ +\infty & \text{otherwise,} \end{cases} \tag{4}$$

where $\Gamma(\mu,\nu)$ is a restricted set of couplings of μ and ν,

$$\begin{aligned} \Gamma(\mu,\nu) := \big\{ &\gamma \in \mathcal{P}(\Omega\times\Omega) : \gamma(A\times\Omega) = \mu(A),\ \gamma(\Omega\times A) = \nu(A) \\ &\text{for all Borel sets } A\subset\Omega, \text{ and } \pi_2(x) = \pi_2(y) \text{ for } \gamma\text{-a.e. } (x,y)\in\Omega\times\Omega\big\}. \end{aligned} \tag{5}$$

This is the usual 1-Wasserstein or Monge-Kantorovich transport distance on $\mathcal{P}(\Omega)$ (see [10]), except for the additional restriction that $\pi_2(x) = \pi_2(y)$ for γ-a.e. (x,y); this restriction forces the transport to move parallel to $b = e_1$.

We then proved the existence of a rate-independent evolution driven by the microscopic total energy $\widetilde{\mathcal{F}}_n$ and by the dissipation d, and used the static Γ-convergence result illustrated above to obtain a rate-independent limit evolution, using the method in [5]. In strong form, the limit continuum dislocation density ρ satisfies the transport equation

$$\partial_t\rho + \operatorname{div}(\rho v) = 0,$$

where velocity v satisfies $v\cdot e_2 = 0$ and

$$-(v(t,x)\cdot e_1)\, \partial_{x_1} \frac{\delta\widetilde{\mathcal{F}}}{\delta\rho}(\rho(t),t), = |v(t,x)|,$$

where $\partial_{x_1}\frac{\delta\widetilde{\mathcal{F}}}{\delta\rho}(\rho(t),t)$ is the horizontal component of the total mesoscopic force acting on a dislocation at x. Hence either $v(x,t) = 0$ or the force equals ± 1. This means that the force has to reach a *threshold* for dislocations to move.

There are several steps we are going to take in the near future towards more realistic and complex systems, including the analysis of dislocation dipoles, and the multiple slip case.

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Evolutionary relaxation of a two-phase model

Alexander Mielke

Here we report on joint work with Sebastian Heinz, which is published in [10] and which was partially supported by DFG through the Research Unit 797 MicroPlast and by ERC through AdG AnaMultiScale.

Microstructures in macroscopic and mesoscopic material models are often described on the basis of the strain tensor and some internal variables such as phase indicators, magnetization, plastic tensor, or hardening variables. In most cases, the stored-energy density depends only on the point values of these variables and thus defines a material model without any length scale. Thus, even steady states, which occur as minimizers of the energy, may develop microstructures on arbitrary fine scales if the energy density lacks quasi- or polyconvexity. For static problems a far-reaching theory for the description of microstructures was initiated by the seminal work [1] on the basis of gradient Young measures.

The modeling of the temporal behavior of such microstructures under changing mechanical or thermal loading is significantly more difficult. For rate-independent systems, which do not have an intrinsic time scale and hence are sufficiently close to static problems, a major step forward was done using incremental minimization problems, namely for finite-strain elastoplasticity in [15, 3] and for shape-memory materials in [12, 14, 9].

These approaches are based on incremental minimization problems, and lead to the theory of energetic solutions for rate-independent systems $(\mathcal{Q}, \mathcal{E}, \mathcal{D})$, see [11], where $\mathcal{Q}$ is the state space, $\mathcal{E} : [0,T]\times\mathcal{Q} \to \mathbb{R}$ is the energy potential, and $\mathcal{D} : \mathcal{Q}\times\mathcal{Q} \to [0,\infty]$ is the dissipation distance. For initial states $q_0 \in \mathcal{Q}$, the *approximate incremental minimization problem* reads

$$\text{(AIMP)} \qquad \begin{aligned} &\text{for } j = 1, ..., J \text{ find } q_j \in \mathcal{Q} \text{ with} \\ &\mathcal{E}(j\tau, q_j) + \mathcal{D}(q_{j-1}, q_j) \le \varepsilon\tau + \mathcal{E}(j\tau, \widehat{q}) + \mathcal{D}(q_{j-1}, \widehat{q}) \text{ for all } q \in \mathcal{Q}, \end{aligned}$$

where $\tau = T/J > 0$ is the time step. Here the error level $\varepsilon = 0$ is allowed, if there exist minimizers of $\mathcal{E}(t,\cdot) + \mathcal{D}(q_{j-1},\cdot)$; but we are interested in cases were minimizers do not exists, whereas approximate minimizers for $\varepsilon > 0$ always exist. In such cases, the solutions q_j^ε develop microstructure for $\varepsilon \to 0$. Defining the piecewise constant interpolants $q_{\tau,\varepsilon} : [0,T] \to \mathcal{Q}$ via $q_{\tau,\varepsilon}(t) = q_{j-1}^\varepsilon$ for $t \in [(j-1)\tau, j\tau[$ the major mathematical task in *evolutionary relaxation* is

(1) to establish convergence of a suitable subsequence for τ_n, $\varepsilon_n \to 0$,
(2) to identify a limit $q : [0,T] \to \mathcal{Q}$, and
(3) to determine an evolution equation for all such limits q.

For nonlinear material models without internal length scale this program is largely open. There are particular results for brittle fracture, see e.g. [6, 5], in damage [7], and for a very particular plasticity model [4].

The work in [10] is a continuation of the two-phase model introduced in [12, 14] with the following new results: (i) the existence result for the separately relaxed problem is generalized, (ii) a numerical convergence result for space-time discretizations is provided, and (iii) the evolutionary relaxation of the rate-independent "pure-state model" is shown to lead exactly to the "separately relaxed model" postulated in [12, 14].

The latter model can described as follows. Consider an elastic material that can be in one of the two phases $z = 0$ or $z = 1$ at each microscopic point $x \in \Omega$, i.e. $z : \Omega \to \{0,1\}$ denotes a "pure-phase indicator". The mesoscopic, separately relaxed model can be described by the "averaged phase portion" $\theta : \Omega \to [0,1]$, where $\theta(x)$ denotes the mesoscopic volume fraction of phase $z = 1$ in a small representative volume element around x. Additionally we consider displacements $\widetilde{u} = g_{\mathrm{Dir}} + u : \Omega \to \mathbb{R}^d$ such that the states for the separately relaxed model are given by $q = (u,\theta) \in \mathcal{Q} = \mathbf{U}\times\mathcal{Z}$ with

$$\mathbf{U} := \big\{\, u \in \mathrm{H}^1(\Omega;\mathbb{R}^d) \,\big|\, u|_{\Gamma_{\mathrm{Dir}}} = 0 \,\big\} \text{ and } \mathcal{Z} = \big\{\, \theta \in \mathrm{L}^2(\Omega) \,\big|\, \theta(x) \in [0,1] \text{ a.e.} \,\big\},$$

while the states for the the pure-state model are given by $q = (u,z)$ with

$$z \in \mathcal{Z}^{\mathrm{pure}} := \big\{\, z \in \mathrm{L}^2(\Omega) \,\big|\, z(x) \in \{0,1\} \text{ a.e.} \,\big\}.$$

The particular structure of the model in [12, 14] is that the energy functional $\mathcal{E}(t,\cdot)$ is quadratic, namely

$$\mathcal{E}(t,u,\theta) = \int_\Omega \frac{1}{2}\Big\langle \mathbb{A}\begin{pmatrix}\mathbf{e}(u)\\ \theta\end{pmatrix}, \begin{pmatrix}\mathbf{e}(u)\\ \theta\end{pmatrix}\Big\rangle \,\mathrm{d}x - \Big\langle l(t), \begin{pmatrix}u\\ \theta\end{pmatrix}\Big\rangle,$$

where $\mathbf{e}(u) = \frac{1}{2}(\nabla u + \nabla u^\top)$ is the linearized strain tensor, and $\mathbb{A}$ is a symmetric positive semidefinite matrix. The dissipation distance has the form

$$\mathcal{D}(\theta, \widetilde{\theta}) = \int_\Omega \max\left\{\kappa_{0\to1}(\widetilde{\theta}-\theta)\,,\, \kappa_{1\to0}(\theta-\widetilde{\theta})\right\} \mathrm{d}x,$$

where $\kappa_{0\to1}$ and $\kappa_{1\to0}$ are positive material constants.

Indeed, the pure-phase model $(\mathbf{U}\times\mathcal{Z}^{\mathrm{pure}}, \mathcal{E}, \mathcal{D})$ is given exactly with the same functionals $\mathcal{E}$ and $\mathcal{D}$ as above, where θ is replaced by z taking only the values 0 and 1. Then, separate relaxation gives theq quadratic and "linear" form of $\mathcal{E}$ and $\mathcal{D}$, respectively. Here separate relaxation simple means that we calculate the weakly lower semicontinuous hulls of $\mathcal{E}(t,\cdot) : \mathbf{U}\times\mathcal{Z}^{\mathrm{pure}} \to \mathbb{R}$ and $\mathcal{D} : \mathcal{Z}^{\mathrm{pure}}\times\mathcal{Z}^{\mathrm{pure}} \to [0,\infty[$, where $\mathcal{Z}$ is simply the weak closure of $\mathcal{Z}^{\mathrm{pure}}$.

The new observation in [10] is that the method of *mutual recovery sequences* of [13], see also [11], can be exploited together with the tools from H-measures, see [17, 8, 16]. Indeed, for each sequence $z^k \in \mathcal{Z}^{\mathrm{pure}}$ with $z^k \rightharpoonup \theta$ in $\mathcal{Z}$ and each $\widehat{\theta} \in \mathcal{Z}$, it is possible to construct a sequence $\widehat{z}^k$ such that

$$\mathcal{D}(\theta,\widehat{\theta}) \;=\; \lim_{k\to\infty} \mathcal{D}(z^k,\widehat{z}^k), \quad \mathrm{sign}\big(\widehat{z}^k(x)-z^k(x)\big) = \mathrm{sign}\big(\widehat{\theta}(x)-\theta(x)\big), \quad \text{and}$$
$$\mathcal{E}(t,U(t,\widehat{\theta}),\widehat{\theta}) - \mathcal{E}(t,U(t,\theta),\theta) \ge \limsup_{k\to\infty} \big(\mathcal{E}(t,U(t,\widehat{z}^k),\widehat{z}^k) - \mathcal{E}(t,U(t,z^k),z^k)\big).$$

Using these mutual recovery sequences, it is possible to show the full evolutionary relaxation result: for any approximate solutions $q_{\tau,\varepsilon}$ for $(\mathbf{U}\times\mathcal{Z}^{\mathrm{pure}}, \mathcal{E}, \mathcal{D})$ obtained via (AIMP) there exists a subsequence q_{τ_k,ε_k} that converges to a limit $q = (u,z) : [0,T] \to \mathbf{U}\times\mathcal{Z}$ which is an energetic solution of the separately relaxed rate-independent system $(\mathbf{U}\times\mathcal{Z}, \mathcal{E}, \mathcal{D})$.

Further results include a simplified and generalized existence theory as well as a convergence analysis for the numerical approximations considered in [2].

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A new quasistatic evolution model for perfectly plastic plates

Maria Giovanna Mora
(joint work with Elisa Davoli)

In this talk we discussed the rigorous derivation of a quasistatic evolution model for perfectly plastic plates, starting from three-dimensional Prandtl-Reuss plasticity and using Γ-convergence techniques. The limit model can be described as follows.

Let ω be a bounded domain in $\mathbb{R}^2$ with a C^2 boundary. The set $\Omega := \omega \times (-\frac{1}{2}, \frac{1}{2})$ represents the reference configuration of a three-dimensional plate. The current configuration of the plate at time t is described by a triplet $(u(t), e(t), p(t))$, where $u(t)$ is the displacement, $e(t)$ is the elastic strain tensor, and $p(t)$ is the plastic strain tensor, satisfying the following conditions:

(sf1) *kinematic admissibility:* $Eu(t) = e(t) + p(t)$ in Ω, $u(t) = w(t)$ on Γ_d, and $e_{i3}(t) = p_{i3}(t) = 0$ in Ω for $i = 1, 2, 3$.

Here $Eu(t)$ denotes the symmetric part of $Du(t)$, while $w(t)$ is a prescribed boundary condition on $\Gamma_d := \gamma_d \times (-\frac{1}{2}, \frac{1}{2})$, where $\gamma_d \subset \partial\omega$. Condition (sf1) implies that $u(t)$ is a Kirchhoff-Love displacement, that is, the vertical displacement $u_3(t)$ is independent of the out-of-plane variable x_3 and the horizontal displacement takes the form

$$u_\alpha(t, x) = \bar{u}_\alpha(t, x') - x_3 \partial_\alpha u_3(t, x') \quad \text{for } x = (x', x_3) \in \Omega,\ \alpha = 1, 2. \tag{1}$$

In particular,

$$(Eu)_{\alpha\beta}(t, x) = (E\bar{u})_{\alpha\beta}(t, x') - x_3 \partial^2_{\alpha\beta} u_3(t, x') \quad \text{for } x = (x', x_3) \in \Omega,\ \alpha, \beta = 1, 2.$$

From a mechanical point of view this structure guarantees that straight fibers that are normal to the mid-surface of the plate in the reference configuration, stay straight and normal after the deformation, within the first order.

Condition (sf1) does not imply, in general, that $e(t)$ and $p(t)$ are affine with respect to x_3. However, one can show that $e(t)$ and $p(t)$ admit the following decomposition:

$$e(t,x) = \bar{e}(t,x') + x_3\hat{e}(t,x') + e_\perp(t,x), \quad p(t,x) = \bar{p}(t,x') + x_3\hat{p}(t,x') - e_\perp(t,x),$$

where the zero-th order moments $\bar{e}(t)$ and $\bar{p}(t)$ satisfy

$$E\bar{u}(t) = \bar{e}(t) + \bar{p}(t) \quad \text{in } \omega$$

while the first order moments $\hat{e}(t)$ and $\hat{p}(t)$ are such that

$$-D^2u_3(t) = \hat{e}(t) + \hat{p}(t) \quad \text{in } \omega.$$

In the above identities and in the following we identify $e(t)$, $p(t)$, and their moments with functions taking values in $\mathbb{M}^{2\times 2}_{sym}$, since their third row and column are zero by condition (sf1).

The strong formulation of the quasistatic evolution problem on a time interval $[0,T]$ consists in finding $u(t)$, $e(t)$, and $p(t)$ such that for every $t \in [0,T]$ equation (sf1) is satisfied, together with the following conditions:

(sf2) *constitutive equation:* $\sigma(t) = \mathbb{C}_r e(t)$ in Ω, where $\mathbb{C}_r$ is the elasticity tensor;

(sf3) *equilibrium:* $-\mathrm{div}_{x'}\bar{\sigma}(t) = f(t)$ and $-\mathrm{div}_{x'}\mathrm{div}_{x'}\hat{\sigma}(t) = g(t)$ in ω, together with suitable Neumann boundary conditions on $\partial\omega \setminus \gamma_d$;

(sf4) *stress constraint:* $\sigma(t) \in K_r$, where K_r is a given convex and compact set, representing the set of admissible stresses;

(sf5) *flow rule:* $\dot{p}(t) = 0$ if $\sigma(t) \in \mathrm{int}\, K_r$, while $\dot{p}(t)$ belongs to the normal cone to K_r at $\sigma(t)$ if $\sigma(t) \in \partial K_r$.

Here $f(t) : \omega \to \mathbb{R}^2$ and $g(t) : \omega \to \mathbb{R}$ are the applied body forces at time t, while $\bar{\sigma}(t) := \mathbb{C}_r\bar{e}(t)$ and $\hat{\sigma}(t) := \mathbb{C}_r\hat{e}(t)$ are the stretching and bending components of the stress, respectively. Condition (sf5) can also be written in the equivalent form:

(sf5′) *maximum dissipation principle:* $H_r(\dot{p}(t)) = \sigma(t) : \dot{p}(t)$, where H_r is the support function of K_r, i.e., $H_r(p) := \sup\{\sigma : p \,:\, \sigma \in K_r\}$.

In [1] it has been proved that system (sf1)–(sf5) describes (up to a suitable scaling) the asymptotic behaviour of the Prandtl-Reuss quasistatic evolutions in a three-dimensional plate, when the plate thickness approaches zero.

We note that the equilibrium condition is purely two-dimensional, while the stress constraint and the flow rule involve the whole stress $\sigma(t)$, whose dependence on the thickness variable x_3 may be not trivial (because of the component $\sigma_\perp(t) := \mathbb{C}_r e_\perp(t)$). Thus, the problem has in general a genuinely three-dimensional nature and differs from the classical two-dimensional plastic plate model of the mechanical literature. This can be also seen by considering the following example.

Let

$$\mathbb{C}_r\xi = 2\mu\,\xi + \frac{2\lambda\mu}{\lambda+2\mu}(\mathrm{tr}\,\xi)I_{2\times 2}$$

for every $\xi \in \mathbb{M}^{2\times 2}_{sym}$, where λ, μ are the Lamé parameters, and let

$$K_r = \Big\{\xi \in \mathbb{M}^{2\times 2}_{sym} : \ |\xi|^2 - \frac{1}{3}(\operatorname{tr}\xi)^2 \le \sigma_c^2\Big\}$$

where $\sigma_c > 0$ is given. These are the elastic tensor and the set of admissible stresses of the reduced problem describing the asymptotic behaviour of an isotropic three-dimensional plate with von Mises yield criterion. We consider the boundary condition

$$w_\alpha(t,x) = -tx_3x_\alpha, \quad w_3(t,x) = \frac{t}{2}(x_1^2 + x_2^2)$$

for $\alpha = 1, 2$ and $t \in [0, T]$, prescribed on the whole lateral boundary $\partial\omega\times(-\frac{1}{2}, \frac{1}{2})$. We assume the body forces to be zero, that is, $f(t) = 0$ and $g(t) = 0$.

One can show (see [2]) that, if $t \mapsto (u(t), e(t), p(t))$ satisfies (sf1)–(sf5), then the stress $\sigma(t,x) = \mathbb{C}_r e(t,x)$ is given by

$$\sigma(t,x) = -\Big(\Big(tx_3 \vee \frac{t_0}{2}\Big) \wedge \Big(-\frac{t_0}{2}\Big)\Big)\frac{2\mu(3\lambda+2\mu)}{\lambda+2\mu} I_{2\times 2},$$

where $t_0 := \sqrt{\frac{3}{2}}\frac{\lambda+2\mu}{\mu(3\lambda+2\mu)}\sigma_c$. Note that $\bar\sigma(t) = 0$ for every $t \in [0, T]$. For $t \le t_0$ we have $\sigma(t) = x_3\hat\sigma(t)$, while for $t > t_0$ we have $\sigma(t) = x_3\hat\sigma(t) + \sigma_\perp(t)$ with $\sigma_\perp(t) \ne 0$. Since the location of the plastic zone (that is, the region where the stress is on the yield surface) depends on the thickness variable x_3, reducing the problem to a two-dimensional setting is not possible in this case. In particular, applying the classical plastic plate model to this set of data would mean to look for a solution that is linear with respect to x_3, and thus would lead to a wrong description of the plastic response.

From a mathematical point of view existence of solutions to (sf1)–(sf5) can be proved by setting the problem in the space $BD(\Omega)$ of functions with bounded deformation in Ω for the displacement $u(t)$, in $L^2(\Omega; \mathbb{M}^{2\times 2}_{sym})$ for the elastic strain $e(t)$ and in the space $M_b(\Omega \cup \Gamma_d; \mathbb{M}^{2\times 2}_{sym})$ of bounded Borel measures on $\Omega \cup \Gamma_d$ for the plastic strain $p(t)$. In this framework the boundary condition $u(t) = w(t)$ on Γ_d is relaxed by requiring that

$$p(t) = (w(t) - u(t)) \odot \nu_{\partial\Omega}\mathcal{H}^2 \quad \text{on } \Gamma_d, \tag{2}$$

where $\odot$ denotes the symmetrized tensor product and $\mathcal{H}^2$ is the two-dimensional Hausdorff measure. The mechanical interpretation of (2) is that $u(t)$ may not attain the boundary condition: in this case a plastic slip is developed along Γ_d, whose amount is proportional to the difference between the prescribed boundary value and the actual value.

Combining these remarks with the kinematic admissibility condition (sf1), we see that $u(t)$ is a Kirchhoff-Love displacement in $BD(\Omega)$, that is, $u_3(t)$ belongs to the space $BH(\omega)$ of functions with bounded Hessian in ω and the averaged tangential displacement $\bar u(t)$ in (1) belongs to $BD(\omega)$. Therefore, $\bar u(t)$ may exhibit jump discontinuities, while, because of the embedding of $BH(\omega)$ into $C(\overline{\omega})$, the normal displacement $u_3(t)$ is continuous, but its gradient may have jump discontinuities.

Since the dependence of $u(t)$ on x_3 is affine, we can conclude that slip surfaces are vertical surfaces whose projection on ω is the union of the jump set of $\bar{u}(t)$ and the jump set of $\nabla u_3(t)$.

Moreover, writing condition (2) in terms of moments yields

$$\bar{p}(t) = (\bar{w}(t) - \bar{u}(t)) \odot \nu_{\partial\omega}\mathcal{H}^1 \quad \text{on } \gamma_d,$$
$$u_3(t) = w_3(t), \qquad \hat{p}(t) = (\nabla u_3(t) - \nabla w_3(t)) \odot \nu_{\partial\omega}\mathcal{H}^1 \quad \text{on } \gamma_d.$$

In this setting the flow rule is proved to hold in the form

$$\mathcal{H}_r(\dot{p}(t)) = \langle \sigma(t), \dot{p}(t) \rangle.$$

This can be seen as an integral version of (sf5′), where the left-hand side is interpreted according to the theory of convex functions of measure, while the right-hand side is meant in the sense of the stress-strain duality introduced in [1].

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Polygonization in Crystal Plasticity

Thomas Blesgen

The heart of the Cosserat model, [5], is the multiplicative decomposition

$$\begin{aligned} F = D\phi &= F_{\mathrm{e}}F_{\mathrm{p}} \\ &= R_{\mathrm{e}}U_{\mathrm{e}}F_{\mathrm{p}}. \end{aligned} \tag{1}$$

Therein, the diffeomorphism $\phi(\cdot, t) : \Omega \to \Omega_t$ controls the deformation of the material at a given reference configuration $\Omega \subset \mathbb{R}^3$ and the deformed material Ω_t at time $t \geq 0$; U_{e} is the stretching component and $R_{\mathrm{e}} \in \mathrm{SO}(3)$ a micro-rotation. It is noteworthy that Eqn. (1) is *not* the polar decomposition of F_{e}.

A further important parameter is the third-order (right) curvature tensor

$$K_{\mathrm{e}} = R_{\mathrm{e}}^t \nabla R_{\mathrm{e}} = (R_{\mathrm{e}}^t \partial_x R_{\mathrm{e}}, R_{\mathrm{e}}^t \partial_y R_{\mathrm{e}}, R_{\mathrm{e}}^t \partial_z R_{\mathrm{e}}).$$

A key assumption of the model is that the time evolution of the material is determined by minimizing the total mechanical energy which consists of a stretching energy $W_{\mathrm{st}}(U_{\mathrm{e}})$, a rotational energy $W_{\mathrm{c}}(K_{\mathrm{e}})$, a dislocation energy $V(\kappa)$, here modeled by a simple quadratic ansatz, and the plastic dissipation. In the rate-independent case, the plastic dissipation can be computed analytically with the help of the Legendre-Fenchel dual $Q^*(\dot{F}_{\mathrm{p}}, \dot{\kappa})$ analogous to the methods in [4], where Q is the plastic potential, for instance given by the Tresca condition.

In addition, the plastic slip is restricted to $I \geq 1$ a-priori given plastic slip systems, i.e.

$$F_{\mathrm{p}} = F_{\mathrm{p}}(\gamma) := \mathrm{Id} + \sum_{a=1}^{I} \gamma_a m_a \otimes n_a,$$

with the parametrisation $\gamma = (\gamma_a)_{1\le a\le I} \in \mathbb{R}^I$ and given slip normals n_a and slip vectors m_a, satisfying $|m_a| = |n_a| = 1$, $m_a \cdot n_a = 0$ for every $1 \le a \le I$.

It is convenient to parameterize the rotation group SO(3) by Euler angles, setting $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{R}^3$ and

$$\begin{aligned} R_{\mathrm{e}}(\alpha) &:= Q_3(\alpha_3)Q_2(\alpha_2)Q_1(\alpha_1) \\ &:= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha_3 & \sin\alpha_3 \\ 0 & -\sin\alpha_3 & \cos\alpha_3 \end{pmatrix} \begin{pmatrix} \cos\alpha_2 & 0 & -\sin\alpha_2 \\ 0 & 1 & 0 \\ \sin\alpha_2 & 0 & \cos\alpha_2 \end{pmatrix} \begin{pmatrix} \cos\alpha_1 & \sin\alpha_1 & 0 \\ -\sin\alpha_1 & \cos\alpha_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned}$$

After introducing a discrete time step $h > 0$ and a regularization r_ε of $|\cdot|$ depending on a small $\varepsilon > 0$, in the traction-free case, the time-evolution of the material is governed by the sequence of minimization problems

$$\begin{aligned} \mathcal{E}_\varepsilon(\phi,\alpha,\gamma) = \int_\Omega \Big[& W_{\mathrm{st}}(R_{\mathrm{e}}^t(\alpha) D\phi F_{\mathrm{p}}(\gamma)^{-1}) + 2\mu_2 |\nabla\alpha|_2^2 - f_{\mathrm{ext}}\cdot\phi - M_{\mathrm{ext}} : R_{\mathrm{e}}(\alpha) \\ & + \rho\Big(\sum_{a=1}^I r_\varepsilon(\gamma_a - \gamma_a^0)\Big)^2 + \sum_{a=1}^I r_\varepsilon(\gamma_a - \gamma_a^0)\Big(\sigma_Y - 2\rho\sum_{a=1}^I \kappa_a^0\Big)\Big] \,\mathrm{d}\mathbf{x} \to \min \end{aligned}$$

subject to $\phi_{|\partial\Omega} = g_d$, $R_{\mathrm{e}|\partial\Omega} = R_D$, where g_d and R_D are given.

As a mayor difficulty in this minimization problem, due to the presence of the rotation group SO(3), compactness is not achieved, causing difficulties in the numerical treatment. A numerical algorithm may get stuck in an unwanted local minimum. In order to test the convergence and correctness of a numerical algorithm, in the case of simple plastic shear analytic solutions can be computed, both in 2D [3], and in 3D, [2]. The convergence to these analytic solutions is studied in [1].

A currently open problem is the simulation of polygonization in bent single-crystal beams, [6], where dislocations align to form polygonization patterns. The numerical methods at present seem unable to compute the physically correct solution. In order to overcome these difficulties, the next step is a deeper analysis to find an effective preconditioning for the micro-rotations.

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Energetics of dislocation networks in the plane via a Peierls-Nabarro model

Sergio Conti

We study a vector-valued phase-field model proposed by Michael Ortiz and coworkers [15, 11, 12] which generalizes the classical Peierls-Nabarro model for dislocations. It incorporates both a local Peierls interplanar nonconvex potential, which characterizes the discrete nature of slip, and long-range elastic energy. Precisely, for $L > 0$ we consider dislocations contained in the two-dimensional set $\mathbb{T} = (0, L)^2$ with periodic boundary conditions. The elastic deformation $U : \mathbb{T} \times \mathbb{R} \to \mathbb{R}^3$ is equally assumed to be periodic in the horizontal variables, and may jump across the $\{x_3 = 0\}$ plane. The energy contains linear elasticity and an additional term representing the short-range interatomic interactions across the slip plane,

$$F_\varepsilon[U] = \frac{1}{\varepsilon} \int_{\mathbb{T}} \operatorname{dist}^2(\gamma, \mathcal{B}) dx + \int_{\mathbb{T}\times\mathbb{R}} \frac{1}{2} \mathbb{C}e(U) \cdot e(U)\, dx\,. \tag{1}$$

Here $e(U) = (\nabla U + \nabla U^T)/2$ is the elastic strain, $\mathcal{B} \subset \mathbb{R}^2 \times \{0\}$ is the two-dimensional lattice of possible slip vectors, $U : \mathbb{T} \times \mathbb{R} \to \mathbb{R}^3$ is the $(0, L)^2$-periodic displacement field, and $\gamma = [U]$ is its jump across the $\{x_3 = 0\}$ plane, i.e., the plastic slip. Further, $\mathbb{C} : \mathbb{R}^{3\times3} \to \mathbb{R}^{3\times3}$ is the (symmetric) tensor of linear elastic coefficients.

We parametrize γ by its components u along the slip directions s_i, $i = 1, \dots, N$, according to

$$\gamma(x) = [U](x) = \sum_{i=1}^{N} u_i(x) s_i\,. \tag{2}$$

The slip vectors s_i form a basis for the lattice $\mathcal{B}$. Minimizing out the displacement field U for fixed u and dropping boundary terms leads to

$$\begin{aligned} E_\varepsilon[u] =& \frac{1}{\varepsilon} \int_{\mathbb{T}} \operatorname{dist}^2(u, \mathbb{Z}^N) dx \\ &+ \sum_{i,j=1}^{N} \int_{\mathbb{T}\times\mathbb{T}} K_{ij}(z)(u_j(x) - u_j(x+z))(u_i(x) - u_i(x+z))\, dx\, dz\,. \end{aligned} \tag{3}$$

The mathematical analysis of this phase-field model highlights the occurrence of microstructures over many different length scales. The asymptotic behavior of E_ε as $\varepsilon \to 0$ has been extensively studied in the regime where the leading-order contribution to the total energy is given by the dislocation line tension. Precisely, the scalar case $N = 1$ was treated in [9, 10], the vectorial one in [1, 3], and the situation of two parallel planes in [2, 7]. These results have the general form

$$\frac{1}{\ln(1/\varepsilon)} E_\varepsilon \xrightarrow{\Gamma} E_0^* \tag{4}$$

with respect to strong L^1 convergence of the slips u, where

$$E_0^*[u] = \int_{J_u} \psi_{\rm rel}([u], n) d\mathcal{H}^1 \text{ for } u \in BV(\mathbb{T}; \mathbb{Z}^N)\,. \tag{5}$$

The relaxed line-tension energy $\psi_{\rm rel}$ is the $\mathcal{H}^1$-elliptic envelope [4] of the energy per unit length of a straight dislocation ψ_0 (see [6] for a variational characterization). Precisely,

$$\psi_{\rm rel}(b,n) = \inf\Big\{\frac{1}{2}\int_{J_u} \psi_0([u],\nu) d\mathcal{H}^1 : u \in BV(B_1, \mathbb{Z}^N),\, u = u^{b,n} \text{ on } \partial B_1\Big\} \tag{6}$$

where $u^{b,n}(x) = 0$ if $x \cdot n < 0$, and b if $x \cdot n > 0$, and B_1 the ball of unit radius centered in the origin.

We study here a situation in which $E_\varepsilon[u_\varepsilon]$ is of order $(\ln \frac{1}{\varepsilon})^2$, and u_ε is itself of order $\ln \frac{1}{\varepsilon}$, so that a continuous distribution of dislocations arises. Specifically, we are interested in the limit $\varepsilon \to 0$, assuming that

$$\frac{u_\varepsilon}{\ln \frac{1}{\varepsilon}} \to u_0 \tag{7}$$

and computing the asymptotic energy (in the sense of Γ-convergence)

$$\frac{E_\varepsilon[u_\varepsilon]}{(\ln \frac{1}{\varepsilon})^2} \to E_0[u_0]\,. \tag{8}$$

This is the same scaling regime discussed in the talk by Lucia Scardia [16], and first considered by Garroni, Leoni and Ponsiglione [8] in a geometrically linear setting with a core regularization approach, and by Müller, Scardia and Zeppieri with a geometrically nonlinear formulation [13, 14]. The kinematics is, however, different, as our dislocations are contained in the plane, whereas all those papers consider an antiplane shear situation where dislocations are lines orthogonal to the considered plane.

The limiting energy E_0 turns out to contain both a long-range elastic energy term and a short-range self-energy term, which characterizes the planar distribution of dislocations. The energy per unit area of an affine slip field $u(x) = Ax$ is defined as the optimal energy of dislocation networks which realize it asymptotically. We start from the rescaled energy density defined in (10). We define $g : \mathbb{R}^{M\times 2} \to [0,\infty)$ by the cell problem

$$g(A) = \inf\Big\{\liminf_{j\to\infty} \frac{1}{\pi}\int_{J_{u_j}\cap B_1} \psi_\infty([u_j], n)\, d\mathcal{H}^1 : u_j \text{ piecewise constant}, \\ u_j(x) \to Ax \text{ in } L^1(B_1)\Big\} \tag{9}$$

where

$$\psi_\infty(b,t) = \liminf_{s\to\infty} \frac{1}{s}\psi_{\rm rel}(sb,t)\,. \tag{10}$$

This leads (see [5]) to the limiting functional

$$E_0[u] = E_{\text{self}}[u] + \int_{\mathbb{T}\times\mathbb{T}} K(z)(u(x) - u(x+z)) \cdot (u(x) - u(x+z))\, dx\, dz\,, \tag{11}$$

where the self-energy of the dislocation network is given for $u \in BV(\mathbb{T};\mathbb{R}^N)$ by

$$E_{\text{self}}[u] = \int_{\mathbb{T}} g(\nabla u) dx + \int_{\mathbb{T}} g(\frac{dD^s u}{d|D^s u|}) d|D^s u|\,. \tag{12}$$

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The Geometry of Discombinations in Nonlinear Elastic Solids

Arash Yavari
(joint work with Alain Goriely)

The geometric formulation of continuum mechanics provides a powerful approach to understand and solve problems in anelasticity where an elastic deformation is combined with a non-elastic component arising from defects, thermal stresses, growth effects, or other effects leading to residual stresses. The main idea is to assume that the material manifold, describing the reference configuration for a body, has an intrinsic, non-Euclidean geometry. Residual stresses then naturally arise when this configuration is mapped into Euclidean space. Here, we consider the problem of *discombinations* (a new term that we have introduceed [1]), that is a combined distribution of fields of dislocations, disclinations, and point defects. Given a discombination, we compute the geometric characteristics of the material manifold (curvature, torsion, non-metricity), its Cartan's moving frames and structural equations. This identification provides a powerful algorithm to solve semi-inverse problems with non-elastic components. As an example, we calculate the residual stress field of a cylindrically-symmetric distribution of discombinations in an infinite circular cylindrical bar made of an incompressible hyperelastic isotropic elastic solid.

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Energy Minimizing Maps and Dislocation Theory

Gianluca Lauteri
(joint work with Stephan Luckhaus)

We study a semi-discrete model for small angle grain boundaries, namely the functional

$$\mathcal{F}_\epsilon(A) := \int_{[-L,L]^2 \setminus B_{\lambda\epsilon}(\mathrm{supp}(\mathrm{Curl}A))} \mathrm{dist}^2(A, \mathrm{SO}(2))\mathrm{d}x + |B_{\lambda\epsilon}(\mathrm{supp}(\mathrm{Curl}A))|,$$

where the square $[-L, L]^2$ represents a two-dimensional section of a crystal, $\epsilon > 0$ is the lattice spacing, $\lambda > 0$ is a parameter giving the core radius and the matrix fields A belong to a class of admissible strain fields, which in particular satisfy a *boundary condition* (i.e. $A \equiv R_{\pm\alpha}$ near $x = \pm L$) and the *first quantization of the Burgers vector*, that is

$$\left(\int_\gamma A \cdot t\mathrm{d}\mathcal{H}^1 \neq 0 \Rightarrow \left|\int_\gamma A \cdot t\mathrm{d}\mathcal{H}^1\right| \geq \tau_0\epsilon\right)$$

for each simple, Lipschitz closed curve $\gamma \subset [-L,L]^2 \setminus B_{\lambda\epsilon}(\mathrm{supp}\,(\mathrm{Curl}A))$. Constructing a column of dislocations, we show the existence of a matrix field $A_{\mathrm{gb}}(\epsilon)$ in such class whose energy satisfies

$$\mathcal{F}_\epsilon(A_{\mathrm{gb}}(\epsilon)) \leq C_0\epsilon\alpha L\left(|\log(\alpha)|+1\right),$$

which can be interpreted as the *Read-Shockley* formula in this context. We claim that this is the best possible energy under such constraints.

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Questions on coarse-graining dislocation dynamics

Amit Acharya

(joint work with Xiaohan Zhang, Anish Roy, Noel Walkington, Jacobo Bielak)

The structure of a pde model of small and finite deformation dislocation dynamics is discussed. The averaging questions that arise in upscaling the model are explained. As illustrations of the microscopic theory involved, results pertaining to supersonic dislocation motion as well as Peierls stress effects under quasi-static loadings of small magnitude in a translationally-invariant pde model are shown. The model implies an additive decomposition of the velocity gradient into elastic and plastic parts at finite deformation as a consequence of the conservation law for Burgers vector content, without invoking any notion of a reference configuration.

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Semicontinuous energies defined in the space of multiple valued maps

Emanuele Spadaro
(joint work with Matteo Focardi and Paolo Maria Mariano)

In this talk we presented some recent results [3] on the lower semicontinuity of integral functionals defined in the space of multiple valued points. Although the original appearance of such energies occurred in geometric analysis in the study of minimal surfaces (cp. Almgren's big regularity paper [1]), this formalism can be further developed in a more general context, also in relation with some model in material science. Indeed, in order to account for the influence of microscopic events on the mechanical behavior of deformable bodies, it is sometimes useful to introduce variables, say ν, describing material features which, depending on the spatial scales involved, can refer to a single microstructure or be a sort of average over a family of microstructures. In our work [3] we consider the case of a detailed description of local families of microstructures made of a given number $Q \in \mathbb{N}$ of indistinguishable elements, and study lower semicontinuous energies for such systems.

The following is a streamlined account of the main results in [3].

1. Function spaces

In the general framework in which we describe material microstructures, we need to define spaces of maps taking values on a complete Riemannian manifold $(\mathcal{M}^n, g)$. We denote by $d_{\mathcal{M}}$ its geodesic distance.

1.1. **Space of Q-points.** We denote by $(\mathcal{A}_Q(\mathcal{M}), \mathcal{G}_{\mathcal{M}})$ the metric space of unordered Q-tuples of points in $\mathcal{M}$ given by

$$\mathcal{A}_Q(\mathcal{M}) := \left\{ \sum_{i=1}^{Q} [\![P_i]\!] \,:\, P_i \in \mathcal{M} \ \text{ for every } i = 1, \dots, Q \right\},$$

where $[\![P_i]\!]$ denotes the Dirac mass in $P_i \in \mathcal{M}$ and

$$\mathcal{G}_{\mathcal{M}}(T_1, T_2) \ := \ \min_{\pi \in \mathscr{P}_Q} \sqrt{\sum_i d^2_{\mathcal{M}}(P_i, S_{\pi(i)})},$$

with $T_1 = \sum_i [\![P_i]\!]$ and $T_2 = \sum_i [\![S_i]\!] \in \mathcal{A}_Q(\mathcal{M})$, and $\mathscr{P}_Q$ denotes the group of permutations of $\{1, \dots, Q\}$. Note that $\mathcal{A}_Q(\mathcal{M})$ is isomorphic to the singular space $(\mathcal{M})^Q / \mathscr{P}_Q$.

1.2. **Q-valued Sobolev maps.** Let $\mathcal{B}$ be a bounded, regularly open subset of the Euclidean space $\mathbb{R}^m$. For $p \in [1, +\infty]$, we say that a map ν belongs to $W^{1,p}(\mathcal{B}, \mathcal{A}_Q(\mathcal{M}))$ if there exists $h \in L^p(\mathcal{B})$ such that, for every $T_0 \in \mathcal{A}_Q(\mathcal{M})$,

(i) the real valued function $x \mapsto \mathcal{G}_{\mathcal{M}}(\nu(x), T_0)$ is $W^{1,p}(\mathcal{B})$;
(ii) and the distributional gradient satisfies $|D\big(\mathcal{G}_{\mathcal{M}}(\nu(\cdot), T_0)\big)| \leq h(\cdot)$ $\mathcal{L}^m$-a.e. in $\mathcal{B}$.

Moreover, we need to introduce the notion of weak convergence: for $p \in [1, \infty]$ and $\nu \in W^{1,p}(\mathcal{B}, \mathcal{A}_Q(\mathcal{M}))$, a sequence $\{\nu_k\}_{k\in\mathbb{N}} \in W^{1,p}(\mathcal{B}, \mathcal{A}_Q(\mathcal{M}))$ converges weakly to ν for $k \to \infty$ in $W^{1,p}(\mathcal{B}, \mathcal{A}_Q(\mathcal{M}))$ – and we write $\nu_k \rightharpoonup \nu$ in this case – if

(i) $\|d(\nu_k, \nu)\|_{L^p(\mathcal{B})} \to 0$ as $k \to \infty$;
(ii) $\sup_k \||D\nu_k|\|_{L^p(\mathcal{B})} < \infty$;
(iii) in case $p = 1$, $(|D\nu_k|)_{k\in\mathbb{N}}$ is equi-integrable.

1.3. **First order calculus: differentiability.** Let $\nu \in W^{1,p}(\mathcal{B}, \mathcal{A}_Q(\mathcal{M}))$, $x_0 \in \mathcal{B}$ be a Lebesgue point for ν and $\nu(x_0) = \sum_{i=1}^Q [\![\nu_i(x_0)]\!]$. We say that ν is approximately differentiable at x_0 if there exist linear maps $L_i : \mathbb{R}^m \to T_{\nu_i(x_0)}\mathcal{M}$, $i = 1, \dots, m$, such that $L_i = L_j$ if $\nu_i(x_0) = \nu_j(x_0)$, and, for all $\varepsilon > 0$, it holds

$$\lim_{r\to 0^+} r^{-m}\mathcal{L}^m\left(\{x \in C_r(x_0) : \mathcal{G}_{\mathcal{M}}\left(\nu(x), T_{x_0}\nu(x)\right) \geq \varepsilon|x - x_0|\}\right) = 0,$$

with

$$T_{x_0}\nu(x) := \sum_{i=1}^{Q} \left[\!\!\left[\exp_{\nu_i(x_0)}(L_i(x - x_0))\right]\!\!\right].$$

When defined, the linear maps L_i are uniquely determined; in such a case we shall denote them respectively by $(d\nu_i)_{x_0}$. This way the first-order approximation $T_{x_0}\nu$ is then unambiguously determined.

The main proposition about the differentiability of Sobolev Q-valued maps is the following Rademacher-type result.

Proposition 1.4. *Every map $\nu \in W^{1,p}(\mathcal{B}, \mathcal{A}_Q(\mathcal{M}))$ is approximately differentiable $\mathcal{L}^m$-a.e. on $\mathcal{B}$.*

2. Quasiconvexity and lower semicontinuity

A measurable map $e_M : \mathcal{B} \times (\mathrm{Hom}(\mathbb{R}^m, T\mathcal{M}))^Q \to [0, +\infty)$ is a *Q-integrand* if for every permutation $\pi \in \mathscr{P}_Q$ we get

$$e_M\big(x, \nu_1, \dots, \nu_Q, N_1, \dots, N_Q\big) = e_M\big(x, \nu_{\pi(1)}, \dots, \nu_{\pi(Q)}, N_{\pi(1)}, \dots, N_{\pi(Q)}\big),$$

where $(\nu_i, N_i) \in \mathrm{Hom}(\mathbb{R}^m, T\mathcal{M})$ for each i.

Given any Sobolev Q-valued function ν, the expression

$$e_M(x, \nu(x), d\nu_x) = e_M(x, \nu_1(x), \dots, \nu_Q(x), (d\nu_1)_x, \dots, (d\nu_Q)_x)$$

is well-defined almost everywhere in $\mathcal{B}$. We choose e_M as the integrand of microscopic energy of a rigid body with microstructure that we call *active* imagining that it may have changes in the energy landscape, induced by external agencies,

such as electric fields. We write $\mathcal{E}(\nu)$ for such a microscopic energy which is then defined by

$$\mathcal{E}(\nu) = \int_{\mathcal{B}} e_M\big(x, \nu(x), (d\nu)_x\big)dx.$$

An extension of the notion of quasi-convexity to the case of multiple valued functions with values on a manifold can be proposed.

Definition 2.1 (Quasi-convexity)**.** Let $e_M : (\mathrm{Hom}(\mathbb{R}^m, T\mathcal{M}))^Q \to \mathbb{R}$ be a locally bounded Q-integrand. We say that e_M is *quasi-convex* if for every

(i) affine Q-valued function $\nu : \mathbb{R}^m \to \mathcal{A}_Q(\mathcal{M})$ given by

$$\nu(x) = \sum_{j=1}^{J} q_j \left[\!\!\left[\exp_{\bar\nu_j}(L_j x)\right]\!\!\right],$$

with $\bar\nu_i \neq \bar\nu_j \in \mathcal{M}$ for $i \neq j$,

(ii) and maps $w^j \in W^{1,\infty}(C_1, \mathcal{A}_{q_j}(T_{\bar\nu_j}\mathcal{M}))$ with $w^j|_{\partial C_1} = q_j \left[\!\!\left[L_j|_{\partial C_1}\right]\!\!\right]$,

the inequality

$$e_M\big(\nu(0), (d\nu)_0\big) \leq \int_{C_1} e_M\big(\underbrace{\bar\nu_1, \dots, \bar\nu_1}_{q_1}, \dots, \underbrace{\bar\nu_J, \dots, \bar\nu_J}_{q_J}, dw_x^1, \dots, dw_x^J\big)dx$$

holds, where we identify the tangent space $T_{w_i^j(x)}(T_{\bar\nu_j}\mathcal{M})$ with $T_{\bar\nu_j}\mathcal{M}$ itself.

This definition generalizes the notion of quasi-convexity introduced by Morrey [5], which characterizes sequentially lower semicontinuous functionals in Sobolev spaces. The main result we have discussed is the following.

Theorem 2.2. *Let $p \in [1, \infty[$ and $e_M : \mathcal{B} \times (\mathrm{Hom}(\mathbb{R}^m, T\mathcal{M}))^Q \to \mathbb{R}$ be a continuous Q-integrand. If $e_M(x, \cdot, \cdot)$ is quasiconvex for every $x \in \mathcal{B}$ and*

$$0 \leq e_M(x, \nu, N) \leq C\left(1 + \mathcal{G}^q_{\mathcal{M}}(\nu, \nu_0) + \sum_{i=1}^{Q} |N_i|^p_{g(\nu_i)}\right) \quad \text{for some constant } C > 0,$$

where $q = 0$ if $p > m$, $q = p^*$ if $p < m$ and $q \geq 1$ is any exponent if $p = m$, then the functional $\mathcal{E}$ in (2) is weakly lower semicontinuous in $W^{1,p}(\mathcal{B}, \mathcal{A}_Q(\mathcal{M}))$. Conversely, if $\mathcal{E}$ is weakly$-*$ lower semicontinuous in $W^{1,\infty}(\mathcal{B}, \mathcal{A}_Q(\mathcal{M}))$, then $e_M(x, \cdot, \cdot)$ is quasiconvex for every $x \in \mathcal{B}$.

3. Final comments

In the seminar we have also discussed a sufficient conditions for the lower semicontinuity of integral functionals $\mathcal{E}$ as above, namely the analogous of the notion of polyconvexity (see [2] for details). In this regard, one of the main problem in this context (originally posed by P. Mattila [4] for quadratic integrands) is the following one:

Open question 1. Let $f : \mathcal{B} \times \mathrm{Hom}(\mathbb{R}^m, T\mathcal{M}) \to [0, +\infty)$ be a quasiconvex function. Is it then true that $e_M : \mathcal{B} \times (\mathrm{Hom}(\mathbb{R}^m, T\mathcal{M}))^Q \to [0, +\infty)$ given by

$$e_M\big(x, \nu_1, \dots, \nu_Q, N_1, \dots, N_Q\big) = \sum_{i=1}^{Q} f\big(x, \nu_i, N_i\big),$$

is quasiconvex in the space of multiple valued functions?

The answer to this question is positive in the case of polyconvex functions f and hence for quadratic quasiconvex integrands in small dimensions (see [2] for the proof).

Similarly, a class of open questions concerns the regularity of the minimizers of quasiconvex energy.

Open question 2. Is there any partial regularity for minimizers of quasiconvex functionals in the space of Q-valued functions? Is there any subclass of functionals for which regularity results hold? (cp. the case of the Dirichlet energy in [1] or of two dimensional quadratic energies in [4]).

Finally we have also mentioned the problem of finding non-trivial branching effects for minimizers: assuming that the boundary value is a multiple of a single valued function, are the minimizers also multiple of a single valued functions?

Open question 3. Let u be a minimizer of a quasiconvex functional: does the following implication hold?

$$u|_{\partial\mathcal{B}} = Q\,[\![\phi]\!] \quad \Longrightarrow \quad u = Q\,[\![\Phi]\!]\,.$$

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Boundary-layer behaviour of a pile-up of dislocations

Lucia Scardia
(joint work with Adriana Garroni, Patrick van Meurs, Mark Peletier)

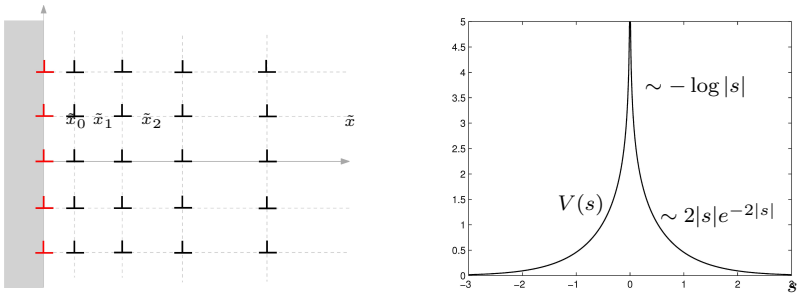
Dislocations are defects in the arrangement of the atoms in a metal lattice, and their distribution and motion greatly affect the macroscopic behaviour of the material. Dislocations do not only interact with other dislocations, but also with impurities, other defects, and interfaces. Understanding the behaviour of dislocations at grain boundaries and phase boundaries, in particular, has been the object of intensive research in academia and industry, but is still far from being achieved.

The analysis of idealised pile-ups in two dimensions is a first attempt to shed light on this complex subject. The simplest case concerns a one-dimensional array of points, corresponding to dislocations in a single glide plane, forced against an obstacle by an external load (see [1]). We consider a model that lies half-way between one and two dimensions. At the microscopic level, the system contains a *large number of periodic walls of edge dislocations* with the same Burgers vector (see Figure 1(a) and [5, 3, 6, 4]). The coordinate system is chosen so that the walls are vertical, and represented by their horizontal positions $\tilde{x}^n = (\tilde{x}^n_i)_{i=0}^n \in [0,\infty)^{n+1}$, with $\tilde{x}^n_0 = 0$, $n \in \mathbb{N}$. The energy of this system is given by

$$\tilde{E}_n(\tilde{x}^n) := K_n \sum_{k=1}^{n} \sum_{j=0}^{n-k} V\left(\frac{\tilde{x}^n_{j+k} - \tilde{x}^n_j}{h_n}\right) + \sigma_n \sum_{i=1}^{n} \tilde{x}^n_i, \tag{1}$$

where K_n measures the elastic properties of the medium, h_n is the distance between consecutive dislocations within a wall, σ_n is an imposed shear stress, and the interaction energy potential V (see Figure 1(b)) is

$$V(s) := s\coth s - \log(2\sinh s) = \frac{2|s|}{(e^{2|s|}-1)} - \log(1-e^{-2|s|}). \tag{2}$$



(a) The walls (b) The interaction energy V

Figure 1. The dislocation configuration considered in this study.

As shown in [3], the problem can be rescaled to depend only on the single dimensionless parameter $\gamma_n = \sqrt{\frac{nK_n}{\sigma_n h_n}}$.

Roughly speaking, γ_n is a measure of the total length of the pile-up, relative to h_n. We will restrict our attention to the case when $1 \ll \gamma_n \ll n$, which corresponds to arrangements where dislocations are closer horizontally than vertically, while the length of the pile-up region is larger than the in-wall spacing h_n. In term of the rescaled positions $x_i = \frac{\tilde{x}_i}{\gamma_n h_n}$ the (suitably rescaled) energy (1) becomes

$$E_n(x^n) := \frac{\gamma_n}{n^2} \sum_{k=1}^{n} \sum_{j=0}^{n-k} V\left(\gamma_n \left(x^n_{j+k} - x^n_j\right)\right) + \frac{1}{n} \sum_{i=1}^{n} x^n_i. \tag{3}$$

In [3] it was shown that the Γ-limit of E_n, for the scaling regime $1 \ll \gamma_n \ll n$, and in the "many-walls" limit $n \to \infty$, is the continuum energy E given by

$$E(\mu) = \frac{1}{2}\Big(\int_{\mathbb{R}} V\Big) \int_0^\infty \rho(x)^2\, dx + \int_0^\infty x\rho(x)\, dx, \quad \text{if } \mu(dx) = \rho(x)\, dx, \tag{4}$$

where $\mu_n := \frac{1}{n}\sum_i \delta_{x_i^n} \rightharpoonup \mu$ as $n \to \infty$. The minimiser ρ^* of the limit energy E is an affine function with slope $-(\int_{\mathbb{R}} V)^{-1}$, and it fits very well the discrete dislocation density profile ρ_n^* in the *bulk* of the pile-up domain. (Note that $\rho_n^*(x_i^*) = \frac{2/n}{x^*_{i+1} - x^*_{i-1}}$, where x_i^* are the components of the minimiser of E_n.) The continuum model, however, fails to capture the distribution of dislocations at the two ends of the domain, where *boundary layers* appear (see Figure 2).

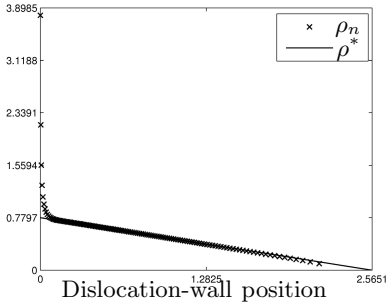


FIGURE 2. Minimisers of E_n and E, for $n = 2^7$ and $\gamma_n = \sqrt{n}$.

Inspired by this observation, we analysed the boundary layer at the lock at $x = 0$, in the scaling regime $1 \ll \gamma_n \ll n$. We did this by studying a Γ-expansion of the energy E_n in terms of the small parameter $1/\gamma_n$. The zero-order term of the expansion is the Γ-limit of the energy (namely E in (4)), which describes correctly the bulk behaviour of the minimiser; the term of order $1/\gamma_n$ in the expansion, instead, is a first-order correction that captures boundary layer effects.

In [2] we studied the limit of the closely related functional $\gamma\left(E_\gamma(\mu) - E_\gamma(\rho^*)\right)$ as $\gamma \to \infty$, where

$$E_\gamma(\mu) := \frac{1}{2}\gamma \int_0^\infty \int_0^\infty V(\gamma(x-y))\mu(dx)\mu(dy) + \int_0^\infty x\mu(dx) \tag{5}$$

is the continuous version of the discrete functional E_n. The limit, boundary-layer energy is

$$F(\nu) = \frac{1}{2}\int_{\mathbb{R}} (V * \nu) d\nu - \rho^*(0) \int_{-\infty}^{0} (V * \nu) dx$$

where ν is the limit (with respect to vague convergence) of the blown-up densities $\nu_\gamma(y) := \mu(y/\gamma) - \rho^*(y/\gamma)$, which capture the (blown-up) difference between the profiles in Figure 2 close to the lock. The minimiser ν^* of F is therefore the sought (blown-up) boundary-layer profile. This can be seen by matching the continuum bulk profile ρ^* with ν^* (namely by defining $\rho^{\gamma_n}(x) := \rho^*(x) + \nu^*(\gamma_n x)$) with the optimal discrete profile, which we show in Figure

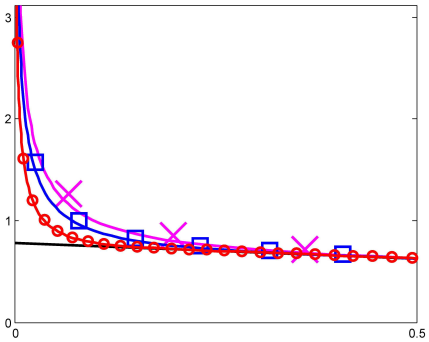


FIGURE 3. Plot of ρ_n^* against ρ^{γ_n} (solid lines), for different values of n. The bulk profile is the line at the bottom.

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