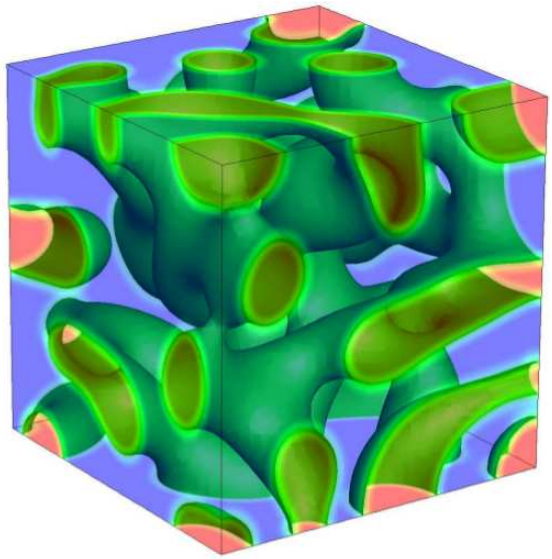
15th GAMM-Seminar on Microstructures



UNIVERSITÉ PARIS 13

Institut Henri Poincaré, Paris

22–23 January, 2016

15th GAMM-Seminar on
Microstructures

General Information

Institut Henri Poincaré, Paris
22–23 January, 2016

Organizers

Postal Address:	15th GAMM-Seminar on Microstructures Prof. Gilles A. Francfort, Ph.D. Université Paris-Nord Laboratoire Analyse, Géométrie et Applications 99, Avenue J.-B. Clément 93430 - Villetaneuse, France
Phone:	(33) 1 49 40 35 86
Email:	gilles.francfort@univ-paris13.fr

Postal Address:	15th GAMM-Seminar on Microstructures Prof. Dr.-Ing. Christian Miehe Stephan Teichtmeister Lukas Böger Universität Stuttgart Insitut für Mechanik (Bauwesen) Pfaffenwaldring 7 D-70550 Stuttgart, Germany
Phone:	+49-711-685-66378
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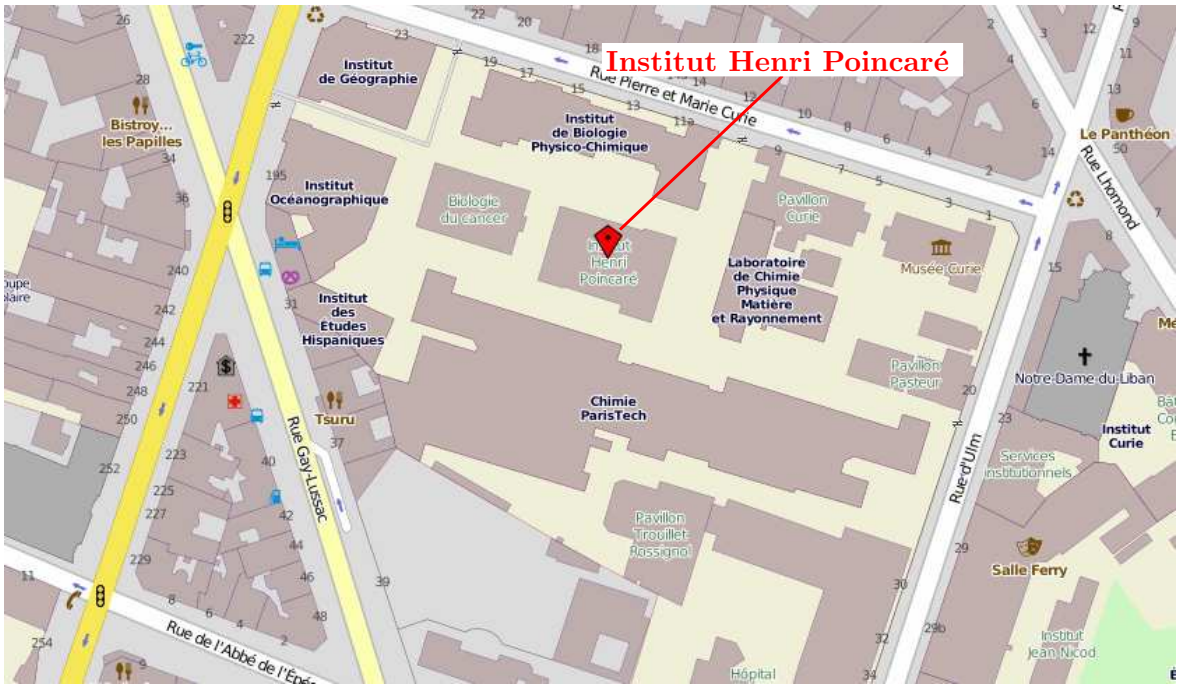
Website:	www.mechbau.uni-stuttgart.de/gamm-micro

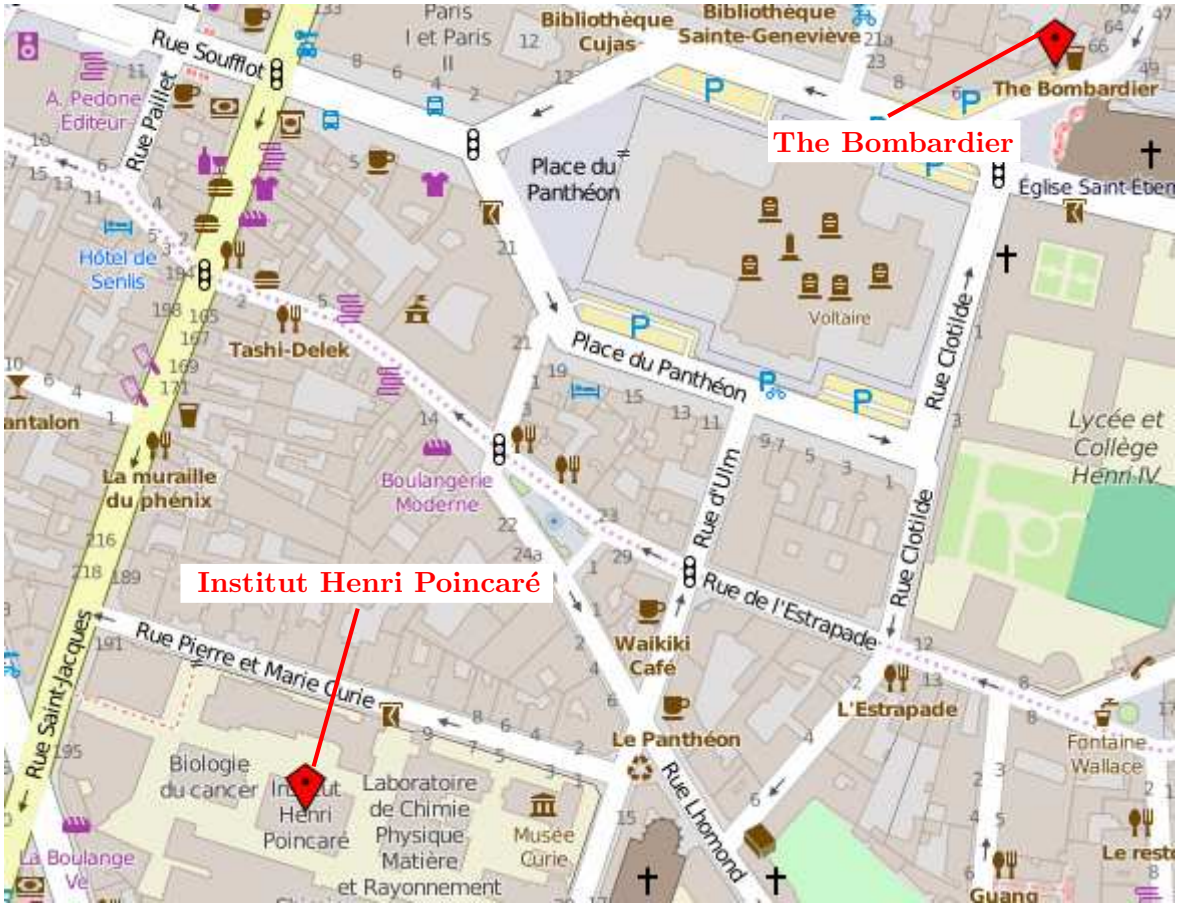
Location of Lectures

The seminar is hosted by the Université Paris-Nord and the University of Stuttgart. The lectures will be given at the Institut Henri Poincaré, 11 rue Pierre et Marie Curie, 75231 Paris Cedex 05.



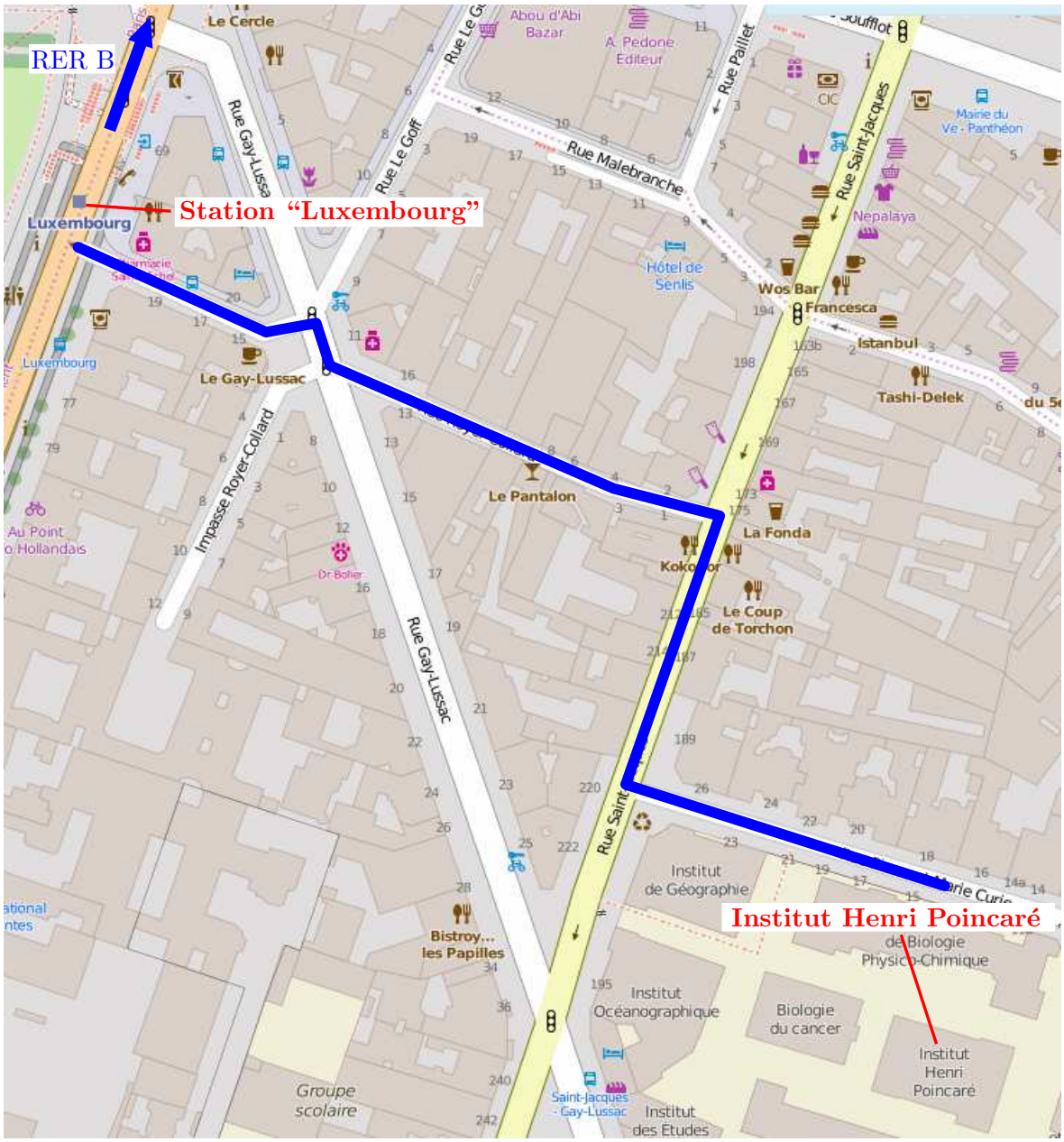
Informal Social Event

On Thursday evening, January 21, at 19:00 there is a coming together at the pub "The Bombardier", 2 Place du Panthon, 75005 Paris, see map below.



Conference Dinner

The conference dinner will take place at the restaurant “La Fresque”, 100 rue Rambuteau, 75001 Paris. From the Institut Henri Poincaré, it is the best to take a 10 minutes walk to the station “Luxembourg”, see map below, and take the train RER B into the direction “Mitry-Claye”. It leaves the station “Luxembourg” at 19:48 and reaches the station “Châtelet-Les Halles” at 19:53. From there, it is a 5 minutes walk to the restaurant, see map on next page.




“La Fresque”
Station “Châtelet-Les Halles”
RER B
Rue Rambuteau
Rue Mondétour
Le Max
L'Artisa du Burg
Les Halles Pierre Lescot
91 Rue Rambuteau 75001 Paris
Châtelet-les-Halles
Place Basse
Porte Lescot
Rue Pierre Lescot
Rue des Prêcheu
Levi's
Rue de la Cossonner
Daisy
Avant Garde
Foot Locker
Quick
Pomme
Rue Saint-Denis
FNAC
Rue Berger
Aire Livraison Nord

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Program

UNIVERSITÉ PARIS 13

Institut Henri Poincaré, Paris
22–23 January, 2016

Friday, January 22, 2016

8:15– 8:25		**registration**
8:25– 8:35		**opening remarks**
8:35– 9:15	**D. Kochmann** (keynote)	On the kinetics of microstructural evolution in ferroelectric ceramics (see page 14)
9:15– 9:40	**M. I. Idiart**	Influence of second-phase inclusions on the electrodeformation of ferroelectric ceramics (see page 26)
9:40–10:05	**M. Labusch**	3D Preisach model for magnetostrictive solids based on orientation distribution functions (see page 31)
10:05–10:30	**M. Wagner**	Elastic anisotropy, compatibility stresses and plastic slip in twinned microstructures (see page 40)
10:30–11:00		**coffee**
11:00–11:40	**M. Peletier** (keynote)	Variational convergence for the analysis of boundary layers in dislocation pileups (see page 17)
11:40–12:05	**J.-F. Babadjian**	Reduced models for linearly elastic thin films allowing for fracture, debonding or delamination (see page 20)
12:05–12:30	**F. Iurlano**	Existence theorem for the Griffith fracture problem in dimension two (see page 27)
12:30–12:55	**R. Knops**	Uniqueness in the linear continuum theory of dislocations (see page 29)
12:55–14:20		**lunch**
14:20–14:45	**H. Petryk**	Sharp versus diffuse interfaces in size-dependent microstructures in crystals (see page 37)
14:45–15:10	**M. E. Jabbour**	Revisiting Surface Instabilities Via Nonequilibrium Thermodynamics (see page 28)
15:10–15:35	**P. Neff**	Loss of ellipticity for non-coaxial plastic deformations in additive logarithmic finite strain plasticity (see page 35)
15:35–16:00	**K. Pham**	Variational formulation and stability analysis of a superelastic shape-memory-alloys model (see page 36)

16:00–16:30		**coffee**
16:30–16:55	**K. Hackl**	Modeling of microstructures in a Cosserat continuum using relaxed energies (see page 25)
16:55–17:20	**S. Conti**	Pattern formation in compressed elastic sheets: the case of indented cones (see page 21)
17:20–17:45	**P. M. Mariano**	Existence of ground states for mixture thin films undergoing large strains (see page 34)
17:45–18:10	**P. P. Castañeda**	Fully optimized second-order variational estimates for nonlinear composites (see page 38)
18:10–19:00		**GAMM activity group meeting**
20:15		**Conference dinner**

For directions to the restaurant "La Fresque", please see page 5.

Saturday, January 23, 2016

8:50– 9:30	**J.-J. Marigo** (keynote)	Gradient Damage Models coupled with Plasticity (see page 15)
9:30– 9:55	**S. Forest**	Nonquadratic potentials in gradient plasticity and phase field models (see page 23)
9:55–10:20	**R. Alessi**	Energetic formulation for rate-independent processes: remarks on discontinuous evolutions with a simple example (see page 18)
10:20–10:45	**K. Danas**	A class of analytical models for porous single crystals with ellipsoidal voids (see page 22)
10:45–11:15		**coffee**

11:15–11:55	**A. Gloria** (keynote)	From Polymer Physics to Nonlinear Elasitcity (see page 13)
11:55–12:20	**B. Schweizer**	Dispersive models for waves in heterogeneous media (see page 39)
12:20–12:45	**T. Yamada**	Design of Periodic Microstructures Considering Dispersive Effect in Wave Propagation (see page 41)
12:45–13:10	**B. Audoly**	One-dimensional models for nonlinearly-elastic and visco-plastic bars (see page 19)
13:10–14:40		**lunch**
14:40–15:05	**V. Kouznetsova**	Multi-scale modelling of locally resonant metamaterials towards an enriched continuum (see page 30)
15:05–15:30	**F. Fritzen**	Reduced basis multiscale variational formulation of multiscale problems (see page 24)
15:30–15:55	**J. LLorca**	Multiscale Micromechanical Model of Needlepunched Nonwoven Fabrics (see page 32)
15:55–16:20	**A. Madeo**	Wave Propagation In Relaxed Micromorphic Continua: Modeling Meta-materials Exhibiting Frequency Band-gaps (see page 33)
16:20–16:35		**closing remarks**

15th GAMM-Seminar on
Microstructures

Abstracts

Institut Henri Poincaré, Paris
22–23 January, 2016

From Polymer Physics to Nonlinear Elasticity

Antoine Gloria[1]
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Rubber-like materials are essentially random networks of interacting polymer-chains. The behaviour of polymer-chain networks is well-understood in the framework of statistical physics, and characterised by meaningful physical parameters. In the continuum setting however, there is hardly a consensus on the form of the energy density to be used to model rubber-like materials, and the associated parameters hardly have a mechanical meaning beyond small deformations. In this talk I will present a state-of-the-art of the long term endeavour to relate the statistical physics description to the continuum mechanics of rubber-like materials. Emphasis will be put on the multidisciplinary aspect of this program, and more specifically on the questions of mathematical analysis it raises.

On the kinetics of microstructural evolution in ferroelectric ceramics

Neel P. Nadkarni[1], **Wei Lin Tan**[1], **Felix Göküzüm**[2], **Dennis M. Kochmann**[1]
[1] Graduate Aerospace Laboratories, California Institute of Technology, Pasadena, U.S.A.
[2] University of Stuttgart, Stuttgart, Germany.

Ferroelectric ceramics such as lead zirconate titanate (PZT) are of utmost technological importance, owing to their electro-mechanical coupling which is exploited in sensors and actuators. Conventional use includes the application of small electric fields to result in small reversible strains (the inverse piezoelectric effect), or the production of a voltage in response to applied strains (the piezoelectric effect). This approximately linear relation between eletrical and mechanical fields breaks down when large electric fields (or large compressive stresses) are applied, which leads to permanent microstructural changes. Specifically, domain switching occurs which irreversibly alters the state of polarization by modifying the complex domain structure at the micron- to nanometer scales. An accurate description of the material behavior subjected to combined electro-mechanical loads thus requires models that account for the intricate mechanisms of domain reorganization.

Most conventional models for ferroelectrics have a rigorous first-principles basis for the thermodynamic formulation of the energetic potentials (including mechanical strain energy density as well as electrical energy and coupling terms). This includes efficient sharp-interface models using, e.g., lamination or convexification strategies [1], as well as diffuse-interface models such as phase field approaches [2,3]. Unfortunately, the kinetics of domain wall motion are insufficiently understood at present, which necessitates phenomenological assumptions for the kinetics of volume fraction changes (in sharp interface models) or for the mobility of domain walls (in diffuse interface models). Microstructural kinetics are particularly challenging since they involve time scales above atomistics, and length scales out of reach for most experiments.

We discuss the state of the art and present continuum models for the microstructural evolution of ferroelectric ceramics that aim for a more accurate description of the microstructural kinetics. In particular, we theoretically link the motion of (sharp) domain interfaces to the (diffuse) phase field description commonly employed in domain switching simulations. The efficient macroscale model is based on a combination of Taylor-type modeling of polycrystals with convexification-based modeling of domain patterns; the microscale model uses a 3D phase field formulation. We also present experimental results that probe the effective, collective impact of the microstructural kinetics in an electro-mechanically-coupled setting for the example of polycrystalline-polydomain PZT [4,5].

References

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Gradient Damage Models coupled with Plasticity

J.-J. Marigo[1]
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It is now well established that gradient damage models are very efficient to account for the behavior of brittle and quasi-brittle materials. Their basic ingredients are: (i) a decreasing dependency of the stiffness $\mathbf{E}(\alpha)$ on the damage variable α; (ii) no more rigidity at the ultimate damage state (say $\mathbf{E}(1) = 0$); (iii) a critical stress σ_c ; (iv) a softening behavior with a decrease of the stress from σ_c to 0 when the damage goes to 1; (v) a gradient damage term in the energy which necessarily contains an internal length ℓ and which limits the damage localization. Accordingly, the process of crack nucleation is as follows [3]: (i) a first damage occurs when the stress field reaches the critical stress somewhere in the body; (ii) then, because of the softening character of the material behavior, damage localizes inside a strip the width of which is controlled by the internal length ℓ; (iii) the damage grows inside this strip, but not uniformly in space (the damage is maximal at the center of the strip and is continuously decreasing to 0 so that to match with the undamaged part of the body at the boundary of the strip); (iv) a crack appears at the center of the strip when the damage reaches there its ultimate value (say $\alpha = 1$). During this crack nucleation process, some energy is dissipated inside the damage strip and this dissipated energy involves a quantity $\mathbf{G}_c$ which can be considered as the effective surface energy of Griffiths theory. Therefore, $\mathbf{G}_c$ becomes a byproduct of the gradient damage model which can be expressed in terms of the parameters of the model (specifically, $\mathbf{G}_c$ is proportional to $\sigma_c^2\ell/\mathbf{E}(0)$). However, this type of quasi-brittle models are not able to account for residual strains and consequently cannot be used in ductile fracture. Moreover there is no discontinuity of the displacement in the damage strip before the loss of rigidity at its center, *i.e.* before the nucleation of a crack. In other words such a model cannot account for the nucleation of cohesive cracks, *i.e.* the existence of surface of discontinuity of the displacement with a non vanishing stress. The natural way to include such effects is to introduce plastic strains into the model and to couple their evolution with damage evolution. Of course, this idea is not new and a great number of damage models coupled with plasticity have been developed from the eighties in the spirit of [2]. But our purpose is to construct such models in a softening framework with gradient of damage terms and to see how these models can account for the nucleation of cracks in presence of plasticity. In our knowledge, the previous works are not able to go so far. Here we will adopt a variational approach in the spirit of our previous works [1]. The main ingredients are the following ones: (i) one defines the total energy of the body in terms of the state fields which include the displacement field and the internal variable fields, namely the damage, the plastic strain and the cumulated plastic strain fields; (ii) one postulates that the evolution of the internal variables is governed by the three principles of *irreversibility*, *stability* and *energy balance*. In particular, the stability condition is essential as well for constructing the model in a rational and systematic way as for obtaining and proving general properties. Besides, we have the chance that the variational approach works and has been already developed both in plasticity and in damage mechanics, even though only separately up to now. So, it suffices to introduce the coupling by choosing the form of the total energy to obtain, by virtue of our plug and play device, a model of gradient damage coupled with plasticity. A part of our paper will be devoted to this task. Specifically, our model, presented here in a three-dimensional setting, contains three state functions, namely $\mathbf{E}(\alpha)$, $\mathrm{d}(\alpha)$ and $\bar{\sigma}_P(\alpha)$ which give the dependence of the stiffness, the local damage dissipated energy and the plastic yield stress on the damage variable. So, our choice of coupling is minimalist in the sense that it

simply consists in introducing this dependence of the yield plastic stress $\sigma_P(\alpha)$ on the damage variable (with the natural assumption that $\sigma_P(\alpha)$ goes to 0 when the damages goes to 1). In turn, by virtue of the variational character of the model, the product $\sigma'_P(\alpha)\bar{p}$ of the derivative of the state function $\sigma_P(\alpha)$ by the cumulated plastic strain $\bar{p}$ enters in the damage criterion and this coupling plays a fundamental role in the nucleation of a cohesive crack.

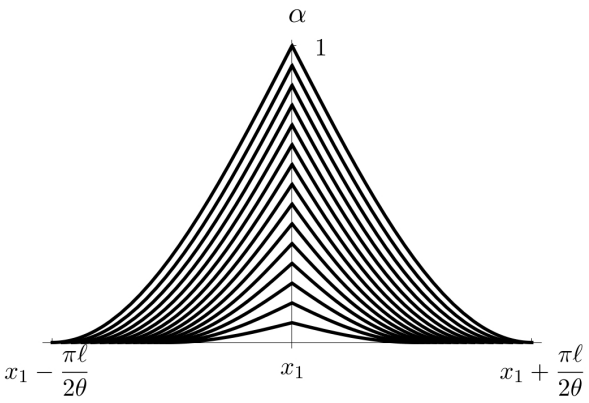

FIGURE 1. Localization damage process with nucleation of a cohesive crack at the center of the damage zone

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Variational convergence for the analysis of boundary layers in dislocation pileups

Mark Peletier[1]
[1] Department of Mathematics and Computer Science, Eindhoven University of Technology, Eindhoven, The Netherlands.

Plasticity, the permanent deformation that one observes in metals, is the net effect of the movement of a large number of microscopic defects in the atomic lattice. These defects, called dislocations, are curve-like topological mismatches, and migrate through the metal under the influence of internal and external forces. Macroscopic, permanent, deformation arises through the concerted movement of a large number of these dislocations.

It is a major challenge to connect a microscopic description of dislocation movement on one hand with models of macroscopic plastic behaviour on the other hand. At this stage we are not able to do this; there is a major gap between the models at these different spatial and temporal scales. Part of the difficulty lies in the complex interactions between dislocations: they attract and repel each other, and form complex higher-level structures that appear to play an important role in determining the macroscopic behaviour.

In this talk I will report on a much more modest result. Dislocations 'pile up' at boundaries of the grains, through which they can not easily pass. These pileups give rise to a net force on the grain boundary, which can have macroscopic consequences. In this talk we study these pileups, and give a description at two levels, corresponding to a 'bulk' behaviour and a boundary-layer behaviour.

The methods we use are those of variational calculus, specifically Gamma-convergence at two different scales. These yield descriptions of the behaviour, both in the bulk and in the boundary layer, in terms of limiting energies.

This work is together with Adriana Garroni, Patrick van Meurs, and Lucia Scardia.

Energetic formulation for rate-independent processes: remarks on discontinuous evolutions with a simple example

Roberto Alessi[1]
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In this work, we discuss in the simplest way some open issues concerning the energetic formulation for the modeling of rate-independent processes by means of a simple one-dimensional example, [1]. Early and unphysical jumps are avoided taking advantage of a time-reparametrization and enforcing an energy imbalance during time-discontinuous transitions. A new energetic selective criterion is then introduced able to predict the final state after a jump and representing intrinsically the energy contribution of rate-dependent phenomena as inertia and viscosity that may arise during fast discontinuous transitions. An improved version of the energetic formulation is finally proposed, preserving completely the rate-independent setting. Some implications of such improved theory will be shown within the field of damage mechanics [2] and superelastic SMA modeling [3].

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One-dimensional models for nonlinearly-elastic and visco-plastic bars

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With the aim to analyze the necking localization of a stretched bar, we derive 1D models by carrying out dimensional reduction on slender prismatic solids. We consider two types of constitutive laws: (*i*) nonlinearly elastic materials, such that the traction curve of homogeneous solutions admits a maximum load (analysis of elastic necking); (*ii*) an incompressible visco-plastic material (analysis of necking in rate-dependent materials). In both cases, we consider non-homogeneous 3D solutions varying slowly in the longitudinal direction, an assumption relevant to the early stage of necking. For the case (*i*), we derive a second gradient model and obtain a simple formula for the second-gradient modulus [4]; this formula is valid for arbitrary cross-sectional geometries and for a compressible of incompressible, orthotropic material. By doing so, we extend to 3D the analysis of Mielke [1], and correct the expressions of the second-gradient modulus found in the classical analyses of circular cylinders [2,3] where the curvature of the cross-sections is ignored. Next, we show that the case of a material of the type (*ii*) can be handled similarly, and we derive a 1D model that allows one to analyze the effect of rate-dependence on necking in a one-dimensional framework.

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Reduced models for linearly elastic thin films allowing for fracture, debonding or delamination

Jean-François Babadjian[1], **Blaise Bourdin**[2], **Duvan Henao**[3], **Andres Leon Baldelli**[4], **Corrado Maurini**[5]

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[3] Facultad de Matemáticas, Pontificia Universidad Católica de Chile, Santiago, Chile
[4] Mathematical Institute, University of Oxford, Oxford, U. K.
[5] Sorbonne Universités, UPMC Univ. Paris 6, Institut Jean Le Rond dAlembert, Paris, France

This talk is devoted to highlight the interplay between fracture and delamination in thin films. The usual scaling law on the elasticity parameters and the toughness of the medium with respect to its thickness gives rise to traditional cracks which are invariant in the transverse direction. We will show that, upon playing on this scaling law, it is also possible to observe debonding effects (delamination as well as decohesion) through the appearance of cracks which are orthogonal to the thin direction. Starting from a three-dimensional brittle elastic thin film, we will first present how both phenomena can be recovered independently through a Γ-convergence analysis as the thickness tends to zero. Then, working on a "toy modelfor scalar anti-plane displacements, we will show how both phenomena can be obtained at the same time. Some partial results in the full three-dimensional case will be presented.

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[2] J.-F. Babadjian, D. Henao: Reduced models for linearly elastic thin films allowing for fracture, debonding or delamination, submitted.

Pattern formation in compressed elastic sheets: the case of indented cones

Sergio Conti[1]
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Elastic thin sheet under compression form a wide range of microstructures. In the case of a flat reference configuration, a complex structure arises, with point singularities connected by ridges. Compressing a spherical shell, as for example a table-tennis ball, different types of deformation are observed: a cylindrically-symmetric pattern at small compression, where the buckled region has a round boundary, and a polygonal-shaped pattern with lower symmetry at large compression [3].
In the case of a conical reference configuration a detailed mathematical analysis is possible [2]. Assuming cylindrical symmetry, a transition between a regime with deformation close to the boundary at small strain and one with buckling close to the center is observed. At larger strain, an extension of the construction from [1] proves that a broken-symmetry buckling pattern has lower energy than any radially symmetric deformation.

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A class of analytical models for porous single crystals with ellipsoidal voids

Armel Mbiakop[1], **Andrei Constantinescu**[1], **Kostas Danas**[1]
[1] LMS, Ecole Polytechnique, C.N.R.S.,École Polytechnique, University Paris Saclay, 91128 Palaiseau, France

A class of rate-dependent and rate-independent constitutive models [1,2] for porous single crystals with arbitrary crystal anisotropy (e.g., FCC, BCC, HCP etc) containing general ellipsoidal voids is developed. The proposed model, denoted as modified variational model (MVAR), is based on the nonlinear variational homogenization method, which makes use of a linear comparison porous material to estimate the response of the nonlinear porous single crystal. Periodic multi-void finite element simulations are used in order to validate the MVAR for a large number of parameters including cubic (FCC, BCC) and hexagonal (HCP) crystal anisotropy, various creep exponents (i.e., nonlinearity), several stress triaxiality ratios, general void shapes and orientations and various porosity levels. The MVAR model, which involves a priori no calibration parameters, is found to be in good agreement with the finite element results for all cases considered in the rate-dependent context. The model is then used in a predictive manner to investigate the complex response of porous single crystals in several cases with strong coupling between the anisotropy of the crystal and the (morphological) anisotropy induced by the shape and orientation of the voids. Finally, a simple way of calibrating the MVAR with just two adjustable parameters is depicted in the rate-independent context so that an excellent agreement with the FE simulation results is obtained. In this last case, this proposed model can be thought as a generalization of the Gurson model in the context of porous single crystals and general ellipsoidal void shapes and orientations.

References

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Nonquadratic potentials in gradient plasticity and phase field models

Samuel Forest[1]
[1] Mines ParisTech CNRS UMR 7633

Quadratic dependence of the Helmholtz free energy potential on gradient variables is widely used in strain gradient plasticity, including crystal plasticity involving the dislocation density tensor, or phenomenological models used for the simulation strain localisation in softening plasticity. This dependence can be shown to lead to unphysical scaling laws in the size-dependent plasticity of metals [4,5]. Power law, rank one and logarithmic potentials will be used to introduce new aspects of plastic deformation mechanisms into the continuum models [3,2]. Applications deal with the cyclic behaviour of laminate microstructures [6,7].
The phase field approach is used to model grain boundary migration in metals at high temperature during heat treatment or under mechanical load [1]. The model involves a non-quadratic potential with respect to lattice curvature.

References

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Reduced basis multiscale variational formulation of multiscale problems

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Solid materials with microstructure show a strong dependence of effective mechanical response with respect to the microscopic distribution of the material properties and their geometrical arrangement. Both the topology and the morphology of the inhomogeneities have a significant impact on the overall response of the material which - viewed from a larger scale - appears homogeneous at first. The prediction of the response of solid materials with consideration of the multiscale character of the problem is a challenging task. First, it involves the postulation of sensible assumptions. Second, these assumptions are translated into mathematical models. Third, due to the lack of reliable (accurate yet feasible) analytical methods for many problem settings, numerical methods are used to solve the often nonlinear problem. Moreover, the microstructural information is statistic in nature: material properties and geometry are not known to arbitrary precision at the smaller scale(s).

In this talk we focus on the computationally efficient solution of the twoscale problem. We refer to the *macroscale* as the scale at which the structural problem is defined and to the *microscale* as a smaller scale asserted to be eligible to a continuum mechanical treatment and spatially clearly separated from the macroscale. Our interest is on the behavior of materials in geometrically linear setting but with full consideration of the rate-dependent dissipative effects at the small (and therefore also large) scale.

The computational efficiency requires two factors to be addressed: the storage memory needs to be reduced significantly and the computing time needs to be lowered by several orders of magnitude. Both aims can be realized by using the pRBMOR (potential bases reduced basis model order reduction) proposed in [1, 2]: a reduced basis approach for the internal variables is combined with micro-mechanical properties of the considered problem. Based on the thereby obtained parameterization of the microscopic model an incremental variational formulation is proposed in order to calculate the evolution of the new degrees of freedom. The new model is not a mere acceleration of FE^2 type simulations but has a new mathematical and algorithmic structure. Only recently the approach was extended to materials with cohesive interfaces [3].

We present a review on the recent developments of the method, e.g., regarding the efficient identification of the reduced order model which can have a strong impact on both accuracy and computing time. A survey on possible extensions towards other problem classes such as large strain elasticity and inelasticity or the modification of the approach for the rapid simulation of structural problems by generalization of the geometry and boundary conditions.

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Modeling of microstructures in a Cosserat continuum using relaxed energies.

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A continuum model for granular materials exhibiting microstructures is presented using the concept of energy relaxation. In the framework of Cosserat continuum theory the free energy of the material is enriched with an interaction energy potential taking into account the counter rotations of the particles. The total energy thus becomes non-quasiconvex, giving rise to the development of microstructures. Relaxation theory is then applied to compute its exact quasiconvex envelope. It is worth mentioning that there are no further assumptions necessary here. The computed relaxed energy yields all possible field fluctuations of displacements and micro-rotations as minimizers. We show that the material behavior can be divided into three different regimes. Two of the material phases are exhibiting microstructures in rotational and translational motion of the particles, respectively, and the third one is corresponding to the case where there is no internal structure of the deformation field. The properties of the proposed model are demonstrated by carrying out numerical computations. The obtained results exhibit a number of unexpected features, for example the transition between distributed and localized microstructures.

Influence of second-phase inclusions on the electro-deformation of ferroelectric ceramics

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Theoretical estimates are given for the overall dissipative response of ferroelectric ceramics with second-phase inclusions, under arbitrary electromechanical loading histories. The ferroelectric behavior of the constituent phases is described via a stored energy density and a dissipation potential in accordance with the theory of generalized standard materials. An implicit time-discretization scheme is used to generate a variational representation of the overall response in terms of a single incremental potential. Estimates are then generated by constructing sequentially laminated microgeometries of particulate type whose overall incremental potential can be computed exactly. Because they are realizable, by construction, these estimates are guaranteed to conform with any material constraints, to satisfy all pertinent bounds, and to exhibit the required convexity properties with no duality gap.
By way of example, the theory is used to study the influence of metallic particles and of microcavities on the electro-deformability of a lead zirconate titanate. In particular, the role of remanent polarization fluctuations on the piezoelectric properties is assessed. The analysis suggests that the popular assumption of material homogeneity within the ferroceramic matrix can lead to inaccurate estimates for the effective piezoelectric properties.

Existence theorem for the Griffith fracture problem in dimension two

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The Griffith model for brittle fracture is based on the balance between elastic and surface energy, the latter assumed to be proportional to the fractured area. In two dimensions the energy functional takes the form

$$E(\Gamma, u) := \frac{1}{2} \int_{\Omega \setminus \Gamma} \mathbb{C}e(u) \cdot e(u) dx + \mathcal{H}^1(\Gamma)$$

and it is complemented by suitable boundary conditions. Here $\Omega \subset \mathbb{R}^2$ is the reference configuration, $\Gamma \subset \Omega$ is the crack, and $u : \Omega \setminus \Gamma \to \mathbb{R}^2$ is the displacement.
The static problem of minimizing E among all pairs (Γ, u), with Γ closed in Ω and u smooth out of Γ, is completely solved in the case of antiplane shear, where u can be assumed to be scalar and $e(u)$ can be replaced by ∇u. This was the object of [1] by De Giorgi, Carriero, and Leaci in the context of image segmentation, where E is known as the Mumford–Shah functional.
Our aim is to extend the work [1] to the general vector-valued case of linearized elasticity in dimension two. The crucial point in the proof is the usage of a new Poincaré-type inequality in SBD recently obtained by the authors.

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Revisiting Surface Instabilities Via Nonequilibrium Thermodynamics

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At the nanoscale, the surface of a crystalline thin film consists of atomic steps separating flat terraces. During growth by, say, molecular beam epitaxy, or sublimation, the surface evolves by diffusion of adsorbed atoms (adatoms) and their attachment to, or detachment from, the steps. In this step-flow regime, two instabilities have been observed: step meandering, whereby flat steps become wavy, and bunching, which consists of a transition from a surface of nearly constant step density to one in which regions of high step density (bunches) are separated by wide terraces. Beyond the scientific challenges that their modeling poses, these instabilities are of technological interest insofar as they pave the way for the patterning of crystal surfaces via the self assembly of nanostructures.
Existing models of step dynamics are, to varying degrees, extensions of the classical work of Burton, Cabrera and Frank [1]. Despite its many successes, several experiments remain at odds with the predictions of this BCF theory. For instance, it does not capture the simultaneous occurrence of step bunching and meandering on metallic and semiconductor surfaces, as observed by N eel et al. [2]. Nor can it account for the multiple stability reversals, with increasing temperature, between a flat surface morphology (equidistant steps) and a facetted one (step bunches), as observed during growth/sublimation of silicon thin films in the presence of an applied electric field, cf. Krug [3] and the references therein. In this talk, based on joint work with N. Kirby and Y. Chen [4], I will present a generalization of the BCF theory, one that is consistent with nonequilibrium thermodynamics and can serve to reconcile it with the aforementioned experiments.

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Uniqueness in the linear continuum theory of dislocations

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Certain aspects of uniqueness, and therefore completeness, are discussed for the static, quasi-static, and dynamic dislocation problems in classical linear elasticity. A continuous distribution of dislocations is assumed whose (evolving) density, taken as principal data, is supplemented by specified standard initial and boundary conditions. Existence of a elastic distorsion tensor is postulated.
In the static and quasi-static traction boundary value problems the stress is uniquely determined by the stated data. By contrast, this data is insufficient to uniquely determine either the stress or total displacement in the quasi-static mixed boundary value problem and in the initial boundary value problems. The inderterminacy is precisely identified and illustrated by the example of a screw dislocation moving uniformly in an infinite region occupied by an isotropic linear elastic body.
The work is joint with Professor Amit Acharya of Carnegie-Mellon University.

Multi-scale modelling of locally resonant metamaterials towards an enriched continuum

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In recent years, significant progress has been achieved in the development of the so-called metamaterials, exhibiting exotic properties, usually not existent in natural materials. One of the examples are the acoustic metamaterials designed to attenuate wave propagation in certain frequency ranges. The unique features of these metamaterials originate from the complex interaction of transient phenomena at the microscopic and macroscopic scales, with local resonance occurring within (one of the) micro-constituents resulting in effective band gaps at the macroscale.
In the previous work, a transient computational homogenization of FE^2 type has been proposed, applicable to general non-linear materials [1]. This approach opens new ways to design of these materials, however the technique is computationally demanding. The present contribution will focus on a particular case of linear elastic materials only. In this case, it is possible to develop a framework leading to a closed-form homogenized ef- fective continuum model, in which the microscale inertia effects, e.g. the local resonance, emerge at the macroscale as the enriched degrees of freedom. To this end, an extended first-order computational homogenization framework is used to establish the scale coupling. At the microscale, static-dynamic superposition of Craig-Bampton type is applied to solve in an off-line stage and subsequently eliminate the microscale problem, resulting in a compact closed form description of the micro-dynamics that captures the local resonance phenomena. Upon substitution of the reduced microscale model into the scale transition relations, the resulting macroscale equations represent an enriched continuum in which additional kinematic degrees of freedom emerge to account for local resonance effects which would otherwise be absent in a classical continuum. Such an approach retains the accuracy and robustness offered by a standard two-scale coupled computational homogenization implementation, while significantly reducing the problem size and the computational time to the on-line solution of one scale only. The approach is validated against the direct numerical simulations and is shown to accurately describe the low-frequency effective behaviour of a local resonant material inside, as well as outside, the frequency band gaps.

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3D Preisach model for magnetostrictive solids based on orientation distribution functions

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Magnetostrictive as well as piezoelectric devices are used in a broad spectrum of technical applications, such as sensor or actuator technologies. They operate on the basis of the special characteristics of the integrated materials, which show a magneto-mechanical or electro-mechanical coupling. By applying an external magnetic or electric field, such materials react with a mechanical deformation. However, the interaction between the applied field and the material response is highly non-linear concerning their magnetization or electric polarization, respectively, as well as their mechanical deformations. Therefore, a realistic and exact modeling of these ferromagnetic- and ferroelectric properties is important to predict the functionality of such devices. In order to simulate the characteristic magnetization and mechanical butterfly hysteresis loops, we employ a three-dimensional Preisach model for magnetostrictive solids. In detail, we decompose the magnetic induction and mechanical deformations into a linear reversible and a non-linear irreversible part, see for example [3]. The irreversible part of the magnetic induction, which describes the remanent magnetization of the material, is approximated with a Preisach operator, see [1], [2], [4] or [5]. This Preisach operator approximates the magnetization by a superposition of multiple relays, which show an "up" or "down" magnetization, described with different switching thresholds. Each relay is further multiplied with a suitable weighting factor such that the superposition of all relays yield the non-linear hysteresis loop. The resulting magnetization is then used to determine the remanent deformations. In contrast to the classical Preisach model, which is based on a scalar valued function, we extended the model to the three-dimensional space. Therefor, we apply the Preisach operator in each direction of an orientation distribution function. Numerical examples show the performance of the implemented model.

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Multiscale Micromechanical Model of Needlepunched Nonwoven Fabrics

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Nonwoven fabrics are a class of textile materials used in many different applications (including thermal insulation, geotextiles, fireproof layers, filtration and water absorption, ballistic impact, etc.) because of their low processing cost and the possibility to tailor the properties by manipulating the fiber nature, the pore size or the interfiber bond. From the viewpoint of the mechanical performance, nonwoven fabrics present lower stiffness and strength than the woven counterparts but much higher ductility and energy-absorption capability. Deformation of nonwoven fabrics involves a number of different mechanisms, including fiber straightening, bond failure and fiber reorientation as well as fiber sliding and fracture, and the sequence of activation and their interaction depend on a number of factors, such as the nature of the fibers and of the interfiber bonds [1]. The analysis of the failure mechanisms is further complicated by the disordered microstructure of the nonwoven and by the development in some cases of non-affine deformation i.e. the macroscopic strain is not homogeneously transferred to the fiber network leading to the formation of loading paths that percolate the network.

A constitutive model for the mechanical behavior of a mechanically-entangled nonwoven fiber network is presented. The model is built upon a detailed characterization of the dominant deformation and failure mechanisms at different length scales (fiber, bundle, network) [2] and accounts for the effects of non-affine deformation, anisotropic connectivity induced by the entanglement points, fiber uncurling and re-orientation as well as fiber disentanglement and pull-out from the knots. The model is intended to be used within the framework of the finite element method and provides the constitutive response for a mesodomain of the fabric corresponding to the volume associated to a finite element and is divided in two blocks. The first one is the network model which establishes the relationship between the macroscopic deformation gradient $\mathbf{F}$ and the microscopic response obtained by integrating the response of the fibers in the mesodomain. The second one is the fiber model, which takes into account the deformation features of each set of fibers in the mesodomain, including uncurling, pull-out and disentanglement. As far as possible, a clear physical meaning is given to the model parameters, so they can be identified by means of independent tests. The numerical simulations based on the model of the tensile deformation of a commercial needle-punched nonwoven fabric along two perpendicular orientations were in very good agreement with the experimental results in terms of the nominal stress - strain curve (including the large anisotropy in stiffness and strength), the specimen shape and the evolution of the fiber orientation distribution function with the applied strain. In addition, the model was able to simulate the effect of fiber orientation on the ballistic response of the material.

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Wave Propagation In Relaxed Micromorphic Continua: Modeling Meta-materials Exhibiting Frequency Band-gaps

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Generalized continuum models are nowadays recognized to be a useful tool for the macroscopic description of the mechanical behavior of materials with heterogeneous microstructures showing exotic properties and/or size effects. In particular, a recently introduced generalized continuum model, which we called *relaxed micromorphic* has been shown to be well-adapted to describe very exotic behaviors of micro-structured materials in the dynamic regime [1], [2]. In particular, a relaxed micromorphic model is, to our knowledge, the only generalized continuum model which is able to describe complete band gaps with respect to wave propagation. We study dispersion relations for the considered relaxed medium and we are able to disclose precise frequency ranges for which propagation of waves is inhibited (frequency band-gaps). We explicitly show that band-gaps phenomena cannot be accounted for by classical micromorphic models of the Mindlin-Eringen type as well as by Cosserat and second gradient ones. We finally point out that such relaxed micromorphic model also gives rise to some very intriguing mathematical questions regarding its well-posedness.

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Existence of ground states for mixture thin films undergoing large strains

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We describe a mixture thin film as a membrane endowed with multiple out-of-tangent-plane vectors at each point, with vector sequence defined to within a permutation to account for the mixing of mixture components. Such a description is motivated by a 2000 proposal for an atomistic-to-continuum derivation of a representation of multi-atomic layer thin films by G. Friesecke and R. D. James, a view not requiring the introduction of phenomenological parameters [2]. Differences between that proposal and the model discussed here are the definition of the values of the layer-descriptor map to within permutations and the explicit introduction of a bending-like term in the energy. We consider surface-polyconvex (see [1]) the membrane energy and a quadratic bending term involving the out-of-tangent-plane multiple vectors, a term which is also quasiconvex. Under appropriate assumption for the energy growth and Dirichlet-type boundary conditions, we prove existence of ground states satisfying a condition of non-degeneracy for the tangent plane. Essential tools in the proofs are special versions of lower semicontinuity results obtained in [3] and 2-currents.

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Loss of ellipticity for non-coaxial plastic deformations in additive logarithmic finite strain plasticity

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We consider the additive logarithmic finite strain plasticity formulation from the view point of loss of ellipticity in elastic unloading [1]. We prove that even if an elastic energy $F \mapsto W(F) = \hat{W}(\log U)$ defined in terms of logarithmic strain $\log U$, where $U = \sqrt{F^T F}$, is everywhere rank-one convex as a function of F, the new function $F \mapsto \widetilde{W}(F) = \hat{W}(\log U - \log U_p)$ need not remain rank-one convex at some given plastic stretch U_p (viz. $E_p^{\log} := \log U_p$). This is in complete contrast to multiplicative plasticity in which $F \mapsto W(F\,F_p^{-1})$ remains rank-one convex at every plastic distortion F_p if $F \mapsto W(F)$ is rank-one convex. We show this disturbing feature with the help of a recently considered family of exponentiated Hencky energies.

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Variational formulation and stability analysis of a superelastic shape-memory-alloys model

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We present a variational framework for the three-dimensional macroscopic modeling of superelastic shape memory alloys in an isothermal setting. Phase transformation is accounted through a unique second order tensorial internal variable, acting as the transformation strain. Postulating the total strain energy density as the sum of a free energy and a dissipated energy, the model depends on two material scalar functions of the norm of the transformation strain and a material scalar constant. Appropriate calibration of these material functions allow to render a wide range of constitutive behaviours including stress-softening and stress-hardening. The quasi-static evolution problem of a domain is formulated in terms of two physical principles based on the total energy of the system: a stability criterion, which selects the local minima of the total energy, and an energy balance condition, which ensures the consistency of the evolution of the total energy with respect to the external loadings. The local phase transformation laws in terms of Kuhn-Tucker relations are deduced from the first-order stability condition and the energy balance condition. Evolutions of homogeneous states are given for proportional and non-proportional loadings in numerical experiments. Finally, in view of an identification process, the issue of stability of homogeneous states in multi-dimensional setting is answered based on the study of second-order order derivative of the total energy.

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Sharp versus diffuse interfaces in size-dependent microstructures in crystals

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Formation of microstructures in single crystals of metal and alloys is generally explained by energy minimization. Either total or incremental energy minimization is considered depending of the physical mechanism of inelastic deformation, e.g. mechanical twinning, martensitic phase transition or incremental plastic deformation by crystallographic slip. Competition between the bulk and interfacial energy contributions provides a natural intrinsic length scale and makes the microstructures size-dependent. The attention is focused here on the differences and similarities between two distinct approaches to the modelling of size-dependent microstructures in which the interfaces are treated as either sharp or diffuse. As the major example, martensitic phase transformation in a shape memory alloy crystal is selected for study. A finite-strain phase field model for shape memory alloys is developed introducing new ingredients. The results calculated by using the finite-element phase-field model with diffuse interfaces have been found in satisfactory agreement with the sharp-interface approach based on the assumption of perfect laminates, in spite of the simplifying assumptions involved in the latter approach. The phase-field model avoids tracking of individual interfaces and leads to an efficient computational scheme for predicting the formation and evolution of microstructures of initially unknown pattern. If the pattern is regarded as known then the effect of strain gradients within diffusive interfaces can be directly compared to the effect of interfacial energy associated with a sharp interface.

Fully optimized second-order variational estimates for nonlinear composites

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A variational method is developed to estimate the macroscopic constitutive response of composite materials consisting of aggregates of viscoplastic single-crystal grains and other inhomogeneities [1]. The method, which builds on earlier work [2-4], derives from a stationary variational principle for the macroscopic stress potential of the viscoplastic composite in terms of the corresponding potential of a linear comparison composite, whose viscosities and eigenstrain rates are the trial fields in the variational principle. The resulting estimates for the macroscopic response are guaranteed to be exact to second-order in the heterogeneity contrast [5], and to satisfy known bounds [3]. In addition, unlike earlier 'second-order' methods, the new method allows optimization with respect to both the viscosities and eigenstrain rates, leading to estimates that are fully stationary and exhibit no duality gaps. Consequently, the macroscopic response and field statistics of the nonlinear composite can be estimated directly from the suitably optimized linear comparison composite, without the need for difficult-to-compute correction terms. The method is applied to a simple example of a porous single crystal, and the results are found to be more accurate than earlier estimates [6,7].

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Dispersive models for waves in heterogeneous media

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Our analysis concerns the linear wave equation of second order. We assume that the spatial operator is in divergence form and that an oscillatory coefficient matrix a^ε is periodic with characteristic length scale $\varepsilon > 0$. Denoting solutions by $u^\varepsilon : \mathbb{R}^n \times (0,\infty) \to \mathbb{R}$, we are interested in

$$\partial_t^2 u^\varepsilon(x,t) = \nabla \cdot (a^\varepsilon(x) \nabla u^\varepsilon(x,t)) \,. \tag{1}$$

We assume that $a^\varepsilon(x) = a_Y(x/\varepsilon)$ where $a_Y : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ is periodic with the periodicity of the unit cell $Y = (-\pi,\pi)^n$. We are interested in the behavior of u^ε in the limit $\varepsilon \to 0$.
Classical homogenization theory allows to describe solutions $u^\varepsilon \approx u^*$ well by a non-dispersive wave equation $\partial_t^2 u^* = \nabla \cdot (a^* \nabla u^*)$ — on fixed time intervals $(0,T)$. Instead, when larger time intervals are considered, dispersive effects are observed. To describe u^ε on intervals $(0, T\varepsilon^{-2})$, we must use a dispersive wave equation. Our main result is that u^ε is close to the solution w^ε of the well-posed, weakly dispersive equation

$$\partial_t^2 w^\varepsilon = AD^2 w^\varepsilon + \varepsilon^2 E D^2 \partial_t^2 w^\varepsilon - \varepsilon^2 F D^4 w^\varepsilon \,. \tag{2}$$

The terms of order ε^2 produce leading order effects, since time intervals of length ε^{-2} are considered. We succeed to compare the norms of the two solutions and obtain uniform error estimates of the form $\|u^\varepsilon(t) - w^\varepsilon(t)\| \le C\varepsilon$ for every $t \in (0, T\varepsilon^{-2})$ in some norm. These estimates are accompanied by computable formulas for the coefficients A, E, and F in the effective models.
Our method relies on a Bloch-wave expansion of the solution u^ε. The Bloch expansion suggests a dispersive equation for the solution. But this formal equation, known as the "bad-Boussinesq equation", cannot approximate solutions, it is not even well-posed. Through a substitution trick we transform the ill-posed equation into a well-posed equation (2). Numerical results in one and two space dimensions show the dispersive behavior in heterogeneous media and confirm the approximation property of the weakly dispersive model.

Elastic anisotropy, compatibility stresses and plastic slip in twinned microstructures

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Twins can form in many materials, mainly as a result of annealing heat treatments, during plastic deformation, or as a mechanism for self-accommodation in martensitic phase transformations. Individual variants (i.e., regions adjacent to a twin boundary) are related by well-defined crystallographic orientation relationships. When a stack of thin twin variants is subjected to mechanical loading, elastic anisotropy gives rise to additional stresses that originate at the twin boundaries, but are constant throughout single variants. In this presentation, I will discuss a simple micromechanical model that fully describes these compatibility stresses. Compatibility stresses can be of the same order of magnitude as the applied stresses, and may therefore significantly alter the local stress state. I will present two examples, illuminating the effect of elastic anisotropy in twins on (i) the activation of dislocation slip systems in nano-twinned copper, and (ii) on the effective compliance matrix (which, for the twinned structure, becomes asymmetric) of B19' martensite twins in NiTi shape memory alloys.

Design of Periodic Microstructures Considering Dispersive Effect in Wave Propagation

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Dispersion is a phenomenon appearing in heterogeneous media, by which waves with different wavelengths propagate with different velocities [1]. It is well known that solutions of the linear wave equation in a periodic inhomogeneous medium can be approximated by solutions of an homogenized wave equation with constant coefficients. Since dispersion does not occur in homogeneous media, it is necessary to include higher order terms (namely a fourth-order term) in the effective model in order to represent those dispersive effects [1], [2], [3]. This fourth-order term can be obtained by the method of two-scale asymptotic expansions or by the Bloch wave method. It was first rigorously justified in [3]. This effect is pretty important for industrial applications, because the periodic size of microstructures is finite in all industrial applications. To begin with, this work shows several numerical simulation, which exhibits the long time behavior of wave propagation in periodic inhomogeneous media in case of one dimension. By the numerical results, we can confirm that the higher order homogenized wave equation is a much better approximation than the usual homogenized wave equation in the long time situation. Next, this study presents the design of two dimensional periodic microstructures to minimize or maximize the dispersive effect with prescribed value of the homogenized coefficient and volume constraint of the inclusion by using a shape optimization technique. As was expected, we obtain microstructures which have different dispersive properties but have the same homogenized coefficients and the same volume of material. For simplicity, our study is restricted to isotropic media, namely the unit cell of the periodic microstructures is assumed to have an 8-fold symmetry.

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