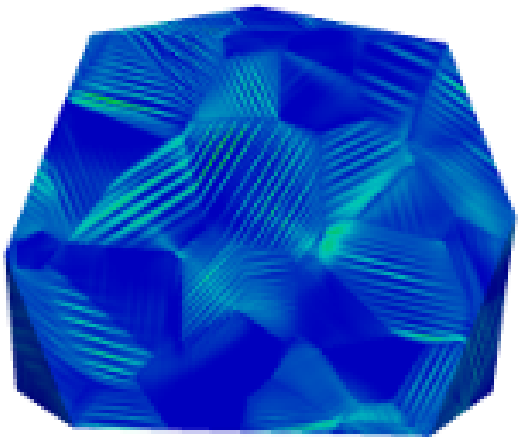
Book of Abstracts



IUTAM Symposium on

Generalized continua emerging from microstructures

19–23 July 2021
Paris, France

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Contents

Scope of the Symposium

The mechanics of generalized continua has become a well-established field of continuum mechanics of materials and structures, with many applications in computational mechanics. It includes gradient approaches (strain gradient media or gradient of mechanical variables like plastic strain or damage parameters) and higher order continua that rely on the introduction of additional kinematic degrees of freedom (Cosserat or micromorphic theories for instance). It is now well-accepted that such approaches are necessary in particular for the analysis of strain localization phenomena, up to fracture. They are also very effective for the description of size effects in the linear and nonlinear mechanical behavior of materials and structures. However, the formulation of such models very often remains purely phenomenological even though the origin of the generalized contributions is attributed to the underlying microstructure.

The objective of this symposium is to bring together experts in the field of generalized continua and homogenization methods in order to elaborate strategies for the construction of higher order theories starting from the detailed knowledge of the properties of the microstructure. The main features of the microstructure are very often of discrete nature: defects in crystalline solids or granular media, beam networks or unit cells in architectured materials or composites. How to predict size effects and the associated effective characteristic lengths from the collective behavior of defects under load or from the unit cell deformation fields in periodic media?

Fruitful discussions are expected between experts in the development of thermodynamically consistent phenomenological strain gradient theories and specialists of homogenization and coarse graining methods. The targeted material and structural properties are the static elastic-plastic and damage responses but also the dynamic behavior of architectured materials. The dispersion of waves in heterogeneous materials like metamaterials can be described successfully by generalized continuum models. We expect that the meeting of experts from different communities will result in common or alternative strategies to address scale bridging from microstructures to generalized continua. Generalized continuum models can be only validated by comparison and identification with field measurements which are now striving in experimental mechanics: crystal lattice orientation and dislocation density field by diffraction, strain field measurements by digital image correlation. This experimental information will be presented in the Symposium.

Conference topics

Theory of generalized continua
Instabilities and localization
Strain gradient plasticity
Crystal plasticity
Homogenization and generalized continua
Discrete defects in solids
Computational mechanics of generalized continua
Metamaterials
Geomaterials
Gradient damage and fracture
Phase field approaches

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Symposium website

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First Session
Theory of Generalized Continua

Monday 19 July 2021
14h00 – 16h00

14:00 *Explicit harmonic structure of bidimensional linear strain-gradient elasticity*
Nicolas Auffray

14:30 *Multiphase continua for fiber-reinforced materials*
Jérémy Bleyer

15:00 *Local micromorphic non-affine anisotropy*
Sebastian Skatulla

15:30 *Microtwist elasticity: Zero modes and polarization in kagome lattices*
Hussein Nassar

Explicit Harmonic Structure Of Bidimensional Linear Strain-Gradient Elasticity

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Abstract:

In the perspective of homogenization theory, strain-gradient elasticity is a strategy to describe the overall behaviour of materials with coarse mesostructure [1]. In this approach, the effect of the mesostructure is described by the use of three elasticity tensors whose orders vary from 4 to 6. Higher-order constitutive tensors make it possible to describe rich physical phenomena. However, these objects have intricate algebraic structures that prevent us from having a clear picture of their modeling capabilities. The harmonic decomposition is a fundamental tool to investigate the anisotropic properties of constitutive tensor spaces [2]. For higher-order tensors (i.e. tensors of order $n \geq 3$), their determination is generally a difficult task. In this talk, a novel procedure to obtain this decomposition is introduced. This method, which we have called the Clebsch-Gordan Harmonic Algorithm, allows one to obtain explicit harmonic decompositions satisfying good properties such as orthogonality and uniqueness. The elements of the decomposition also have a precise geometrical meaning simplifying their physical interpretation. This new algorithm is here developed in the specific case of 2D space and applied to Mindlin's Strain-Gradient Elasticity [4]. We provide, for the first time, the harmonic decompositions of the fifth- and sixth-order elasticity tensors involved in this constitutive law. The Clebsch-Gordan Harmonic Algorithm is not restricted to strain-gradient elasticity and may find interesting applications in different fields of mechanics which involve higher-order tensors [5, 6].

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Multiphase continua for fiber-reinforced materials

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Abstract: Fiber-reinforced materials exhibit interesting size effects due to the material contrast between fiber and matrix materials and the slenderness of the fibers. Homogenization theory cannot account for such effects when considering standard Cauchy continua. Multiphase continuum models [1, 2] are a class of generalized continua which consist of different media (fiber and matrix phases) possessing their own kinematics and in interaction with each other. An interaction energy depending on the difference of both phases displacements is at the origin of a size effect. Moreover, different boundary conditions can be prescribed at the same point for each phase, enabling to simulate, at the macroscopic level, matrix cracks bridged by intact fibers for instance. We will describe an extended homogenization procedure for deriving the generalized material parameters in the elastic setting. This procedure will be then validated by comparing against finite-element computations on the heterogeneous structure. Finally, by considering a phase-field brittle fracture model for the matrix and a damage model for the interface, we will show that periodic microcracking can be obtained using this generalized continuum model as commonly observed for such reinforced materials.

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Local micromorphic non-affine anisotropy

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Abstract: There has been increasing experimental evidence of non-affine elastic deformation mechanisms in biological soft tissues. These observations call for novel constitutive models which are able to describe the dominant underlying micro-structural kinematic aspects, in particular relative motion characteristics of different phases. This work proposes a flexible and modular framework based on a micromorphic continuum encompassing matrix and fiber phases. In addition to the displacement field, it features so-called director fields which can independently deform and intrinsically carry orientational information. Accordingly, the fibrous constituents can be naturally associated with the micromorphic directors and their non-affine motion within the bulk material can be efficiently captured. Furthermore, constitutive relations can be formulated based on kinematic quantities specifically linked to the material response of the matrix, the fibres and their mutual interactions. Associated stress quantities are naturally derived from a micromorphic variational principle featuring dedicated governing equations for displacement and director fields. This aspect of the framework is crucial for the truly non-affine elastic deformation description.
In contrast to conventional micromorphic approaches (e.g. [1][2]), any non-local higher-order material behaviour is excluded, thus significantly reducing the number of material parameters to a range typically found in related classical approaches.
In the context of biological soft tissue modeling, the potential and applicability of the formulation is studied for a number of academic examples featuring anisotropic fiber-reinforced composite material composition to elucidate the micromorphic material response as compared with the one obtained using a classical continuum mechanics approach.

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Microtwist elasticity: Zero modes and polarization in kagome lattices

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Abstract: The triangles of a kagome lattice can rotate with respect to one another with little effort. This twisting motion is at the origin of a whole space of zero-energy modes that the lattice can accommodate. Such modes are non-uniformly distributed in space: some are bulk modes and produce a distortion that reaches deep in the lattice; others are edge modes and prefer to localize near boundaries. More importantly, edge modes can be oddly distributed. In that case, they will prefer a boundary (say one with outward normal $\mathbf{n}$) over its opposite (say one with outward normal $-\mathbf{n}$). Thus, a finite sample of the lattice will appear to be soft if indented on one side and stiff if indented on the opposite side [1]. A polarized, i.e., parity-asymmetric, behavior of this kind goes beyond what (homogeneous) Cauchy elasticity, be it isotropic or not, can produce. Here, we report on an effective medium theory, baptized "microtwist elasticity", that can model the polarized behavior of kagome lattices on the macroscopic scale as well as the underlying odd distributions of edge zero modes [2]. The theory is of the generalized, kinematically enriched, type with one extra DOF carried by a periodic low-energy twisting motion. The extra DOF is interpreted as an angle but can also be understood as a change in area or in length. In that case, microtwist elasticity appears to be isomorphic to micro-dilatational elasticity.

The constitutive and balance equations of the theory are derived based on two-scale asymptotic expansions valid in the homogenization limit for (2D) kagome lattices that are weakly-distorted, i.e., when the triangles have homologous sides that are nearly aligned. For such lattices, localization occurs over macroscopic distances and polarization effects manifest themselves in the leading-order effective medium theory. Equivalently, weakly-distorted lattices exhibit a low-frequency optical dispersion branch that is strongly coupled to the acoustic branches. From that standpoint, the carried asymptotics are reminiscent of degenerate, or nearly-degenerate, $\mathbf{k}\cdot\mathbf{p}$ perturbation theory used in condensed matter physics [3]. Finally, we comment on how the theory accounts for certain topological properties of kagome lattices in connection to current trends in "topological insulators" which motivated the study in the first place.

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Second Session
Theory of Generalized Continua

Monday 19 July 2021
16h30 – 18h00

16:30 *Gradient materials: The different behavior of free boundaries of a body and the fictitious cut around some subbody*
Arnold Krawietz

17:00 *Modelling contact interactions of generalized continua: microblock contact model for a Cosserat body*
Stanislaw Stupkiewicz

17:30 *Three-dimensional solids and structures within strain gradient elasticity: numerical methods and model comparisons*
Jarkko Niiranen

Gradient materials: The different behavior of free boundaries of a body and the fictitious cut around some subbody

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Abstract: When dealing with simple materials, no distinction has to be made between the boundary of a real body and the fictitious cut around some subbody. A recent investigation ([1], open access) demonstrates, however, that the situation is different with gradient materials: A crust shell exists at the free surface of a third gradient material with forces and moments as cutting loads and an edge beam exists where patches of the free surface meet. This beam has a cutting force and can be loaded by forces and moments per unit length. At vertices where several beams meet, a single force can be applied.

The simplest gradient theory is that of the Kirchhoff plate. Its boundary conditions were analyzed by Thomson and Tait almost 150 years ago.

It shall be demonstrated why an edge beam must be present at a free boundary of a plate but not anywhere in the interior. At first, the acceptance of this fact may seem hard, but fortunately, we can gain an insight into it by treating the elastic torsion of a board: On the one hand by the two-dimensional theory of plates and on the other hand by de Saint-Vénant's three-dimensional theory of torsion. The pattern of the shear stress trajectories reveals our interpretation as the only possible one.

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Modelling contact interactions of generalized continua: microblock contact model for a Cosserat body

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Abstract: Microstructured materials may exhibit size effects when the characteristic dimension of the body is small relative to the characteristic size of the microstructure. One of the feasible approaches to the modelling of the size effects is to resort to generalized continuum theories that include higher-gradient terms and the related intrinsic length-scale parameters. Formulation of a contact problem for such a continuum necessarily requires that adequate contact conditions are formulated for the additional kinematic variables or for the respective generalized tractions. The simplest choice is to assume that the related generalized tractions are equal to zero, see e.g. [1], but this choice is not necessarily justified from the physical point of view. In this work, we address several related open problems, namely, (i) how to enhance the classic contact conditions to include the effects of the additional kinematic variables, (ii) how to link the enhanced contact model to the underlying microstructure of the solid, and (iii) how to do it in a consistent manner.

As a first step towards a new class of contact models for generalized continua, a microblock contact model has been derived [2] for a Cosserat continuum based on simple micromechanical considerations. The essential feature of the model is that contact tractions and contact micro-moments are coupled in a consistent manner. In particular, for an elastic microstructured solid, the potential structure of the problem is preserved.

Two sample problems are studied in order to illustrate the non-trivial effects introduced by the non-standard boundary conditions imposed by the microblock contact model. First, the problem of compression of an infinite strip with nonaligned microblocks is considered, and an analytical solution is derived for the corresponding boundary layers. Second, a Hertz-like contact problem is solved numerically by means of the finite element method, thus revealing non-standard features of the solution and the related size effects.

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Three-dimensional solids and structures within strain gradient elasticity: numerical methods and model comparisons

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Abstract: Literature on the most common dimensionally reduced structural models within different theories of generalized continuum mechanics is vast, most probably due to the relative commonness, simplicity and applicability of the corresponding well-known models of the classical continuum mechanics. The small amount of generalized constitutive parameters incorporated into these reduced models has definitely been an attraction for scholars as well [1]. On the contrary, literature on the three-dimensional formulations of generalized continuum mechanics is still quite limited, partly due to the large number of constitutive parameters incorporated into the models and partly due to the relatively high complexity and computational cost of the related numerical methods [2, 3].

This contribution focuses on comparing the structural dimension reduction models to the corresponding three-dimensional "parent" models of strain gradient elasticity, especially in the context of microarchitectural, lattice or cellular, structures [3, 4]. These comparisons rely on analytical and numerical solutions of the different models and incorporate constitutive parameters obtained by different computational homogenization techniques. For microarchitectural structures, non-homogenized fine-grain models of classical elasticity provide reference solutions, and hence enable a simulation-based model validation. Ritz–Galerkin methods, in the form of higher-order finite element methods, are adopted for obtaining reliable numerical solutions for those problems which are lacking for analytical benchmark solutions.

Some of the main characters of the structural models, e.g., the so-called stiffening effect for beams, are in accordance with the three-dimensional models – and with the fine-grain reference models when regarding microarchitectural structures – whereas some features, e.g., the so-called boundary layers for bars, can be questioned according to the model comparisons.

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First Session
Crystal Plasticity

Tuesday 20 July 2021
8h30 – 10h30

8:30 *A FFT-based approach for Mesoscale Field Dislocation Mechanics: applications to internal length scale effects in polycrystals and steel matrix composites*
Stephane Berbenni

9:00 *A mesoscale continuum approach of dislocation dynamics and the approximation by discontinuous Galerkin methods*
Christian Wieners

9:30 *Modeling plastic slip localization within polycrystals*
Aldo Marano

10:00 *On the control of elastic gaps in Gurtin-type strain gradient crystal plasticity theories using uncoupled dissipation assumption*
Mohamed Jebahi

A FFT-based approach for Mesoscale Field Dislocation Mechanics: applications to internal length scale effects in polycrystals and steel matrix composites

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Abstract: An enhanced crystal plasticity elasto-viscoplastic FFT (Fast Fourier Transform) formulation coupled with a mesoscale continuum dislocation mechanics theory (MFDM) is presented [1,2]. The present numerical approach, named "MFDM-EVPFFT", accounts for plastic flow and hardening from densities of geometrically necessary dislocations (GNDs) in addition to statistically stored dislocations (SSDs). The model also captures GND density evolution through a filtered numerical spectral approach [3], which is here coupled with stress equilibrium through the elasto-viscoplastic FFT method (EVPFFT) [4]. The discrete Fourier transform method together with finite difference schemes is applied to solve both lattice incompatibility problem and Lippmann-Schwinger equation (see [5] and [6] for numerical details). Numerical results are first shown for two-phase laminate composites with plastic single crystal channels and elastic precipitates for both monotonous and reversible shear loadings. A grain size effect is obtained due to the influence of GND densities on the overall and local hardening behaviors [7]. In addition, the role of GND densities on the Bauschinger effect is reported during reversible loadings, where the hardening mechanisms due to piling-up/unpiling-up of GNDs is examined [8]. 3D face-centered cubic (FCC) polycrystals using periodic Voronoï tessellations are considered using different RVEs with various average grain sizes. In comparison with conventional crystal plasticity models, it is shown that GND density accumulations at grain boundaries modify both intra-granular plastic fields and stress profiles, which is at the origin of the grain size effect on the flow stress of polycrystals [9]. Lastly, the MFDM-EVPFFT model is also applied to particle interspacing effects on the mechanical behavior of a Fe-TiB2 metal matrix composite [10].

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A mesoscale continuum approach of dislocation dynamics and the approximation by discontinuous Galerkin methods

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Abstract: We consider a mesoscale continuum model for the evolution of dislocation density in small-strain crystal plasticity. The model is based on the continuum dislocation dynamics theory and extended by a formulation for impenetrable grain boundaries. We introduce a fully coupled numerical method combining a conforming finite element approximation of elasto-plasticity with an implicit Runge-Kutta discontinuous Galerkin discretization of the dislocation microstructure which allows for 3d computations including multiple slip systems and dislocation interaction. In our scheme, we use an explicit coupling scheme by alternately incrementing the dislocations solving the CDD system, and then updating the plastic strain by a flow rule depending on the dislocations and the stress which results from the equilibrium equation for the displacement.

In our numerical model we consider the 3d dislocation density evolution for face-centered cubic (fcc) crystals with 12 slip systems. Similar to DDD, grain boundaries are modeled as impenetrable obstacles retaining dislocations in the respective grain. By this means, a continuum plasticity model is accomplished including a physically based representation of grain boundaries. The theory is validated considering a fcc tricrystal under tensile loading showing that dislocation density gradients close to the boundary can be reproduced dependent on the grain orientations without additional fitting parameters. The numerical results are compared with DDD simulations derived in the literature.

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Modeling plastic slip localization within polycrystals

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Intragranular localization of plastic slip plays a key role in the deformation and fracture mechanisms of polycrystalline materials. As shown by Asaro & Rice [1], softening crystal plasticity (CP) equations predict the formation of two types of localization bands as bifurcation modes in homogeneous crystals: slip bands and kink bands. With the advances of high performance numerical simulation, those equations can be integrated over large polycristalline unit cells with a high-resolution, in order to bridge together the localization band and polycrystalline scales. This work explores the potential of this approach to achieve accurate simulation of slip localization and its consequences on polycrystalline materials mechanics, through massively parallel FFT-based simulations [2].

We first link the degree of localization to the macroscopic mechanical behavior of materials through a pragmatic modeling approach. Polycrystalline simulations with prescribed slip band networks where carried out, varying the spacing and width of the bands. Results show that degree of localization strongly influences the macroscopic kinematic hardening of the material. Besides, this approach is able to capture the increased intergranular fracture susceptibility induced by localization.

Then, we investigates the ability of crystal plasticity theory to simulate intense slip localization bands, by conducting a systematic analysis of the fields simulated, to characterize localization bands geometry, number and nature. It is shown that classical CP models fundamentally cannot accurately predict realistic bands networks, as they predict slip and kink bands as two equivalent localization modes. Hence, they predict similar amounts and characteristics for both type of bands, whereas in reality they are two distinct phenomena.

To break the modes equivalence, a class of Nye's tensor based gradient plasticity models are used [3]. It is evidenced that these models change qualitatively the nature of simulated slip localization. They significantly reduce the amount of simulated kink bands, allow to control their width separately and can predict their decomposition in a dense succession of slip bands. This results in physically more accurate localization networks, mostly composed of slip bands, and where slip and kink bands have distinct and realistic features.

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On the control of elastic gaps in Gurtin-type strain gradient crystal plasticity theories using uncoupled dissipation assumption

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Abstract: The excellent capabilities of strain gradient plasticity (SGP) theories in capturing small scale effects have motivated numerous SGP studies in the last two decades. However, despite the great progress made on these theories, several challenging issues related to them remain to be addressed.

One of these issues is concerned with the description of the dissipative processes due to plastic strains and their gradients. In almost all existing SGP works, such processes are described using generalized effective plastic strain measures, which imply plastic strains and their gradients in a coupled manner. This kind of measures makes the issue of proposing robust and flexible dissipation formulations and the control of important dissipative effects difficult. Using such measures, it is not easy to control, for example, the elastic gaps under certain non-proportional loading conditions [3].

In most cases, the coupling between dissipative processes is only used by assumption with no physical confirmation. In spirit of multi-criterion approaches [1], the present work proposes a flexible uncoupled dissipation assumption to describe dissipative processes. These processes are assumed to be derived from a pseudo-potential that is a sum of two independent functions of plastic strains and plastic strain gradients. Using this assumption, a strain gradient crystal plasticity (SGCP) model based on the model of Gurtin *et al.* [2] is developed and applied to simulate various two-dimensional plane-strain tests under proportional and non-proportional loading conditions.

Results associated with these tests show the great flexibility of the proposed model in controlling some major dissipative effects, such as elastic gaps. A simple way to remove these gaps under certain non-proportional loading conditions is provided [4].

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Second Session
Crystal Plasticity

Tuesday 20 July 2021
11h00 – 12h30

11:00 *Microstructural aspects of gradient-enhanced crystal plasticity*
Henryk Petryk

11:30 *Plastic flow and dislocation strengthening in a continuum formulation of dislocation dynamics*
Katrin Schulz

12:00 *Analytic solutions for strengthening of a strain gradient plasticity material reinforced by small elastic particles*
Jonas Faleskog

Microstructural aspects of gradient-enhanced crystal plasticity

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Abstract: The classical continuum theory of single crystals deformed plastically by multislip, established at arbitrary strain by Hill and Rice [1], involves no internal length scale. To incorporate size effects, a number of strain-gradient theories of plasticity have been developed, notably [2], also referred to here to honour Quoc-Son Nguyen's memory. Nevertheless, the internal length scale is rarely not set arbitrarily but has a physical meaning related to the evolving internal microstructure of a crystal [3].

To determine the dissipation rate in a gradient-enhanced theory, besides the free energy rate also a non-classical external power component must be defined. It is shown, in reference to slip-gradient and micromorphic theories, that this component cannot be arbitrary but is subject to a thermodynamic condition [4, 5]. The thermodynamic condition, in turn, provides a basis for deriving, rather than assuming, the boundary conditions and the expression for internal power. Existence of microstructural interpretation of the non-classical external power component can be helpful in verifying physical soundness of a gradient theory and is thus worth investigating.

In the minimal gradient enhancement of crystal plasticity [3], the external power is still classical while an evolving internal length scale appears in the extra term in the hardening law. It is shown that this length scale is uniquely expressed through standard parameters of a non-gradient hardening law. Remarkably, the experimentally observed indentation size effect in a Cu single crystal is captured correctly [6] in spite of the absence of any adjustable length-scale parameter in this 'minimal' framework. This may be due to the fact that the internal length scale is closely linked to the mean free path of dislocations and thus to the evolving microstructure.

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Plastic flow and dislocation strengthening in a continuum formulation of dislocation dynamics

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Abstract: The dynamics of dislocations causing plastic deformation in crystalline materials depends on the applied stress fields and the stress interaction in the dislocation microstructure. Regarding the kinematic evolution of curved dislocation lines, recently rigorous techniques have been developed for performing meaningful averages over systems of moving, curved dislocations, yielding evolution equations for a dislocation density tensor, see [1,2].
However, the evolution of a dislocation system is significantly characterized by the formation of dislocation networks due to dislocation interaction and reactions of different slip systems. Modeling dislocation multiplication due to interaction and reactions and the corresponding dislocation network evolution on a mesoscopic scale is an important task for the physically meaningful description of stage II hardening in face-centered cubic crystalline materials. The complexity of the detection and incorporation of the underlying processes has been revealed in [3,4].
In this contribution, we analyze plastic flow and dislocation strengthening in discrete dislocation networks and derive a formulation of dislocation multiplication and network evolution in a dislocation-based continuum formulation of plasticity. A mechanism-based homogenization considering different reaction types is proposed in three-dimensional fcc systems. As a key feature, the presented model includes the generation of dislocations based on an interplay of dislocation density on different slip systems. This particularly includes slip systems with vanishing shear stress. The results show, that the proposed continuum formulation allows for a physically meaningful microstructural evolution of dislocation networks without self-replication of dislocations density. The results are discussed in comparison to discrete dislocation dynamics simulations as well as experiments exposing the coupling of different slip systems as the central characteristic for the increase of dislocation density on active and inactive slip systems.

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Analytic solutions for strengthening of a strain gradient plasticity material reinforced by small elastic particles

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Abstract: Small particles or precipitates introduced in metallic alloys through different types of heat treatments may lead to a remarkable strengthening and increase in yield stress [1]. The primary cause for this strengthening is that particles serve as obstacles to dislocation glide or cross slip as proposed in the pioneering work of Orowan. For example, the yield stress has experimentally been observed to increase up to a factor five in some aluminium alloys [2] and by a factor of two or more in Ni-based superalloys and in maraging steels [3]. A common denominator in those precipitation strengthened materials is that particles are small, and typically smaller than a material length scale ℓ arising in strain gradient plasticity (SGP) theories motivated by dislocation mechanics.

Here, this problem is analysed by a higher order strain gradient plasticity (SGP) theory [4]. By recasting the governing equations on non-dimensional form, the structure reveals that the plastic strain in the matrix material is to zeroth order approximation constant for a sufficiently small particle size a in comparison to the material length scale ℓ associated with the SGP theory employed. Based on this observation, a perturbation solution has been developed by expansions of all field variables in terms of a/ℓ and the volume fraction of particles f. The simple structure of the plastic strain field is also exploited to derive an upper bound solution from the principles of virtual work and maximum plastic dissipation. These analytical solutions are then used to derive expressions for the yield stress that account for a random distribution of particles of various size and shape with elastic constants that differ from the matrix. The accuracy and range of validity of these solutions are demonstrated by comprehensive 2D and 3D finite element analyses [5,6] of material volumes containing realistic distributions of particles of spherical and spheroidal shape of various elastic modulus. The results show that significant strengthening will arise provided that the representative particle size is smaller than the material length scale ℓ of the SGP material.

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First Session
Strain gradient plasticity

Tuesday 20 July 2021
14h00 – 16h00

14:00 *Distortion gradient plasticity modelling of the small-scale behaviour of metals under non-proportional loading*
Lorenzo Bardella

14:30 *A phase field fracture and strain gradient plasticity-based model for predicting hydrogen embrittlement*
Emilio Martinez-Paneda

15:00 *Modeling micron-scale compression molding*
Christian Niordson

15:30 *Enhanced Strength of Cu-Gr-Cu nanolaminate*
Jeff Kysar

Distortion gradient plasticity modelling of the small-scale behaviour of metals under non-proportional loading

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Abstract: In the context of strain gradient plasticity (SGP) under general loading histories, we build on the Mixed energetic-dissipative Potential (MP) proposed in [1], following earlier contributions by Chaboche, Ohno, and co-workers for nonlinear kinematic hardening within size-independent metal plasticity. The MP is given by M quadratic terms that each transitions, at a distinct threshold value, into a linear dissipative contribution. Therefore, the MP involves $2M$ positive material parameters, consisting of the M threshold values and M moduli weighing each quadratic recoverable term. Our analysis [2] demonstrates that, under proportional loading, the MP limit for $M \to \infty$ converges to a *less-than-quadratic* (LTQ) potential with specific properties. This is a key result for the material parameters identification. Moreover, we provide a formula for the characterisation of the recoverable and dissipative contributions of any possible MP limit, showing that, in relation to the predicted size effects with diminishing size, one can select the MP such that its contribution to the strengthening (that is, increase in yield point) is mostly dissipative, while its contribution to the strain hardening increase is mostly energetic.

On this basis, we plug the MP into our previous finite element model for the torsion problem [3], which implements a logarithmic LTQ potential into Gurtin's SGP relying on Nye's dislocation density tensor (that is, *distortion* gradient plasticity). This allows the accurate fitting of the experimental data of Liu et al. [4] on the cyclic torsion of copper wires of diameter spanning from 18 to 42 micrometres. We identify the MP material parameters by resorting to the Coliny evolutionary algorithm coded in Dakota (https://dakota.sandia.gov/). The results show unprecedented good agreement between experimental data and model predictions [5].

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A phase field fracture and strain gradient plasticity-based model for predicting hydrogen embrittlement

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Abstract: We present a new theoretical and computational framework for predicting hydrogen assisted cracking in elastic-plastic solids. Non-local constitutive choices are adopted for both damage and plasticity [1]. The model combines, for the first time: (i) stress-assisted diffusion of solute species, (ii) higher order strain gradient plasticity [2], and (iii) a hydrogen-sensitive phase field fracture formulation [3], inspired by first principles calculations. The theoretical model is numerically implemented using a mixed finite element formulation and several 2D and 3D boundary value problems are addressed to gain physical insight and showcase model predictions. The results reveal the critical role of plastic strain gradients in rationalising decohesion-based arguments and capturing the transition to brittle fracture observed in hydrogen-rich environments. Large crack tip stresses are predicted, which in turn raise the hydrogen concentration and reduce the fracture energy. The computation of the steady state fracture toughness as a function of the cohesive strength shows that cleavage fracture can be predicted in otherwise ductile metals using sensible values for the material parameters and the hydrogen concentration. In addition, we compute crack growth resistance curves in a wide variety of scenarios and demonstrate that the model can appropriately capture the sensitivity to the plastic length scales, the fracture length scale, the loading rate and the hydrogen concentration. Finally, the modelling framework is coupled with in-line inspection measurements to predict structural failure from a given distribution of defects. The paradigmatic case of a pipeline subjected to pit corrosion damage is addressed, showcasing the capabilities of the model in delivering large-scale multi-physics predictions as a function of the environment, the material properties and the loading conditions.

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Modeling micron-scale compression molding

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Micron-scale metal forming is highly influenced by material size effects due to plastic strain gradients. While compression molding with characteristic feature sizes above about 100 microns exhibits intrinsic size-effects mainly through the Hall-Petch relation, molding with smaller feature sizes is explicitly affected by hardening due to plastic strain gradients and related geometrically necessary dislocations. Recent experimental studies have shown how the characteristic molding pressure increases with decreasing feature size. While this effect is well modelled using strain gradient plasticity theory, capturing the details of the imprinted features in terms of their sharpness has proven challenging. The present study demonstrates how a finite strain version of Gudmundson's strain gradient plasticity theory can capture the size effects in compression molding of copper in terms of the characteristic pressure. However, the feature geometry is poorly represented by the plastic flow model alone, leading for example to difficulties in accurately assessing the contact pressure between the punch and the molded material. It is argued that plastic damage and the creation of new surface is essential in compression molding of sharp features on the micron-scale, and a simple shear cohesive zone model is proposed in order to improve modeling capabilities.

Enhanced Strength of Cu-Gr-Cu nanolaminate

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Understanding the deformation mechanism in nanocomposites is critical to realizing a host of next-generation technologies. Graphene's unparalleled mechanical properties -- owing to its two-dimensional geometry, high intrinsic strength, and Young's modulus -- provide us with an opportunity to engineer metal/graphene composites with strengths that do not naturally occur. Graphene's (Gr) ability to act as a strength enhancer depends on the interface interactions and the composite's microstructure. Here we demonstrate an industrially scalable and transfer-free microstructure design of Cu-Gr-Cu nanolaminate that enhances the composite's strength. Bending tests performed on fabricated Cu-Gr-Cu nanolaminate cantilever beams exhibit a remarkable strengthening effect over a control Cu-Cu nanolaminate. A significantly higher load is required to deflect a Cu-Gr-Cu cantilever beam indicating that the presence of single atomic layer of graphene enhances the strength of the composite. The enhancement in strength of Cu-Gr-Cu nanolaminate suggests a build-up of dislocations at the Cu-Gr interface, which limits the plastic slip that can occur at the internal interface. We developed a strain gradient plasticity computational model of the experimental system based upon Gudmundson's higher order theory and implemented it as a user element in ABAQUS. A set of material parameters is identified that reproduce the experimental force vs. displacement results for both the Cu-Cu and the Cu-Gr-Cu nanolaminate. The only difference in the simulations is that zero plastic strain boundary conditions are enforced at the Cu-Gr interfaces in the Cu-Gr-Cu nanolaminate. The results give insight into the design of metal-graphene composites as well as structure of strain gradient plasticity theories.

Second Session
Strain gradient plasticity

Tuesday 20 July 2021
16h30 – 18h00

16:30 *The evolution of Hooke's law under finite plastic deformations* for fiber reinforced materials
Albrecht Bertram

17:00 *A stochastic solver based on the residence time algorithm for crystal plasticity models*
Jaime Marian

17:30 *Gradient models for softening thermo-plasticity at large strain*
Jerzy Pamin

The evolution of Hooke´s law under finite plastic deformations for fiber reinforced materials

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Abstract: For the simulation of plastic deformations it is necessary to calculate the current stresses by an elastic law associated with the current elastic range. In most cases a linear isotropic or anisotropic elastic law is chosen. However, this elastic law cannot be assumed to be constant since the plastic deformation also influences its properties. The modeling of this evolution of Hooke´s law under finite plastic deformations has been a challenge within finite plasticity modeling, and will probably also be in the future.

For special classes of materials we have a clear picture of this evolution, while for others no solutions have yet been given, and can hardly be expected. Within the context of crystal plasticity, the concept of *isomorphy* of elastic ranges almost perfectly applies [1]. The isomorphic elastic law is determined by just one tensorial variable which we identify as the plastic deformation tensor from the multiplicative decomposition, for which a flow rule is needed.If we consider polycrystals the situation changes completely. Here the evolution of the elastic behavior is dominated by the evolving crystallographic texture. We know from metal forming processes that a material may be almost isotropic in its initial state, while it can go through almost all classes of minor symmetry in the course of the deformation, see, e.g., [2] .

A different situation is presented by a material which consists of fibers and a matrix material both assumed to be (isotropic) elastoplastic. Here the plastic deformations lead to changes of the configuration of the fibers which influences the elastic behavior of the compound material in an obvious way. In the present approach, the elastic behavior of regular fiber arrangements is modeled by a superposition of transversely isotropic stiffnesses linked to each individual fiber bunch [3]. During the plastic deformation, the direction of these bunches is varied under the plastic deformation. So the elastic anisotropy is directly linked to the plastic deformation. This effect has been called *material plasticity* [1], [4].

In the presentation, the compound material is modeled by a representative volume element. The overall elastic stiffnesses have been numerically calculated by FEM. The macro behavior has been modeled by the approach above and compared to the numerical results. Both results exhibit good conformity. Therefore, the presented approach is justified.

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A stochastic solver based on the residence time algorithm for crystal plasticity models

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Abstract: The deformation of crystalline materials by dislocation motion takes place in discrete amounts determined by the Burgers vector. Dislocations may move individually or in bundles, potentially giving rise to intermittent slip. This confers plastic deformation with a certain degree of variability that can be interpreted as being caused by stochastic fluctuations in dislocation behavior. However, crystal plasticity (CP) models are almost always formulated in a continuum sense, assuming that fluctuations average out over large material volumes and/or cancel out due to multi-slip contributions. Nevertheless, plastic fluctuations are known to be important in confined volumes at or below the micron scale, at high temperatures, and under low strain rate/stress deformation conditions. Here, we present a stochastic solver for CP models based on the residence-time algorithm that naturally captures plastic fluctuations by sampling among the set of active slip systems in the crystal. The method solves the evolution equations of explicit CP formulations, which are recast as stochastic ordinary differential equations and integrated discretely in time. The stochastic CP model is numerically stable by design and naturally breaks the symmetry of plastic slip by sampling among the active plastic shear rates with the correct probability. This can lead to phenomena such as intermittent slip or plastic localization without adding external symmetry-breaking operations to the model. The method is applied to body-centered cubic tungsten single crystals under a variety of temperatures, loading orientations, and imposed strain rates.

Gradient models for softening thermo-plasticity at large strain

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Abstract: Engineering materials subjected to large loads and/or high temperatures often exhibit softening. It can be caused by material, geometrical or thermal effects, or their interactions. The phenomenological modelling of such material (or structural) response requires regularization to preserve well-posedness of the problem and reduce discretization sensitivity of numerical simulations. In this paper higher order gradients of a selected field variable are introduced via an additional averaging equation.

The considered thermo-plastic models admit large deformations in a static process. Three model variants are considered: the extension of the model of Geers [1] to thermo-plasticity, the coupled model with a gradient-dependent yield function proposed by de Borst and Mühlhaus [2] and modified according to Peerlings [3], and finally the model with temperature averaging proposed by Wcisło and Pamin [4].

The numerical tests are performed using finite element programs implemented using the automatic code generator *AceGen* within *Mathematica* environment, cf. Korelc and Wriggers [5]. The benchmark of a plate in tension is used to compare the features of the models, whereby the importance of heat conduction in strain localization is analyzed. Algorithmic aspects are also discussed. Moreover, simulations of the evolution of Lueders bands in a bone-shape specimen are performed to examine the influence of temperature on the modelled phenomenon, see Mucha et al [6].

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First Session
Homogenization and generalized continua

Wednesday 21 July 2021
8h30 – 10h30

8:30 *Green functions and integral representation of anisotropic second gradient continua The case of pantographic lattices*
Claude Boutin

9:00 *Predictive strain-gradient homogenization of a pantographic material with compliant junctions and experimental evidence*
Arthur Lebée

9:30 *Nonlinear gradient models in hyper-elasticity: from slender structures to architectured materials*
Claire Lestringant

10:00 *Direct FE2 for concurrent multiscale modelling of heterogeneous thin plate structures*
Leong Hien Poh

Green functions and integral representation of anisotropic second gradient continua. The case of pantographic lattices

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Abstract: This paper addresses the integral representation methods in generalized elastic continua by considering the case of pantographic lattices (PL). In the general case, this problem is rather unexplored because it requires the knowledge of fundamental (generalized) solutions. Such Green's functions exist for isotropic second gradient media where the effects of the second gradient slightly perturb the effects of the simple gradient, [1]. However, PLs do not fullfil these assumptions because, (i) the single gradient and second gradient energies are of the same order, and (ii) they are extremely anisotropic media [2].

First, we determine analytically the Green's functions for orthogonal lattices in small deformations. These solutions provide the kinematic field in infinite PL media, subject to point forces or couples. In accordance with the morphology, they exhibit a very strong directivity (in the lattice directions) and a singularity in $1/\sqrt{x)}$ at the point of application of a force [3].

Second, using distribution theory, we establish the representation of the kinematic variables, in the form of surface integrals of the boundary conditions (in force (stress) and couple (hyperstress)) which are radiated by the corresponding Green's functions.

Hence, it is shown that the solution of a well-posed boundary problem can be performed in two steps. First, the resolution of two Fredholm integrals, enable to determine the unknown boundary conditions (i.e. that which are not prescribed). Then, the transfer of these into the integral formulation, yields the field(s) at any point of the PL. The homogenization of PL media [2] allows a clear and satisfactory physical micro-macro- interpretation of these results.

Beyond the PLs, this study provides a first analytical Green's function for second gradient anisotropic media that cannot be reduced to Cauchy media. It opens the possibility of using integral representation methods for generalized continua. Such a formulation allows to reduce the dimension of the numerical problem. Moreover, the exploitation of Green's functions which encapsulate the physics of the micro-structure allows to better tackle ill-conditioned problems.

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Predictive strain-gradient homogenization of a pantographic material with compliant junctions and experimental evidence

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Abstract: This work presents an architectured material featuring significant strain-gradient effects and called pantographic material. It is a plate made of a single and continuous linear elastic material containing voids and thus is easy to fabricate. The pattern consists of triangles connected by thin junctions and arranged in such a way that two floppy strain modes are present. A homogenization scheme based on the two-scale asymptotic expansion is suggested, keeping only significant strain-gradient contributions in the homogenized energy by means of an adequate projection. The predictions from the homogenization scheme are validated against a full-scale simulation and yield very good L^2 error estimates whereas the classical first-gradient homogenization fails [1]. Furthermore, samples of the pantographic material were laser cut, tested and revealed strain gradient effects comparable to the homogenization scheme predictions.

References

[1] Durand B, Lebée A, Seppecher P, Sab K (2021) Predictive strain-gradient homogenization of a pantographic material with compliant junctions. submitted

Nonlinear gradient modelsin hyper-elasticity: from slenderstructures to architectured materials.

Claire Lestringant

In this talk, I will discuss the parallel between slender structures and architectured materials. Both classes of problems can be described using macroscopic models: 1D models for slender structures and homogenised continuum descriptions for architectured materials. Macroscopic approaches assume a separation of scales governed by the aspect ratio for thin structures or by the microstructural length scale for periodic materials.

Phenomena such as localisation and scale effects occur in these systems and require the macroscopic approaches to describe non linearities and to introduce a length scale, typically through a gradient term. However, classical approaches to homogenisation and dimension reduction rarely combine these two aspects. Classical rod theories for example account for the stretching, bending,and twisting strains of slender structures in a linear way and do not represent finite cross-sectional strains or finite-thickness effects. Therefore,describing the compression of wide columns, predicting the emergence of shape due to heterogeneous pre-stress in growing filaments or describing localisation phenomena such as necking remain challenging tasks.

Using dimension reduction as a starting point, I will introduce a systematic method to establish 1D models for non-linear, slender elastic structures starting from the three-dimensional description of a hyper-elastic prismatic solid. Using a formal asymptotic expansion performed near a finitely pre-strained state, I will derive 1D models that account for stretching, bending,and twisting in a non-linearway. The resulting models retain sources of nonlinearity coming from the geometry and the constitutive law, include higher-order terms depending on strain gradient and thus accurately capture interfaces during localisation. I will illustrate the dimension reduction method on elasto-capillary necking and discuss how it can be extended to derive nonlinear gradient models for architectured materials.

Direct FE^2 for concurrent multiscale modelling of heterogeneous thin plate structures

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Abstract:

The FE^2 method systematically translates macro kinematic constraints to the underlying (micro) RVEs, and extracts the effective RVE responses to macro continuum in an energetically consistent manner. In the literature, many researchers have demonstrated the predictive capability of FE^2 across a wide range of problems. The conventional FE^2 numerical framework adopts a staggered solution strategy between the macro and micro analyses. This limits the adoption of FE^2 method by inexperienced researchers / engineers to solve practical engineering problems using commercial FE software, because a generally complex subroutine needs to be written. Moreover, the reading and writing of data from a macro point to the micro RVE, and vice versa, typically expends significant computational time in a commercial FE software. To this end, a direct FE^2 method has been proposed in [1] and implemented in the commercial software ABAQUS, where macro kinematic constraints are applied directly on the RVEs superimposed on the macro elements. This results in a monolithic numerical framework, without the need to write any subroutines. Compared to the conventional FE^2 implementation using commercial software, the overall computational time is also reduced since the reading and writing of data are now omitted [2]. In this contribution focusing on thin plate structures, the direct FE^2 method is extended based on Kirchhoff-Love thin plate kinematics, and implemented in ABAQUS without the need for subroutines. The predictive capability of the direct FE^2 method for this higher order formulation is demonstrated by comparing against reference solutions from direct numerical simulations, via two problems involving reinforced concrete slabs.

References

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Second Session
Homogenization and generalized continua

Wednesday 21 July 2021
11h00 – 13h30

11:00 *Interpretation of the moduli of isotropic micromorphic elasticity by harmonic decomposition and analytical homogenisation*
Geralf Hütter

11:30 *Hashin–Shtrikman bounds on the effective properties of stress-gradient materials*
Karam Sab

12:00 *Enhanced flexoelectricity in heterogeneous piezoelectric composites using topology optimization*
Julien Yvonnet

12:30 *Analysis of the failure of heterogeneous materials: a bottom-up approach*
Julien Réthoré

13:00 *Direct and energy based homogenization approaches within the second gradient elasticity theory: examples and general relations*
Yuri Solyaev

Interpretation of the moduli of micromorphic elasticity by harmonic decomposition and analytical homogenisation

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Abstract: Since the pioneering works of Mindlin and Eringen in 1964, the micromorphic theory has gained much attention and it has been used to model different kinds of size effects, from the atomic scale up to macroscopic applications of foams, meta-materials and biological materials. Still a challenge is the large number of constitutive parameters in the general theory which amounts to 18 even for isotropic (centro-symmetric) linear-elastic material in 3D. That is why reduced micromorphic theories are mostly used, where certain of these constitutive parameters are set to zero a priori based on more or less heurstic considerations.

The present contribution elucidates the interpretation of the 18 constitutive parameters of the full micromorphic theory. For this purpose, a harmonic decomposition of the respective tensors is performed as done by Glüge et al. [1] for the strain gradient theory. The individual modes like the spherical, deviatoric and skew parts of the classical displacement gradient and respective modes for the nonclassical tensors of microdeformation and its gradient are interpreted by means of the micromorphic homogenisation theory [2] for Hashin's composite shell model [3] of a spherical volume element with inclusion or pore.

It is demonstrated that the harmonic decomposition allows a favorable solution of the resulting elasticity problem at the microscale in terms of spherical harmonics. Thus, all constitutive parameters of the micromorphic theory can be computed in closed-form. The resulting parameters are used to predict size effects under basic loading conditions like simple shear, bending or torsion for which the analytical micromorphic solution has been found recently [4]. In particular, it is shown that the predicted size effect vanishes for microhomogeneous material as expected and that the approach yields good predictions for foam-like materials.

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Hashin–Shtrikman bounds on the effective properties of stress-gradient materials

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Abstract: Stress-gradient materials, introduced by Forest and Sab [1], are generalized continua with two generalized stress variables: The Cauchy stress field and its gradient. Such models are relevant for nanocomposites exhibiting “negative” size-effect [2] and foams [3]. In this presentation, we introduce, for homogenization purposes, an extension to stress-gradient materials of the principle of Hashin and Shtrikman. The variational principle is first stated within the framework of periodic homogenization, then extended to random homogenization. Contrary to the usual derivation of the classical principle, we adopt here a stress-based approach, much better suited to stress-gradient materials. We show that, in many cases of interest, the third-order trial eigenstrain may be discarded, leaving only one (second-order) trial eigenstrain in the functional to optimize. For N-phase material, the bounds are very similar in structure to their classical counterpart. One notable difference is the fact that, even in the case of isotropy, the bounds depend on some additional microstructural parameters (besides the usual volume fractions) as shown in [4].

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Enhanced flexoelectricity in heterogeneous piezoelectric composites using topology optimization

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Abstract: Flexoelectricity is the property of an insulating material to polarize when subjected to strain gradient (inhomogeneous deformation). However, these properties are usually very low in natural materials. In this work, we present a topology optimization framework to design periodic composites comprised of piezoelectric constituents that exhibit large flexoelectric constants. The novelty of the approach is that it leverages a representative volume element (RVE)-based computational homogenization approach that enables the analysis of periodic composites where the characteristic dimensions of the microstructure are significantly smaller than those of the structure, and as such requires only the optimization of a single RVE rather than that of the entire structure. We utilize this approach to analyze the enhancement in flexoelectric constants that can be achieved in different types of PZT-based composites, including hard–hard (PZT–PZT), and hard–soft (PZT–polymer composite, and porous PZT) structures [1]. In all cases, significant enhancements are observed, with improvements between 2 and 15 times those of a naive guess, with some designs reaching a factor of one order of magnitude larger than BTO. In addition to classical flexoelectric constants, we also investigate the enhancement of other higher-order electromechanical coupling terms, including the converse flexoelectric tensor [2].

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Analysis of the failure of heterogeneous materials: a bottom-up approach

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Abstract: Generalized continuum models are appealing for incorporating the effects of material microstructure at the macroscopic scale; notably by incorporating internal lengths that smooth out gradients. Whereas this strategy has been shown to be effective when focusing on the macroscopic global response of the material, local kinematics at the vicinity of structural features inducing strong gradients has been shown to be less convincing [1], when comparing gradient-elasticity simulations to full displacement field measurements. Further, while higher-order homogenization strategies are efficient to estimate the effective parameters of a generalized continuum subjected to loading invoking wave lengths larger than the internal lengths of the model / the microstructure, they cannot be applied when these wave lengths vanish.

Using simulations of the failure of heterogeneous materials (different lattices of holes), we proposed in [3] a coarse-graining strategy inspired by [2]. These simulations are carried out using a well established phase field model. A crack propagates through the lattice of holes which topology strongly influences the results. Then, from the definition of a coarse-graining length ℓ_c, averaged mesoscopic fields that satisfy the fundamental conservation laws of continuum mechanics are computed. These averages are used to estimate the first-order elasticity parameters of a brittle material.

It is shown that elastic parameters converge to a constant value for ℓ_c greater or equal to 3 times the typical size of the considered microstructure. Ultimate stress and failure energy are also estimated from mesoscopic fields by following crack propagation over the continua at different ℓ_c. Contrary to elastic parameters, ultimate stress and fracture toughness are strongly dependent on ℓ_c. From the analysis of the frequency content of the spatial distribution of these fields of material properties, it is shown that characteristic lengths of the hole lattices persist even for very large ℓ_c. These typical lengths also remain in the mesoscopic crack topology. The main conclusion of this work is that unlike elastic properties, failure properties are difficult to homogenise. To be fully consistent, a first-order elastic mesoscopic model must have heterogeneous failure properties (ultimate stress, fracture toughness). The fields defining these material parameters should incorporate variation consistent with the microstructure topology.

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Direct and energy based homogenization approaches within the second gradient elasticity theory: examples and general relations

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Abstract: In this presentation we consider the problem of evaluation of the effective elastic properties of composites materials within the strain gradient elasticity theory (SGET). Assuming that the energy density of phases depends not only on strain but also on the strain gradients, one can evaluate the effective properties of elastic composites taking into account the influence of the inclusions size. In classical models such opportunity also arises when we consider, e.g. the models with additional interphase layers. Within SGET the size dependent predictions for the effective properties is the natural consequence of the extended constitutive equations that contain additional length scale parameters.

In the presentation we discuss possible homogenization approaches that can be used for evaluation of the effective elastic properties of composites within SGET. Considering the examples for the composites with spherical and cylindrical inclusions we compare several analytical and numerical homogenization methods [1,2]. We show, that using averaged values of the strain concentration tensor (or the averaged Eshelby tensor) within direct homogenization methods of SGET leads to the underestimation of the effective elastic properties of composites. Nevertheless, for small volume fractions of inclusions the use of averaged concentration tensors can be appropriate for the approximate evaluation of the effective properties. Corresponding comparison with known experimental data is also provided.

Finally, we prove in general form that using of standard homogeneous boundary conditions within SGET leads to the coincidence between the predictions within the direct and energy based homogenization approaches for the classical elastic constants. This result is obtained by using Eshelby integral formulas that were generalized for SGET in the authors previous works [3]. It is notable, that established coincidence is realized only in the case when one evaluates the averaged field quantities within direct approach without introduction of concentration tensors (i.e. by direct volume averaging of strain, stress, etc.).

For the more general boundary conditions with non-zero strain gradients we also found that the energy and direct homogenization approaches may not coincide within SGET. Such boundary conditions are used for the evaluation of the effective length scale parameters (gradient materials constants) of composites. And it turns out that the identification of such constants can be non-unique within SGET and it may strongly depends on the type of the averaging method.

References

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Session
Instabilities and generalized continua

Thursday 22 July 2021
8h30 – 10h30

8:30 *Generalized continuum models confronted to cell-commensurate instabilities in structured media*
Christelle Combescure

9:00 *Capturing microscopic and macroscopic instabilities in mechanical metamaterials by micromorphic computational homogenization*
Ron Peerlings

9:30 *Determination of homogenized continua behaviors from actual printed microstructures*
Maxence Wangermez

10:00 *A gradient-extended large-strain anisotropic damage model with crack orientation director*
Stephan Wulfinghoff

Generalized continuum models confronted to cell-commensurate instabilities in structured media

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Abstract: This work focuses on the ability for two generalized continuum models to capture mesoscale cell-commensurate instabilities in structured media using a very simple base model. Indeed, [1] have shown that a periodic arrangement of atoms, linked by complex interactomic potential could lead to short-wave commensurate and incommensurate instabilities and [3] proposes a quasi-continuum model based on strain gradients able to capture both long and short wavelength instabilities. On the other hands, using non-linear springs,[2] studied the ability of a strain-gradient model to capture long wavelength instabilities. As a consequence, the example of a periodic arrangement of non-linear springs, as presented in Fig.1a) below has been proposed. This simple example has been shown to display both long and short-wavelength instabilities depending on the values of the model's non-linear parameters (Fig.1b)).
Two generalized media have been compared: micromorphic and second order strain-gradient media. It is thus shown that the short-wavelength bifurcation points can only be captured by a micromorphic-type medium while the long-wavelength bifurcation points are captured by both models. This concludes that if short-wavelength instabilities are possible, micromorphic-type media are more appropriate to describe, in a contiunous way, the buckling of the mesoscopic stucture.

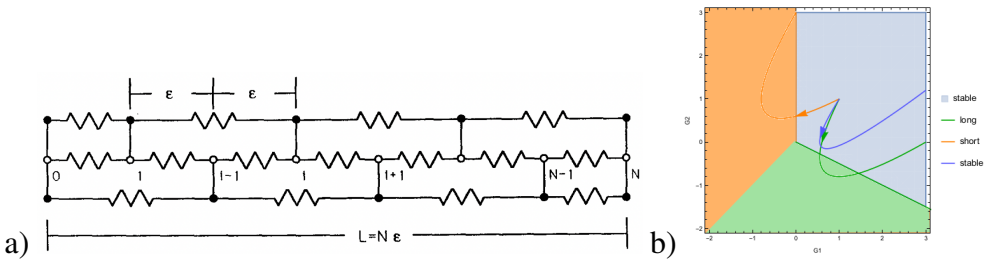

Figure 1: a) Schematic diagram of the studied periodic arrangement of non-linear springs. b) Stable (blue) and unstable long (green) and short (orangle) -wavelength regions for combinations of non-linear parameters.

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Capturing Microscopic and Macroscopic Instabilities in Mechanical Metamaterials by Micromorphic Computational Homogenization

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Abstract: Mechanical metamaterials feature microstructures which have been designed to exhibit exotic, and often counter-intuitive, effective behavior. Such responses are often achieved by instability-induced transformations of the, generally periodic, microstructure into one or multiple patterning modes. Due to a strong kinematic coupling of individual repeating microstructural cells, non-local behavior and size effects emerge. In addition, the individual patterning modes can mutually interact in space as well as in time, while at the engineering scale the entire structure can buckle globally.

Conventional homogenization approaches are limited in capturing these effects. In this contribution we therefore develop an extended computational homogenization approach which takes into account the possible emergence of patterns and the associated microscale and macroscale instabilities. The methodology is based on an additive split of the deformation into a coarse-scale contribution, a quasi-periodic patterned contribution and a remaining microstructural fluctuation field. The coarse-scale part and the amplitude of the pattern are assumed to vary only at the macroscopic scale. Injecting this Ansatz into a variational formulation of the full-scale problem results in governing equations for the macroscopic fields which have a micromorphic character. In order to compute the stress quantities featuring in these equations, a microstructural periodic cell problem needs to be solved for each point of interest in the macro-structure – i.e. in each integration point of the macroscopic discretization.

The potential of the methodology is demonstrated by several examples, focusing in particular on the competition between local and global instabilities, as well as on the tracking of multiple emerging patterning modes.

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Determination of Homogenized Continua Behaviors From Actual Printed Microstructures

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Abstract:

In recent years, architected materials and 3D printing technologies have become important research topics for industries. Numerous models have been developed to design and model these materials, yet there are large discrepancies between CAD geometries and actual parts in terms of geometric and mechanical properties ([1]).

The objective of this work is to develop an experimental device (**Fig. 1**) and an associated methodology to measure the effective mechanical behavior of architected materials directly from a specimen without using numerical models.

The concept of the proposed experimental device, initiated by the work of [2], is based on an arrangement of pantographic structures which allows performing first-order kinematic homogenization tests (KUBC) on plate structures. The homogenized behavior is measured by the dedicated device of the machine.

In addition to the macroscopic components of the first-order elasticity tensor, some components from generalized continua can be measured. Moreover, the device allows measuring directly the invariants of the elasticity tensor of a structure.

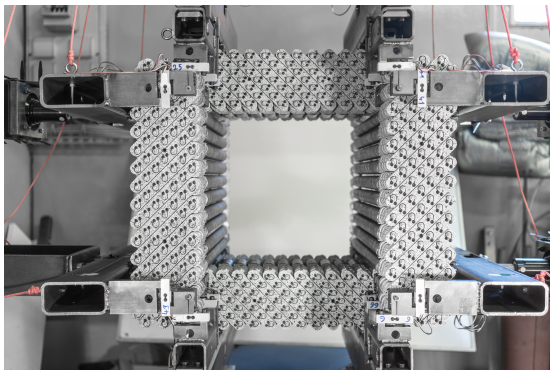

Figure 1: KUBC testing machine

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A Gradient-extended Large-strain Anisotropic Damage Model with Crack Orientation Director

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Abstract: Tension-compression splits are frequently introduced to remedy the symmetric behavior of phase-field models of fracture. These splits can suffer from an overly stiff model response. We propose a gradient- extended damage model with crack orientation director which locally represents the kinematics of fracture modes I , II and III . The kinematics of the model are asymmetric in tension and compression. Other authors which follow this approach are often times concerned with cleavage systems with well- known cleavage planes. In our model the crack surface orientation is not known a priori and thus treated as a degree of freedom. The formulation within the generalized standard material framework yields thermodynamic consistency. Two outstanding features of our approach are the straightforward implementation of anisotropic damage behavior and the traction free crack surface which emerges from the model. We demonstrate our findings with numerical examples for different load cases, different sample geometries and isotropic as well as anisotropic damage behavior. We showcase advantages of our approach when compared to a model which features a spectral tension-compression split.

References

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First Session
Fracture of materials

Thursday 22 July 2021
11h00 – 12h30

11:00 *A strain-gradient plasticity model of ductile failure in porous single crystals*
J.M. Scherer

11:30 *Thermal pressurization of earthquake faults under large co-seismic slip using Cosserat continuum*
Ioannis Stefanou

12:00 *A granular-based elasto-plastic–damage energy formulation for strain gradient solids*
Luca Placidi

A strain-gradient plasticity model of ductile failure in porous single crystals

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Abstract: In metallic alloys voids are known to play a crucial role for ductile failure. These defects embeded in a so called matrix material may evolve during mechanical loading. Their individual growth or shearing can eventually lead to coalescence. At this point, deformation localizes in ligaments between voids until failure is reached. Tremendous efforts have been put into observing, understanding, modeling and simulating these mechanisms. Most models developed to predict ductile failure rely either on variational methods, on homogenization techniques, or on thermodynamical approaches applied to porous materials [1]. These techniques are used to find the material behaviour of an equivalent homogeneous material which behaves as closely as possible as the heterogeneous porous material. Additional fields of internal variables are used to model the actual heterogeneus microstructure. The core of most models is based on a strong coupling between a scalar measure of the void volume fraction, called the porositiy, and the plastic behaviour of the matrix. In the early models the plastic behaviour of the matrix is considered as isotropic, resulting in a isotropic plastic behaviour of the equivalent homogeneous material. These models have been generalized to orthotropic plastic behaviour of the matrix material. However, voids are typically subgrain defects. Therefore, their local environment is a single crystal which was the motivation for coupling a void growth model with crystal plasticity in [2]. The crystallographic nature of the material surrounding voids shall have its greatest effect when only few slip systems are active. This is for instance the case in crystals with few available slip systems or in some irradiated materials which display a channel deformation mechanism with essentially one activated slip system. Existing porous crystal plasticity models account for crystal orientation during void growth or void coalescence. However a full model, combining growth and coalescence is not available. Ductile failure simulations of single crystals are also missing in the literature. The objective of this work is thus to couple a void coalescence criterion to an existing void growth model developed in the framework of crystal plasticity in order to simulate ductile failure of single- and oligo-crystal samples. First, an existing coalescence criterion [3] is compared to a revisited internal necking coalescence criterion. Both criteria are supplemented with evolution laws and coupled to the existing void

Thermal pressurization of earthquake faults under large co-seismic slip using Cosserat continuum

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Abstract: In this paper, we study the role of thermal pressurization in the frictional response of a fault under large coseismic slip. The majority of the slip is concentrated in the principal slip zone (PSZ) inside the fault gouge, a region of fine ultracataclastic granular material [1], which we model as a linear elastic perfectly plastic Cosserat continuum [2]. The Cosserat continuum introduces a characteristic length in the problem allowing us to model the PSZ as an instability of finite width inside the fault gouge thus avoiding strain localization on a mathematical plane and mesh dependency of the numerical results. The mechanical behavior is coupled with the energy and mass balance equations incorporating the effect of thermal pressurization as in [3]. We investigate the role of the seismic slip velocity, mixture compressibility, characteristic length and viscosity parameter in the frictional response of the fault by means of velocity stepping analyses, with seismic slip velocities $\dot{\delta}$ ranging from 0.01 to 1 m/s. We investigate the rate independent and the rate dependent frictional response and compare with existing models found in literature [4]. We show that our model is capable of predicting strain-rate hardening and velocity softening without the assumption of a state variable. We observe traveling instabilities that lead to oscillations in the fault's frictional response (see Figure 1). This behavior is not captured by the existing model of uniform shear [5] and shear on a mathematical plane [6], which predict a strictly monotonous behavior during shearing. Experimental analyses in [7], identifying thermal pressurization from the other weakening mechanisms, corroborate our numerical results.

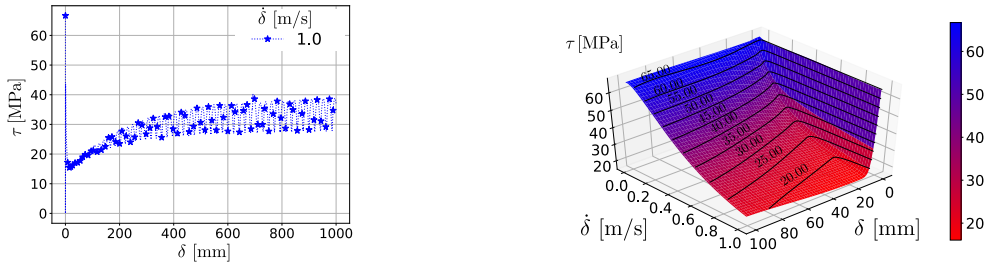

Figure 1: Left: Evolution of τ_{21} with slip δ. Right: 3D fitted surface of τ_{21} with slip δ and slip velocity $\dot{\delta}$.

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A granular-based elasto-plastic–damage energy formulation for strain gradient solids.

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Abstract: This work is devoted to the presentation of a continuum theory for materials having granular microstructure and accounting for tension–compression asymmetry of grain interactions and for dissipative phenomena like damage and plasticity. The continuum description is constructed by assuming expressions of elastic and dissipation energies as well as postulating a hemi-variational principle, without incorporating any additional postulates like flow rules. Granular micromechanics is connected kinematically to the continuum scale through Piola's ansatz. Mechanically meaningful objective kinematic descriptors aimed at accounting for grain–grain relative displacements in finite deformations are proposed. Karush–Kuhn–Tucker (KKT)-type conditions, providing evolution equations for damage and plastic variables associated with grain–grain interactions, are derived solely from the fundamental postulates. Numerical experiments have been performed to investigate the applicability of the model. Results show interesting damage and plastic induced anisotropy evolution including the emergence of a type of chiral behavior and formation of finite localization zones. Besides, loading–unloading histories have been considered to elucidate the material hysteretic features of the continuum. We also assess the competition between damage and plasticity, each having an effect on the other. Further, the evolution of the load-free shape is shown not only to assess the plastic behavior, but also to make tangible the point that, in the proposed approach, plastic strain is found to be intrinsically compatible with the existence of a placement function.

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Second Session
Fracture of materials

Thursday 22 July 2021
14h00 – 16h00

14:00 *Development, implementation and application of a second-gradient model for porous ductile solids*
Jean-Baptiste Leblond

14:30 *An FFT framework for simulating non-local ductile failure in heterogeneous materials*
Javier Segurado

15:00 *Energetic versus dissipative gradient damage models: A comparative analysis*
Djimedo Kondo

15:30 *Damage in periodic composite materials resulting from a micromechanics-based phase field approach*
Marco Paggi

Development, implementation and application of a second-gradient model for porous ductile solids

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Abstract: This talk is about a second-gradient model for porous ductile solids, which was proposed some years ago by Gologanu et al. [1] with the aim of solving the fundamental problem of potentially unlimited localization of strain and damage, resulting in mesh sensitivity in finite element computations. Our aim is three-fold : (i) briefly expound the theoretical foundations of the model ; (ii) discuss its efficient numerical implementation into some finite element code ; (iii) present some applications to some problems of practical interest, with some comparisons between model predictions and experimental observations.

The model does not rely on purely heuristic grounds, but on some theoretical (though admittedly approximate) homogenization procedure. Second-gradient effects at the macroscopic scale do not arise from some complex behavior at the microscopic scale, but from the incorporation into the homogenization procedure of possible quick variations of the mechanical fields over small distances, of the order of the void spacing. Such an incorporation is obtained by assuming the velocity to vary quadratically - instead of linearly as usual - with coordinates on the boundary of the "representative cell" considered.

The numerical implementation relies on the introduction of some extra nodal tensorial variable aimed at representing the strain tensor. Actual coincidence of these two quantities is enforced approximately through some weak formulation, in which the left-hand side matrix is lumped so as to permit to express the components of the new nodal variable explicitly in terms of nodal displacements, and finally eliminate them. The output is a numerical algorithm wherein the nodal degrees of freedom include the sole displacements, like for a standard first-gradient model.

Two applications are finally presented. The first consists of 2D numerical simulations of an experiment of ductile rupture of some pre-notched and pre-cracked CT specimen. Two important conclusions are reached: (i) the procedure of elimination of the nodal strains proposed permits to easily mix elements obeying first- and second-gradient models, so as to use the more complex model only in those zones where it is really needed ; (ii) a good agreement between model predictions and experimental observations is obtained with the second-gradient model - unlike with its simpler first-gradient version - using physically reasonable values of the coalescence parameters. The second application concerns the 3D numerical simulation of crack propagation over a long distance in a multiphase material. Again, experimental observations of the initial fracture locus are noted to agree better with the predictions of the second-gradient model than with those of the first-gradient version.

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An FFT framework for simulating non-local ductile failure in heterogeneous materials

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Abstract: A novel FFT-based staggered algorithm for simulating gradient ductile damage in homogenization problems is proposed [1] with the aim of suppressing the pathological discretization dependence caused by strain localization in damage models. In particular, the Helmholtz-type equation of the implicit gradient approach is properly generalized to model the regularization of damage in multi-phase media, where multiple damage variables and different characteristic lengths may come into play.
In the proposed iterative algorithm, two distinct problems are solved in a staggered fashion: (i) a conventional mechanical problem via a FFT-Galerkin solver with mixed macroscopic loading control and (ii) the generalized Helmholtz-type equation using a Krylov-based algorithm combined with an efficient pre-conditioner.
The technique is applied to study particle size effect in the mechanical response of particle reinforced composites. In particular, a strain gradient phenomenological plasticity model will be combined with the implicit gradient ductile damage approach in order to predict the yield, flow stress and ductility as function of the particle size

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Energetic versus dissipative gradient damage models: a comparative analysis

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Abstract: The study relies on the Generalized Standard Materials (GSM) framework for gradient plasticity models, recently overviewed by Nguyen [8] (see also [9]). This framework is adapted and implemented in order to provide a comparative analysis of two classes of gradient damage models, similarly to the current debate for gradient plasticity models (see for instance [1], [2] and [3]). In the first class of gradient damage models, denoted energetic models, the regularization term is in the form of a stored energy (examples are [4], [5], [6]), while in the second class (dissipative models, [7]) it enters in the dissipation potential. For both cases, the corresponding variational formulation is constructed. Implications of the two modeling choices are also discussed. Finally, we compare their predictions through suitable numerical simulations of 2D and 3D structures.

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Damage in periodic composite materials resulting from a micromechanics-based phase field approach

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Abstract: This study focuses on computational methods to simulate damage evolution in composite materials with microstructures. The phase field approach to nonlocal damage, which is usually cast for homogenous continua, leads to a progressive degradation of the Cauchy material constitutive relation based on the level of damage. However, in presence of a microstructure, the damaged constitutive tensor should reflect the specific physical assumptions on damage evolution occurring in the material microstructure. To provide a modeling solution to this problem, the phase field damage evolution equation is herein coupled with the weak form of the mechanical equilibrium equations through asymptotic homogenization. Therefore, depending on the level of nonlocal damage, first order asymptotic homogenization is applied to identify the damaged homogenized constitutive tensor of the heterogenous material. A case study concerning damage evolution in fiber-reinforced composites with linear elastic ceramic fibers and a metal matrix undergoing damage is provided as a representative engineering problem. Clearly, the basic computational approach may lead to a variety of possible interesting developments in case of higher order elastic continua approximations derived from asymptotic homogenization. Moreover, the enriched continua would also lead to multiple internal length scales, whose identification and relation between each other would demand specific research.

Acknowledgements

Support of the Italian Ministry of Education, University and Research to the Research Project of National Interest (PRIN 2017) “XFASTSIMS: Extra fast and accurate simulation of complex structural systems” (CUP: D68D19001260001) is gratefully acknowledged.

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Session
Diffusion and phase field methods

Thursday 22 July 2021
16h30 – 18h00

16:30	*Mass transport and shape changes in nonhomogeneous sintering* Sinisa Mesarovic
17:00	*Phase field modeling of deformation twinning in β-metastable titanium alloys* Benoît Appolaire
17:30–18:00	*A phase-field enhanced Cosserat model for prediction of microstructure evolution* Anna Ask

Mass transport and shape changes in nonhomogeneous sintering

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Abstract: Sintering of nano and/or microparticles is a critical step in many advanced manufacturing processes. The key obstacles in realizing complex structures using such methods are the part shape distortion and residual stresses during sintering. The mechanisms of particle transport required to realize part distortion during sintering (or residual stresses if deformation is constrained) have never been fully understood. Distortions in sintering, although common, are the result of a complex process and have been difficult to quantify in experiments. Freeform (statically determinate) structure of metallic needles and walls made of stacked individual nanoparticles exhibit measurable distortion in the form of permanent curvature upon sintering. The curvature increases in the early stages of sintering, then decreases until it settles at the final permanent curvature. Temperature measurements (using a thermal camera) and heat transfer simulations indicate bending towards higher temperature side. Note that any sintering model which takes into account only the standard sintering mechanisms – shortening of central distance between nearest neighbors and contact neck formation – cannot predict the permanent curvature. Unless a mass transfer mechanism is taken into account, no permanent curvature can be predicted. Two mass transfer mechanisms are possible: atomic level diffusion and particle displacement under sintering gradient (with unknown relative contribution).

Sintering is driven by the minimization of the surface energy of the pores. We assume that the density of surface energy is a function of porosity. In addition to the *sintering strain*, the network of particles changes volume as a result of material flow relative to the network, resulting in the *mass flow strain* (e.g., network swelling as the result of material inflow). Buildup of the microscopic, self-equilibrating stresses under sintering strain gradient is the main driving force for the mass transport. The resulting elastic energy is relaxed by the mass flow. The simplest model for micro-strain energy describing the physics of the process is characterized by quadratic form of gradients of the sintering the sintering strain and the mass flow strain (positive definite with respect to the former and negative definite with respect to the latter). The resulting continuum formulation is a micro-polar continuum. Its power conjugates (couple stresses) have clear physical meaning.

The computational results for a simple problem of freeform sintering (typical for additive manufacturing) exhibit a remarkable agreement with experiments: (i) needles and walls bend toward the hotter side, (ii) they first develop high transient curvature, and, (iii) finally settle at a lower permanent curvature. Parameters fitted to a series of experiments on the same powder, with different geometries and different temperature gradients, exhibit numerical consistency.

Phase field modeling of deformation twinning in β-metastable titanium alloys

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Recently, new β-metastable titanium alloys have been developed that combine TRIP and TWIP behaviors. They display improved mechanical properties, such as high strength (up to 1200 MPa in UTS) and ductility of about 45% at fracture, accompanied by an unprecedented strain hardening for titanium alloys at ambient temperature [1]. These mechanical properties are attributed to very complex microstructures produced by the mechanical destabilization of the initial bcc phase (β) in the course of the deformation. Indeed, the microstructure features numerous twins following the peculiar $\{332\}\,\langle 11\bar{3}\rangle$ twinning mode of the β phase, specific to β-titanium alloys, as well as α" and ω phases ensued from concomitant displacive transformations.

In order to better understand the formation of the complex microstructures described above, we have implemented a phase field model. As a first step, we focus only on the $\{332\}\,\langle 11\bar{3}\rangle$ twinning system. Contrary to recent works using phase field methods to investigate deformation twinning, we do not resort on some anisotropic twin boundary energy to control the shape of the twins, but rather investigate the importance of the framework for mechanics, i.e. either geometrically linear or nonlinear. In both cases, static mechanical equilibrium is solved using FFT based solvers. The capabilities of the model to describe the $\{332\}\,\langle 11\bar{3}\rangle$ anisotropic twin growth will be illustrated on a simple configuration, and the importance of considering a geometrically nonlinear framework will be addressed.

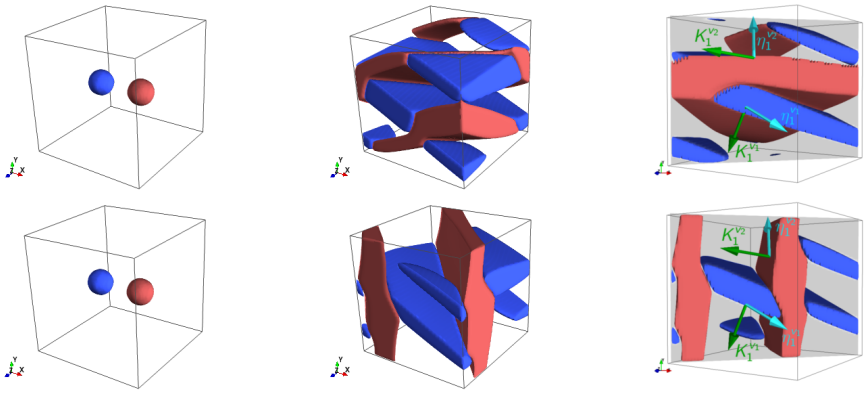

Figure 1: Evolution of two twin variants (red and blue) in the geometrically linear (upper row) and nonlinear (lower row) frameworks.

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A phase-field enhanced Cosserat model for prediction of microstructure evolution

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Abstract: The properties of a metal or metallic alloy can be manipulated by thermomechanical treatment to alter the crystalline microstructure. Large inelastic deformations lead to the appearance of deformation substructures and heterogeneous accumulation of stored energy in the form of dislocations. A new microstructure may form via transformation of low angle subgrain boundaries to high angle grain boundaries, nucleation of new grains, and grain growth. Modeling these processes in a coupled fashion is a major challenge that remains partly unresolved. In this work, an approach combining a Cosserat crystal plasticity model with a phase-field model is used to predict the microstructure evolution [1, 2]. The Cosserat crystal plasticity framework contains three additional degrees of freedom $\underline{\boldsymbol{\theta}}$ at each material point accounting for a local microrotation. The model proposed by [1, 2] associates the Cosserat degrees of freedom with the crystal lattice orientation. It also contains an additional degree of freedom ϕ which represents a phase-field order parameter that distinguishes between the ordered grain interior and the disordered grain boundaries. By adopting a free energy density inspired by the orientation phase-field model proposed by [3], the Cosserat rotational degrees of freedom behave as a phase-field and their evolution is coupled to the evolution of the order variable ϕ, thereby allowing for local reorientation of the crystal lattice due to both plastic deformation and grain boundary migration. The model has already been applied to two-dimensional problems [4] where it has been demonstrated to be able to capture several aspects of the microstructure evolution such as subgrain boundary formation and grain boundary migration.

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First Session
Metamaterials

Friday 23 July 2021
8h30 – 10h30

8:30 *Some perspectives on the Willis equations*
Graeme Milton

9:00 *Interfacial wave between two acoustic bianisotropic materials*
Gengkai Hu

9:30 *An examination of primitive causality in linear generalized continuum theories*
Venkata Mutnuri

10:00 *Elastic wave propagation in non-centrosymmetric and chiral architectured materials: insights from strain gradient elasticity*
Giuseppe Rosi

Some perspectives on the Willis equations

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Abstract: The Willis equations are non-local wave equations where the stress depends not only on the strain but also on the acceleration and the time derivative of the momentum density depends not only the acceleration but also on the strain. Willis first obtained them by ensemble averaging the standard equations of linear continuum elastodynamics. Later, motivated by the works of Greenleaf, Lassas, and Uhlmann, and Pendry, Schurig, and Smith on transformation based cloaking for conductivity and electromagnetism, local variants of the Willis equations, the Milton-Briane-Willis equations, were obtained from the standard linear continuum elastodynamics via a change from Cartesian to curvilinear coordinates reinterpreted as new physical equations in Cartesian coordinates. These are the natural generalizations to linear elasticity of the bianisotropic equations of electromagnetism and the form of both is invariant under a change from Cartesian to curvilinear coordinates. Like the original Willis equations, they involve an anisotropic density and various metamaterial models also exhibit anisotropic density. Metamaterial models coupling stress with acceleration and time derivative of the momentum density with strain have also been developed. Here we argue that the non-local Willis equations are unnecessarily complicated, and can be reduced to a form where the coupling vanishes. On the other hand, this is not true of the Milton-Briane-Willis equations if one wants a local consitutive law. Various other insights into these local and nonlocal equations will be given.

INTERFACIAL WAVE BETWEEN TWO ACOUSTIC BIANISOTROPIC MATERIALS

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Abstract: Acoustic bianisotropic materials present unconventional coupling between pressure and velocity, as well as momentum and strain. This unusual coupling, known also as Willis' coupling [1] provides an additional dimension to control acoustic wave through material microstructure design, however their characterization is beyond ability of traditional acoustic theory.

For two homogeneous bianisotropic materials with properly patterned Willis' coupling coefficients (represented by a vector), we demonstrate that an interfacial mode between these two materials can survive. The existence of this kind of interfacial mode depends closely on Willis' coupling vectors of the two materials, it emerges when the two coupling vectors point apart and disappears otherwise. Microstructure design based on C-shaped Helmholtz resonator unit cell [2] for the acoustic bianisotropic materials is carried out by using retrieval method [3], the designed acoustic bianisotropic material consists of C-shaped Helmholtz resonator array(Fig.1). The direction vector of the opening of the resonator coincides with Willis' coupling vector. A special 2D waveguide is also built, interfacial waves with different Willis' coupling vector patterns are measured. The measurements are in good agreement with the simulations (Fig.2).

This finding presents a new progress on passive acoustic bianisotropic materials, and provides additional tool to control acoustic waves.

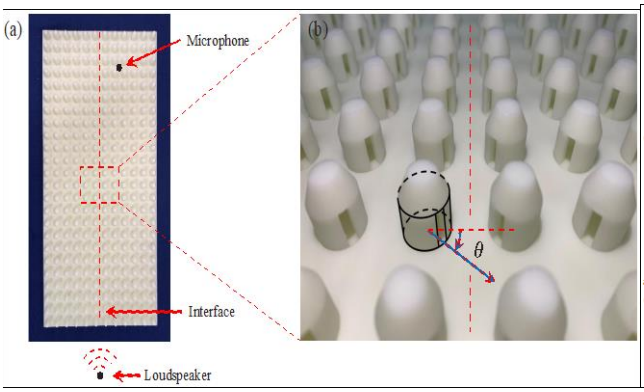

Fig.1 2D wave guide with the sample

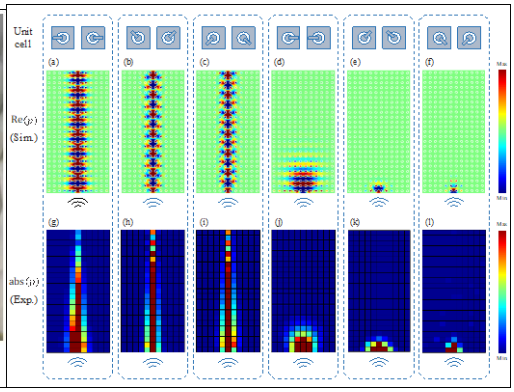

Fig.2 Simulation and experiment

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An examination of primitive causality in linear generalized continuum theories

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Abstract: As an aid in understanding the influence of micro scale physics on the macro scale behaviour of solids, there exist various generalized continuum theories modelling a micro-structured solid. Wave motion phenomena in the linear theories of generalised continua has caught attention due to possibility of wave dispersion engineering. Negative group speeds (NGS) is one of the interesting phenomena that arises due to interactions between length scales within a solid [1]. By definition, NGS waves travel backward, leading to a fundamental question, do these waves agree with the principle of causality? In literature, the subject of examination of causality in any linear media is a well established research topic [2]. However, examination of the relationship between wave motion behaviour in a solid and the causality has been a subject of recent research. Within this subject, although there exist studies relating wave dispersion characteristics to the principle of relativistic causality or the Einstein's causality[3], there do not exist many studies with respect to the principle of primitive causality. The importance of primitive causality arises naturally due to existence of NGS waves. Therefore, this paper studies the relation between primitive causality and wave motion behaviour in a class of generalized continuum theories, including mono-scale and multi-scale theories.

Methodology involves a Fourier frequency based spectral analysis and utilizes Kramers-Kronig (K-K) relations analysis framework [2]. Firstly, frequency spectrum of wavenumber or wave modes (WM) are obtained and utilized to obtain the frequency response function (FRF) for an impact type of loading problem. Following observations are made upon examining the WM and the FRF. There may exist differences between wavenumber spectrum of frequency and WM, especially in the multi-scale models. Existence of NGS waves leads to discontinuities in the wavenumber behaviour in the WM. This in-turn leads to discontinuities in the FRF. Time histories of wave motion responses obtained by the Fourier frequency analysis shows existence of NGS waves before the time of application of external load. Existence of responses before load application and also existence of discontinuities in the FRF are the features that seem to violate Titchmarsch's theorem of primitive causality[2].

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Elastic wave propagation in non-centrosymmetric and chiral architectured materials: insights from strain gradient elasticity

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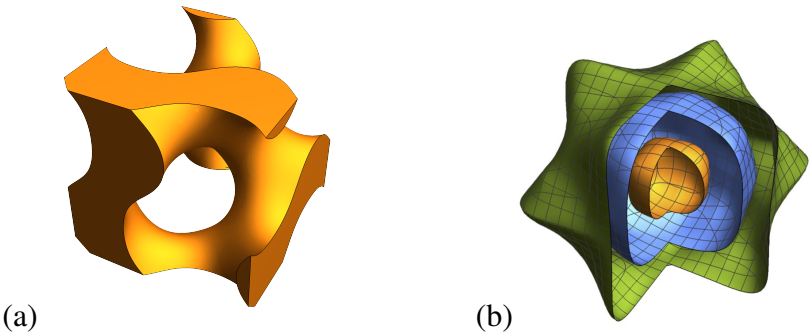
Abstract:

The study of elastic wave propagation is a fundamental tool in different fields, from non-destructive damage evaluation (NDE) to ultrasonic imaging. Usually NDE and characterisation techniques rely on inversion methods based on homogenised theories, that are valid only when the wavelength of the perturbation is considerably larger than the characteristic size of the heterogeneities of the materials. When the wavelength approaches this characteristic size, an upscaling occurs and mesoscopic effects can be transferred to the macro-scale. In this case, classic models used in the aforementioned inversion procedures can fail to predict the correct response [1] and they need to be improved [2].

In this work, we address those architectures for which the unit cell does not have any centre of inversion (non-centrosymmetric) nor symmetry plane (chiral). It will be shown that unconventional effects, in terms of dispersion and polarisation, can be observed even for large wavelengths. We will also show that, in order to describe these materials using an equivalent homogeneous continuum, the use of an enriched or generalised theory, such as the strain gradient elasticity, is mandatory. Moreover, the analysis of the generalised acoustic (or Christoffel) tensor defined in this framework can give a useful insight on the dynamic features of the architectured material. The example of the gyroid unit cell will be detailed.



(a) (b)

Figure 1: Gyroid unit cell (a) and slowness sufaces of plane elastic waves.

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Second Session
Metamaterials

Friday 23 July 2021
11h00 – 13h00

11:00 *An enriched continuum framework for metamaterial panels obtained through computational homogenization and model order reduction*
Varvara Kouznetsova

11:30 *Wave propagation control in active metamaterial with shunted piezoelectric microstructure*
Maria Laura De Bellis

12:00 *Local material symmetry group for first- and second-order strain gradient materials with application to fluids and subfluids*
Victor Eremeyev

12:30 *Piola transformation of stress and double stress in second gradient continua*
Francesco dell'Isola

An enriched continuum framework for metamaterial panels obtained through computational homogenization and model order reduction

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Attenuation of low-frequency flexural waves in lightweight thin structures, such as beams or plates, presents an important engineering challenge. New promising solutions addressing this problem may be found in the emergent field of dynamic metamaterials. In particular, locally resonant acoustic metamaterials (LRAM) may be promising candidates for the low-frequency flexural wave attenuation in beam and plate structures, since they present exceptional wave manipulation properties in a subwavelength regime compared to the size of the unit cell.

The development and design of such metamaterials in general, and LRAMs in particular, and devices/structures made thereof, requires advanced computational techniques. Such techniques should, on one hand, be capable of dealing with complex geometries, boundary conditions and excitations, and on the other hand be computationally more efficient than direct numerical simulations. The latter become quickly computationally infeasible for LRAMs due to the need to accurately resolve the fine scale resonator features, which are much smaller than the size of the large scale structure.

To enable the efficient analysis and design of LRAM beam/plate structural elements for practical applications, a multi-scale computational homogenization method for modelling wave propagation phenomena in LRAM panels is presented in this work. The macroscopic LRAM panel is modelled as a thin continuum beam/shell enriched with extra macroscale field variables representing the micro-inertia effects of the embedded resonators. The evolution equations for these generalized fields emerge naturally through the consistent upscaling procedure. Under the assumption of linear elasticity, using the static-dynamic decomposition and mode synthesis [1], the macroscale effective material properties can be computed once and for all ‘off-line’ for a given unit cell, hereby enabling a significant model reduction. Such an approach retains the accuracy and robustness offered by a two-scale coupled computational homogenization implementation [2], while significantly reducing the problem size and the computational time to the ‘on-line’ solution at the macro-scale only. Moreover, the obtained closed-form enriched formulation can be written in the time, as well as the frequency domains, thus enabling an efficient solution of both transient and steady-state problems. The capabilities of the proposed framework will be illustrated on several representative examples.

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Wave propagation control in active metamaterial with shunted piezoelectric microstructure

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Abstract: An innovative class of tunable periodic metamaterials is designed for realizing high performance acoustic metafilters with tunable real-time capabilities, see [1]. The metamaterial is made up of a phononic crystal coupled to local resonators. Such local resonators consist of masses enclosed into piezoelectric rings, shunted by either dissipative or non-dissipative electrical circuit. In this framework the constitutive properties of the shunting piezoelectric material can be fully adjusted by modifying the impedance/admittance of the electrical circuit. As a consequence, the acoustic properties of the metamaterial can be properly modified in an adaptive way, opening up new possibilities for the control of pass- and stop-bands. By exploiting a generalization of the Floquet-Bloch theory, the free wave propagation in the tunable metamaterial is investigated, by varying a certain tuning parameter, with the aim of showing the efficiency of the proposed shunting piezoelectric system as a wave propagation control device. Special attention is paid to determining the in-plane constitutive equations of the shunting piezoelectric phase in the transformed Laplace space. Finally, we also provide broad design directions of tunable acoustic filters aiming to a changing performance requirement in real-time.

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Local material symmetry group for first- and second-order strain gradient materials with application to fluids and subfluids

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Abstract: Nowadays the strain gradient elasticity found various applications to modelling of composite materials such beam-lattice metamaterials or materials at small scales, see, e.g. [1]. For strain gradient materials there exists a potential energy density which depends on strains and their gradients up to a certain order. As a result, the constitutive equations become rather complex. Thus, the possible simplifications of the constitutive relations could play an important role for further applications.

The aim of this lecture is to discuss the material symmetry group for strain gradient materials. Following [2] we introduce the local material symmetry group for first and second strain gradient media undergoing finite deformations. The local material symmetry group is formed through such transformations of a reference placement which cannot be experimentally detected within the considered material model. We show that considering maximal symmetry group, i.e. material which strain energy is independent on the choice of a reference placement, one comes to the constitutive equations of gradient fluids introduced independently on general strain gradient continua. Considering relations between capillary fluids and general strain gradient elasticity models, we have demonstrated in [3] that the local material symmetry group constitutes an unified approach to material modelling, i.e. to classification and further of constitutive equations of gradient elastic media. Indeed, defining a gradient fluid as a material insensitive to any mass density preserving transformations of a reference placement, we came to the constitutive relations of capillary fluids. In a similar way more complex cases related to strain gradient subfluids can be analyzed. The latter could be useful for the group description of some beam-lattice metamaterials modelled as gradient-incomplete media [4].

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Piola Transformation of Stress and Double Stress in Second Gradient Continua

Francesco dell'Isola, S. Eugster, R. Fedele and P. Seppecher

Second gradient continua are continua with internal virtual work contributions that depend linearly and continuously on the first and second gradient of the virtual displacement. These virtual work contributions can be postulated either in Lagrangian (referential) or Eulerian (spatial) form and define respectively the Piola-Lagrange stresses as well as the Cauchy-Euler stresses. We show how the principle of virtual work in Lagrangian form emerge as a generalization of the minimum of potential energy and derive the Piola transformation of the appearing stress contributions. We give in both the Eulerian and Lagrangian description the expression of surface and edge contact interactions for second Gradient continua in terms of the normal and the curvature of contact boundary surfaces and edge shapes. Moreover, we formulate the complete boundary value problems in both representation.

Speakers Index