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ABSTRACTS

CIRM (Centro Internazionale per la Ricerca Matematica)

MUR - PRIN Project "Free Boundary Problems, Phase Transitions and Models of Hysteresis"

Università degli Studi di Trento

invited lectures

The sharp interface limit of phase field models – is the Allen-Cahn equation a good model?

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This talk reports on a joint work with Peicheng Zhu. The Allen-Cahn equation is a well known model for diffusionless phase transitions in elastic solids. Yet, by studying the sharp interface limit we show that its applicability is limited to the case where the mean curvature is part of the driving force of the interface and where the constitutive relation between driving force and normal speed is "almost linear". More precisely, we show that the constitutive relation in the sharp interface limit is obtained from the constitutive relation of the Allen-Cahn equation by a compact integral operator, which is not surjective. However, for diffusionless (also called martensitic) transformations the mean curvature should not be part of the driving force. We discuss a phase field model, which we have proposed earlier and which originates from a transport equation, and show that the sharp interface limit of this model does in fact not contain the curvature in the driving force and that the constitutive relation in the phase field model and the sharp interface limit coincide even when this constitutive relation is nonlinear.
Therefore this phase field model can be used for solids with diffusionless phase transitions, and it can be used when the constitutive relation between normal speed and driving force is fully nonlinear. This last property suggests to extend it to a phase field model for crack propagation. Besides these questions we discuss the existence proof for the original transport model in one space dimension given in [2], where it is shown in a novel way that the weak limit of measures can be interchanged with a nonlinear function.

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Nonlinear-Dynamical-System Approach to Magnetization Dynamics in Ferromagnets

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The space-time magnetization dynamics in ferromagnetic systems is governed by the Landau-Lifshitz-Gilbert (LLG) equation coupled with Maxwell equations. Numerical solutions of the LLG equation are routinely used in the development of magnetic-recording and spintronics devices. If one limits the analysis to nanomagnets with spatially uniform magnetization, though, a wealth of interesting features can be revealed by recognizing the fact that a LLG system is nothing but a nonlinear dynamical system evolving on the surface of the unit sphere [1]. The dynamical-system perspective reveals basic aspects of the magnetization dynamics which are topological in nature and for this reason are particularly general and robust. On the other hand, the full comprehension of spatially uniform magnetization dynamics is an essential first step before moving to the numerical study of complex spatially non-uniform configurations. The general form of dynamic equation consistent with the spherical character of the phase space will be derived and discussed. It will be shown that this general equation contains as particular cases a number of situations of applicative interest, like precessional magnetization dynamics leading to fast (picosecond-scale) magnetization reversal; microwave-field-assisted magnetization dynamics; spin-transfer-driven magnetization dynamics in the presence of spin-polarized electron currents. For this last case, the conditions leading to the appearance of limit cycles will be discussed, as well as the bifurcation conditions leading to abrupt transitions from fixed-point to limit-cycle solutions and vice versa. This case is of particular applicative interest in view of the development of current-controlled oscillators and microwave generators of nanometric dimensions.

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MATHEMATICAL MODELS FOR ACID-MEDIATED TUMOUR INVASION

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About ten years ago the experimental evidence was produced of the existence of a necrotic gap between some specific tumour and the surrounding host tissue. Such a phenomenon was interpreted as the result of acidic aggression. As a consequence acid-mediated tumour invasion has received great attention in the framework of cancer modelling.
Indeed the increase of H+ ions concentration around tumour cells can be explained on the basis of their glycolytic metabolism. Recent measurements of the pH level inside tumour cells have shown that they are able to keep it slightly above 7, even in the presence of an acidic environment, which on the contrary proves to be lethal for normal cells. This kind of aggression is believed to facilitate the spread of the tumour.
We will illustrate some recent literature dealing with acid-mediated tumour invasion, including models based on travelling waves systems.

Interacting Fluids in Cosmology

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The recent astronomical measurements of the relative brightness with the red-shift of type-IA supernovae and the analysis of the precise measurements of the spectrum of the Cosmic Microwave Background anisotropy provided strong evidence for a present accelerated expansion of the Universe; the nature of the responsible entity, called dark energy, still remains unknown. All usual types of matter with positive pressure generate attractive forces and decelerate the expansion of the Universe. For that reason, a dark energy component with negative pressure was suggested to account for a fluid that drives the current accelerated expansion. Furthermore, the measurements of the rotation curves of spiral galaxies as well as other astronomical observations suggest that the luminous matter represents only a small amount of the massive particles of the Universe, and that the more significant amount is related to dark matter. That offered a new setting for cosmological models with dark energy and dark matter and in these contexts many interesting phenomenological models appear in the literature analyzing the interaction of dark matter with dark energy. In these models the dark matter and the dark energy are coupled, do not evolve separately and the coupling is either motivated by high energy particle physics considerations or is constructed by requiring the final matter to dark energy ratio to be stable against perturbations.
In the present work a cosmological model — for a homogeneous, isotropic and flat Universe — is analyzed whose constituents are a non-interacting baryon matter field and interacting dark matter and dark energy fields. The dark energy and dark matter are coupled through their effective barotropic indexes, which are considered as functions of the ratio of their energy densities. Two asymptotically stable cases are investigated for the ratio of the dark energy densities which have their parameters adjusted by considering best fits to Hubble function data. It is shown that the deceleration parameter, the density parameters, and the luminosity distance have the correct behavior which is expected for a viable present scenario of the Universe. The perturbation evolution of the model is also investigated showing that the energy density perturbation becomes asymptotically stable.

Global energetic solutions for finite-strain plasticity with gradient regularization

Alexander Mielke

Finite-strain plasticity is based on the multiplicative decomposition of the strain tensor $\nabla\varphi = F_{\mathsf{el}}P$ into an elastic part F_{el} and a plastic part P. The former is used for calculating the stored elastic energy, whereas the latter is driven by a plastic flow rule.

We reformulate the flow rule as an internal force balance (Biot's equation) using a dissipation potential R, i.e., the flow rule is associative and obeys the principle of maximal dissipation. From the dissipation potential we construct a dissipation distance D, which allows us to define time-incremental minimization problems that perfectly respect the underlying matrix-group structure. In particular, we emphasize the fact that $\nabla\varphi = F$ lies in the general linear group $\mathsf{GL}^+(\mathbb{R}^d) = \{\, A \in \mathbb{R}^{d\times d} \mid \det A > 0 \,\}$ and the plastic tensor P in another Lie group, usually $P \in \mathsf{SL}(\mathbb{R}^d) = \{\, A \in \mathbb{R}^{d\times d} \mid \det P = 1 \,\}$.

We reformulate the evolutionary boundary-value problem in terms of the energetic formulation that consists of a purely static global stability condition **(S)** and a total energy balance **(E)**. We denote by $\boldsymbol{q} = (\varphi, P, p) : \Omega \to \mathbb{R}^d \times \mathsf{SL}(\mathbb{R}^d) \times \mathbb{R}^m$ the state of the system, where φ is the deformation, P the plastic tensor and p plastic hardening variables. The energy stored is $\mathcal{E}(t, \boldsymbol{q})$ and the dissipation distance $\mathcal{D}$ between two states $\boldsymbol{q}$ and $\widehat{\boldsymbol{q}}$ is given by integrating D over Ω. Then, triple $\boldsymbol{q} : [0,T] \to \mathcal{Q}$ is called an *energetic solution* for the rate indpendent system $(\mathcal{Q}, \mathcal{E}, \mathcal{D})$ if for all $t \in [0,T]$ conditions **(S)** and **(E)** hold:

$$\textbf{(S)} \quad \mathcal{E}(t, \boldsymbol{q}(t)) \le \mathcal{E}(t, \widehat{\boldsymbol{q}}) + \mathcal{D}(\boldsymbol{q}(t), \widehat{\boldsymbol{q}}) \text{ for all } \widehat{\boldsymbol{q}} \in \mathcal{Q},$$

$$\textbf{(E)} \quad \mathcal{E}(t, \boldsymbol{q}(t)) + \mathsf{Diss}_{\mathcal{D}}(\boldsymbol{q}, [0,t]) = \mathcal{E}(0, q(0)) + \int_0^t \partial_s \mathcal{E}(s, \boldsymbol{q}(s)) \, \mathrm{d}s.$$

This energetic formulation has the major advantage that it avoids time-derivatives of the desired solutions and it avoids derivatives of the energy and dissipation potentials. Hence, energetic solutions are rather weak and allow for jumps in time. We show that solutions of the time-incremental problems exist and that, after choosing a suitable subsequence, we have convergence to an energetic solution if the timestep goes to 0.

The mathematical analysis relies strongly on a gradient regularization, which provides the desired compactness and thus prevents formation of microstructures. However, the formulation is so general that it includes isotropic situations as well as crystal plasticity with latent hardening.

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Analysis of model equations for stress-enhanced diffusion in coal layers

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(joint work with Hans Bruining (Delft), to appear in SIAM J. Math. Analysis 2008)

This work is motivated by the study of the sorption processes in the coal. They are modelled by a nonlinear degenerate pseudo-parabolic equation for stress enhanced diffusion of carbon dioxide in coal

$$\partial_t \phi = \partial_x \left\{ D(\phi)\, \partial_x \phi + \frac{D(\phi)\, \phi}{B} \partial_x \left(e^{-m\phi} \partial_t \phi \right) \right\},$$

where B, m are positive constants and the diffusion coefficient $D(\phi)$ has a small value when the CO_2 volume fraction ϕ is $0 \leq \phi < \phi_c$, representative of coal in the glass state and orders of magnitude higher value for $\phi > \phi_c$, when coal is in the rubber like state. These type of equations arise in a number of cases when non-equilibrium thermodynamics or extended non-equilibrium thermodynamics is used to compute the flux.

For this equation existence of the travelling wave type solutions was extensively studied. Nevertheless, the existence seems to be known only for sufficiently short time. We use the corresponding entropy functional in order to get existence, for any time interval, of an appropriate weak solution with square integrable first derivatives and satisfying uniform L^∞-bounds. Due to the degeneracy, we obtain square integrability of the mixed second order derivative only in the region where the concentration ϕ is strictly positive. In obtaining the existence result it was crucial to have the regularized entropy as unknown for the approximate problem and not the original unknown (the concentration).

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Homogenization of dislocation dynamics

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Dislocations are microscopic defects present in crystals that are one the main explanations of the plastic behaviour of metals. These defects can be seen as curves moving in crystallographic planes. The typical length of these defects is of the order of the micrometer. The normal velocity of these curves is proportional to one component of the stress in the material (called the resolved Peach-Koehler force). One important fact, is that every dislocation curve creates its own stress field. In the framework of linear elasticity, the total stress appears naturally to be the sum of the contributions created by each defect in the material.
We are interested in the collective behaviour of such defects and present here homogenization results on this dynamics of defects. In other words, we explain how to replace this microscopic dynamics, by an effective macroscopic dynamics at large scales. To be able to perform rigorously this homogenization, we restrict our study to a particular geometry where all dislocation curves are contained in a single slip plane and have the same nature (namely have the same Burgers vector). In this particular situation, we can develop nonlinear homogenization techniques in the framework of viscosity solutions for nonlocal PDE's. As a result of this homogenization procedure, we predict a viscoplastic law at the macroscopic level.
For some pedagogical reasons, we will illustrate this procedure in the particular case of the fully overdamped dynamics of particles with two-body interactions. We will also present some numerical simulations to compute the effective macroscopic dynamics.

A multi-component theory of solid mixtures with higher gradients and its application to binary alloys

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A theory of mixture for multi-component materials is presented based on a straightforward evaluation technique for the exploitation of the Second Law of thermodynamics. In particular the constitutive equations for entropy, heat and diffusion flux as well as the stress tensor are formulated as a consequence of the non-negative entropy production. Furthermore we derive a Gibbs equation as well as a Gibbs-Duhem relation which also follow from the formalism. Moreover, it is illustrated, how local mechanical strains due to eigenstrains or external loadings, modify the free energy and, consequently, change the chemical potentials of the components. All consecutive steps are illustrated, first, for simple mixtures and, second, for a system containing two different phases. So-called higher gradients of the concentrations are considered, which take the nonuniform composition into account. It will also become apparent that more/other variables of modified/different physical problems beyond the illustrated ones can be easily treated within the presented framework. This work ends with the specification to binary alloys and with the presentation of various numerical simulations.

Optimal nonlinear stability for reaction-diffusion and fluid dynamics models

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It is well known that, in the study of stability of the constant solutions to a nonlinear ordinary differential system, the classical "canonical reduction method", which transforms the associated linearized system in an uncoupled system or in a canonical Jordan form, plays a fundamental role. The reduction method also permits to define an *optimal* Lyapunov function for the linear and nonlinear stability (see eg. [1, p. 45]). (The Laypunov function E is optimal if the critical instability parameter of linearized eigenvalue problem, R_c, and the critical stability parameter obtained with the Lyapunov method, R_E, *coincide*).

Recently, this method has been generalized to some PDE's systems which include some reaction-diffusion systems and fluid-dynamics problems. Optimal Lyapunov functions have been constructed and a known (computed) radius of attraction for the initial data has been given (see [2] - [6]). We point out that what we have established, in [2] - [6], is more than just a linearization principle. A linearization principle simply shows that linear stability implies nonlinear stability, but does not necessarily determine the class of initial data for which one has nonlinear stability (radius of attraction) nor need it yield a bound for the rate of solution decay.

We recall here some of these results in the case of ecological systems (the symmetric and the asymmetric May-Leonard system for three competing species, with diffusion (see [7], [8, p. 373])), biological models (a system for aggregation of glia cells, which are the support structure for the central nervous system, in the brain [9], [6]) and some convection problems in fluid dynamics, [2], [3].

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Traffic flow on networks : conservation laws models

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The aim of the talk is to present recent developments for macroscopic traffic flow models on networks; more precisely we focus on the approach based on conservation laws. The underlaying equations for the models we consider are hyperbolic systems of conservation laws in one dimension:

$$u_t + f(u)_x = 0,$$

where $x \in \mathbb{R}$, $u \in \mathbb{R}^n$ and $Df(u)$ is assumed to have real distinct eigenvalues. The main mathematical novelty is to describe the dynamics on a network, represented by a directed topological graph, instead of a real line. The more advanced results are available for the scalar case, i.e. $n = 1$.

Various fluidodynamic models were developed in the literature: they treat traffic from a macroscopic point of view considering the evolution of macroscopic variables, such as density and average velocity of cars. The interest was also motivated by other applications: data networks [2], supply chain, air traffic management, gas pipelines, irrigation channels etc.

The main interest is in the Cauchy problem for a complex network. The dynamics happens to be undertermined at nodes. Indeed the only conservation of u through a node is not sufficient to describe a unique solution, see [1, 3].
To construct solutions to Cauchy problems, we consider wave-front tracking approximations, thus it is natural to define Riemann problem at a node a Cauchy problem with constant initial data on each arc entering or existing the node. One relies on the notion of Riemann solver, i.e. a map providing solutions to Riemann problems as function of the initial data. Then to pass to the limit on approximate solutions, one has to rely on estimates on the total variation of the flux of the solution.
We provide a general strategy to overcome the technical problems: three key properties of Riemann solvers are defined, which guarantee the needed bounds and thus existence of solutions to Cauchy problems.

The continuous dependence of solutions with respect to initial data is an open problem in the general case. For instance the Lipschitz continuous dependence with respect to initial data may fail; see [1]. However, it was proved for the solver of [2], by viewing L^1 as a Finsler manifold and considering "generalized tangent vectors".

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Phase-field models for moving boundary problems: from the physics of phase transitions to applications in mechanics

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The phase-field method has become widely popular in recent year as a simple and elegant numerical method to treat moving boundary problems. It is rooted in out-of-equilibrium thermodynamics: the time evolution of hydrodynamic variables and order parameters is obtained by variational principles from suitable free energy functionals. In the first part of the talk, the construction of the phase field model and its capabilities will be illustrated by examples from metallurgy: the microstructures formed during the solidification of metallic alloys. Complex morphologies such as dendrites or cellular structures arise from a subtle interplay between the dynamics of the solid-liquid interfaces and instabilities linked to the transport of heat and matter. Fully quantitative three-dimensional simulations can nowadays be carried out on the scale of a few microstructural units, which has made it possible to directly compare simulations and experiments, and to critically assess existing models and theories of pattern formation in solidification.
For achieving this precision, a careful asymptotic analysis of the phase-field equations is needed in order to link the parameters of the phase-field model to the quantities that appear in the corresponding moving boundary problem. It turns out that in some cases it is useful to give up the variational principle in order to obtain more efficient models for a given free boundary problem. These methods can then also be applied to problems for which a variational formulation is not readily available. This will be illustrated in the second part of the talk by examples from mechanics: viscous fingering in non-Newtonian fluids and the propagation of fractures in brittle materials.

Atomistic and continuum descriptions of fluids: some examples of their inter-relations

Errico Presutti
(University of Roma `Tor Vergata')

Focus of my talk is on the relation between atomistic and continuum descriptions of fluids. In a first part I will consider the case of states in local thermodynamic equilibrium and outline the way they are studied from a macroscopic, mesoscopic and microscopic viewpoints. The way such different approaches are related is by now well understood at least at the level of their equilibrium properties, but there are also results about dynamics, in particular on the microscopic derivation of free boundary problems. This first part of the talk is a short survey on well established works in the fields. The second part describes states where a current flows in the system (as for instance when heat flows through a conductor whose sides are kept at different temperatures). I will discuss some recent works on the subject by Jona-Lasinio and coworkers, see J. Stat. Phys. 123, 237{276 (2006), and by Bodineau and Derrida, C.R. Physique, 8, 540{555, (2007). Their analysis of some stochastic particle models leads to interesting problems at the macroscopic level and in my talk I will mainly focus on the latter and discuss some variational problems which arise concluding with some of the many open questions in the field.

2-D constrained Navier-Stokes equation and intermediate asymptotics

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I introduce a modified version of the two-dimensional Navier-Stokes equation, preserving energy and momentum of inertia, which is motivated by the occurrence of different dissipation time scales. Such an equation is strongly related to the gradient flow structure of the 2-D Navier-Stokes equation, which is interesting in itself. The ultimate hope is to understand intermediate asymptotics. My presentation is based on a joint work with E. Caglioti and F. Rousset.

Identifcation of an average temperature and a dynamical pressure in a multi-temperature mixture of fluids

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We first present the different models of a mixture of compressible fluids and we discuss in the case of Euler fluids the local and global well-posedness of the relative Cauchy problem for smooth solutions. Then we present a classical approach of mixture of compressible fluids when each constituent has its own temperature. The introduction of an *average temperature* together with the entropy principle dictates the classical Fick law for diffusion and also new constitutive equations associated with the difference of temperatures between the components. The constitutive equations fit with results recently obtained through the *Maxwellian iteration* procedure in extended thermodynamics theory of multi-temperature mixtures. The differences of temperatures between the constituents imply the existence of a new *dynamical pressure* even if the fluids have a zero bulk viscosity. The non-equilibrium dynamical pressure can be measured and may be convenient in several physical situations as for example in cosmological circumstances where - as many authors assert - a dynamical pressure played a major role in the evolution of the early universe.

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Towards multi-scale continuum elasticity theory

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We propose a new method of constructing a series of nested quasicontinuum models which describe linear elastic behavior of crystal lattices at successively smaller scales. The relevant scales are dictated by the interatomic interactions and are not arbitrary. The novelty of the model is in the use of a decomposition of the displacement field into the coarse grained part and the micro-level corrections. The coarse contribution is the conventional homogenized displacement field used in classical continuum elasticity. The micro-level corrections are sub-continuum fields representing the fine structure of the boundary layers exhibited by the discrete equilibrium configuration. Joint work with M. Charlotte.

Onsager-like Relation and Shock Structures for Hyperbolic Balance Laws

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In this talk, I would like to propose an Onsager-like relation as an entropy-dissipation principle for balance laws—the main mathematical models in extended thermodynamics. This principle not only has a clear and solid physical interpretation, but also provides a convenient framework to develop mathematical theories for the balance laws. Here I will show that, together with the new principle, a Kawashima-like condition is sufficient for the existence of smooth shock structures. As an application, the existence of shock structures for radiation hydrodynamics will been discussed.

contributed talks

Materials with Memory: Free Energies & Solution Exponential Decay

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A rigid linear heat conductor with memory conductor is considered in the framework of the model developed by Fabrizio, Gentili and Reynolds [2]. An evolution problem which arises in studying the thermodynamical state of the material with memory is considered. Specifically, the time evolution of the temperature distribution within a rigid heat conductor with memory is investigated. The constitutive equations which characterize heat conduction with memory, involve an integral term since the temperatures time derivative is connected to the heat flux gradient. Suitable expressions of the minimum free energy [1] allow to construct functional spaces which are both meaningful under the physical as well as the analytic viewpoint since therein the existence and uniqueness results can be established. Here, in particular, the attention is focused on those conditions which guarantee that solution exponentially decay at infinity. Connections with nonlinear wave-type equations are also mentioned [3].

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Free boundary problems in partially saturated porous media

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We deal with the filtration of liquid in a partially saturated porous medium in the one-dimensional case. We assume a given constitutive relation between saturation and pressure; the analyse both the cases with and without gravity. Under different kinds of boundary conditions, we analyse the occurrence of free boundary problems and formulate the correspondent mathematical models for which we look for well-posedness results. If time is left, we assume a constitutive relation with hysteresis between saturation and pressure and analyse under which kinds of boundary conditions we have the occurrence of free boundary problems.

A model of grain boundary motion: Existence of a weak solution

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This is a joint work with A. Ito and N. Yamazaki.
We consider a phase-field model of grain structure evolution:

$$\eta_t - \kappa\Delta\eta + g(\eta) + \alpha'(\eta)|\nabla\theta| = 0 \ \text{ in } Q_T := \Omega \times (0,T),$$

$$\alpha_0(\eta)\theta_t - \nu\Delta\theta - \mathrm{div}\left(\alpha(\eta)\frac{\nabla\theta}{|\nabla\theta|}\right) = 0 \ \text{ in } Q_T,$$

$$\frac{\partial\eta}{\partial n} = 0, \quad \theta = 0 \quad \text{on } \Sigma_T := \partial\Omega \times (0,T),$$

$$\eta(\cdot,0) = \eta_0, \quad \theta(\cdot,0) = \theta_0 \ \text{ in } \Omega,$$

where Ω is a bounded domain in $\mathbf{R}^N$ $(N \geq 1)$; $\kappa > 0$ and $\nu > 0$ are constants; $g(\cdot)$, $\alpha(\cdot) \geq 0$ and $\alpha_0(\cdot) \geq 0$ are given functions on $\mathbf{R}$; η_0 and θ_0 are initial data.

This model of two dimensional grain structure was proposed by R. Kobayashi, J.A. Warren and W.C. Carter (Pysica D, Vol.140(2000),pp.141-150), which was derived from the following free energy functional

$$F(\eta,\theta) = \frac{\kappa}{2}\int_\Omega |\nabla\eta|^2 + \int_\Omega \hat{g}(\eta) + \frac{\nu}{2}\int_\Omega |\nabla\theta|^2 + \int_\Omega \alpha(\eta)|\nabla\theta|;$$

the variable θ is an indicator of the mean orientation of the crystalline and η is an order parameter for the degree of crystalline orietational order. The case of Kobayashi-Warren-Carter is that $\alpha(\eta) = \alpha_0(\eta) = \eta^2$, $\hat{g}(\eta) = \frac{1}{2}(1-\eta)^2$ and $\Omega \subset \mathbf{R}^2$.

We shall give a result on the existence of a weak solution of the above system.

An alternative approach to Saint-Venant's principle

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The minimum strain energy principle together with other standard properties is shown to be sufficient to establish a general form of Saint-Venant's principle valid for broad range of materials. As illustration, decay estimates are derived for elastic cylinders. Differential inequalities are not required. The approach is motivated by contributions due to Zanaboni (1937) and represents joint work with Professor P Villaggio (Pisa).

KINETIC EQUATIONS FOR ANOMALOUS DIFFUSION: A FRACTIONAL CALCULUS APPROACH

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In recent decades the field of anomalous diffusion processes has won more and more interest in applications in the sciences, in physics and chemistry, and even in finance, see the Bibliography. We will give here some views into this rapidly developing field according to the allotted time, paying attention to some deterministic and stochastic aspects related to kinetic master equations of fractional order governing these generalized diffusion processes. As a matter of fact these equations contain pseudo-differential operators that can be interpreted as space and/or time derivatives of non-integer order. In particular we outline the recent work carried out by our research group on these topics.

Homogenisation of a coupled nonlinear parabolic system in a two-phase medium

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The homogenisation problem of a coupled system of two semi-linear parabolic partial differential equations valid in each part of a two-phase medium is considered. The equations are coupled by a nonlinear Robin-type condition. This system arises in different applications in materials science and mathematical biology. Based on two-scale convergence, the limit problems are found in a rigorous way. Several scalings of the internal boundary condition with the homogenisation parameter are considered leading to different types of limit problems. For certain scalings, the same limit problems are obtained as for the corresponding linearised boundary condition. Implications for modelling of particular real-world phenomena are discussed.

This is joint work with J. Sneyd (University of Auckland).

Entropy Principle and the Secondary Balance Laws

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Entropy principle of continuum thermodynamics states that the entropy balance of a thermodynamical system has to be satisfied by any solution of the system of field equations – system of balance equations for all the basic dynamical fields.

We study the structure of the "secondary balance laws" extending the technique used for implementing the entropy principle (see [1,2,3]) to the arbitrary determined systems of balance laws (balance systems).

Secondary balance laws generated by symmetries of a balance system are described by the appropriate version of the Noether Theorem.

Using technique of Exterior Differential Systems ([4]) we present the system of first order linear PDE for the densities and fluxes of secondary balance laws in the domain of the constitutive relations.

In many cases (Rational Extended Thermodynamics, constitutive relations depending on all first derivatives of dynamical fields) the solvability conditions of this system take the form of overdetermined system of linear 2^{nd} order PDE for the density of a secondary balance law.

Solutions of these systems are presented for the Cattaneo heat propagation (all secondary balance laws), 5-fields TD system, 8-fields TD systems and some model balance systems.

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The First Principle of Thermodynamics and the Virtual Temperatures Theorem

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The first principle of thermodynamics is reformulated as a variational principle, in which the test fields are piecewise constant virtual temperatures. This simple trick opens the way to get the proof of the existence of a square integrable covector field, the cold flow field, in duality with the vector field of thermal gradients. To build up a proper functional context which meets the principle of reproducibility, we define the thermal space of Green-regular temperature fields, which is the pre-Hilbert space of square integrable scalar fields with piecewise square integrable distributional gradients. This means that each field in the thermal space is associated with a regularity patchwork in whose elements the temperature field has a square integrable distributional gradient. The trial-constraints are assumed to define in the thermal space a closed linear subspace of conforming temperature fields, admitting a common regularity patchwork. The set of conforming temperature fields is then a Hilbert space. The existence proof is based on the closed range property of the distributional gradient and is a straightforward consequence of Banach's closed range theorem. The square integrable cold flow covector fields are the Lagrange multipliers corresponding to the implicit form of the test-constraint imposing that virtual temperature fields are piecewise constant. The cold flow vector fields are associated with the covector fields by Riesz isomorphism. The first principle of thermodynamics, expressed as a variational principle in terms of these fields of Lagrange multipliers, provides a variational equality which is called the principle of virtual temperatures to underline the perfect analogy with the principle of virtual works of mechanics, stemming from the isometry constraint in the variational condition of equilibrium. It follows that these statements, in spite of their traditional names, are rather theorems than principles since their proof, based on the variational equations, can be performed by standard results of functional analysis. By assuming that the trial-constraints define a boundary value problem, i.e. that zero boundary valued fields are conforming, and that the cold flow vector field is square integrable with piecewise square integrable divergence, an application of Green's formula shows that the generalized divergence and the boundary flux of the cold vector field, are respectively the sources and the outflows of the cold content in the body. This fact provides the explicit representation of the vector field as the cold-flow in the body. A standard localization argument provides the boundary and differential equations of thermodynamics. Another simple instance in which this reasoning can be applied, is provided by the flow of a fluid across a control volume of a porous medium. Then conservation of mass leads to the proof of the existence of a mass-flow vector field. A similar analysis can be applied to any balance law in continuum mechanics and thermodynamics. Introducing maximal monotone and conservative constitutive relations between the fields of Lagrange multipliers and the fields expressing the implicit test-constraint, minimum or saddle point principles equivalent to problems in heat conduction, permeability, elastostatics, ect. are got in the various contexts.

Thermal effects in adhesive contact

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We present a model for contact with adhesion between a body and a rigid support, derived within an approach proposed by Michel Frémond, which combines the theory of unilateral contact with the theory of damage, and also accounts for thermal fluctuations both in the body and in its support. The resulting PDE system has been analysed in collaboration with E. Bonetti and G. Bonfanti, leading to results on the global well-posedness and long-time behaviour of the solutions.

Rate-independent processes in solids

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Recent results in selected applications of theory of rate-independent processes will be presented, focused on problems like damage or transformation processes in ferroic materials and/or combination with rate-depedent processes like viscosity.

HOMOGENIZATION OF MANY-BODY STRUCTURES UNDER GLOBAL INJECTIVITY CONSTRAINTS

PHILIPP EMANUEL STELZIG

ABSTRACT. Let $\Omega \subseteq \mathbb{R}^N$, $N \in \{2, 3\}$ be a bounded Lipschitzian domain and $\mathcal{D} \subseteq \mathbb{R}^N$ represent a periodic structure composed by translations and rotations of finitely many open Lipschitzian "basic" domains, such that $\mathrm{vol}\,(\mathbb{R}^N \setminus \mathcal{D}) = 0$. For $\eta > 0$ a small parameter, $\Omega^\eta := \Omega \cap \eta\mathcal{D}$ occupied by a homogeneous hyperelastic material and adhesive surface forces acting on the contact boundaries $\Omega \cap \partial\Omega^\eta$, the author provides Γ-convergence results for the elastic energies corresponding to the many body structures Ω^η as $\eta \to 0$. Motivated by the modelling of tire reinforcing cord belts, two specific structures $\mathcal{D}$ in two and three space dimensions, respectively, are considered. Γ-convergence is carried out w.r.t. the strong $L^1(\Omega; \mathbb{R}^N)$-topology over a rich subclass of $SBV^p(\Omega; \mathbb{R}^N)$, subject to global injectivity constraints modelled by the Ciarlet-Nečas noninterpenetration condition and to positivity of the jacobian determinant. Suggestions for future work are given.

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On the formulation of the Quantum Extended Thermodynamics for the hot carriers in semiconductor materials.

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By using a semiclassical interpretation of the Wigner function [1, 2, 3] we derive a set of quantum hydrodynamic balance equations, in the framework of the Extended Thermodynamics [4], to describe the properties of hot carriers transport in semiconductor materials. We analyze the closure problem for the hydrodynamic system by using the Quantum Maximum Entropy Principle (QMEP) [5, 6, 7, 8] and the Moyal expansion [2] of the Wigner function, for an arbitrary number of scalar and vectorial moments in the case of a nondegenerate gas. The QMEP is applied to a conducting band within a total average energy-scheme. As first simplified approximation we use the usual classic expressions for the collisions electron-phonon [9, 10, 11], and considering a linear expansion around the local equilibrium, we obtain a closed system of Quantum hydrodynamic equations in which all the unknown constitutive functions are completely determined including non-local terms. We remark that, for $\hbar \to 0$ we obtain the usual expression for the Lagrange multipliers, for the distribution function and for the closure relations determined in the framework of classic MEP approach [10,11].

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On the tolerance modelling of functionally graded materials (FGM) with the locally-periodic microstructure

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A tolerance modelling of composites with the periodic or locally-periodic microstructure can be regarded, from the physical point of view, as a certain generalization of the well-known homogenization approach. This generalization leads to the macroscopic (averaged) field equations with coefficients depending on the microstructure length, cf. [1]. So far, the tolerance modelling was based on some heuristic assumptions related to the decomposition of microscopic fields (like the temperature and displacement fields) into the averaged and fluctuation parts.

The aim of this contribution is to outline a formalized approach to the tolerance modelling of FGM with the locally-periodic microstructure. To this end the new definitions of slowly-varying and locally-periodic functions as well as the new definition of tolerance averaging are proposed. The crucial role in the modelling formalism plays the fundamental micro-macro decomposition lemma. This lemma makes it possible to represent a microscopic field under consideration by its averaged part and by the extra macroscopic fields which are referred to as the fluctuation amplitudes. The averaged microscopic field together with the fluctuation amplitudes are slowly-varying functions representing new basic macroscopic unknowns.

Governing macroscopic equations for those unknowns are derived from the principle of stationary action after the tolerance averaging of the pertinent microscopic Lagrange function. It is shown that by neglecting in the governing macroscopic equations terms depending on the microstructure length, the obtained results coincide with those derived from the homogenization approach.

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Instability and breakup process of a compound liquid jet

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We analytically examine instabilities and breakup processes of a compound liquid jet which consists of a core and a surrounding annular phase. By applying long wave approximations to both phases, we obtain reduced nonlinear evolution equations for large deformation of the jet. The equations are found to be more refined than the past ones based on the Stokes approximation in the sense that both inertial terms in the momentum equations and velocity shear between the phases are taken into consideration. When the jet is doubly infinite, numerical analysis of the equations shows that breakup appears through a periodic sealing-off of the annular part, whose profiles are largely affected by the surface tension and density ratios as well as velocity shear between the phases. On the other hand, for the semi-infinite jet the analysis shows that the breakup appears near the nozzle exit and its profile strongly depends upon the input wave profile for small Weber number. For larger Weber number, however, the breakup appears more and more downstream and its profiles hardly depends upon the input waves, which may result from the absolute instability in the linear regime. In addition, sufficient increase of the viscosity in both phases cause the breakup by ballooning of the annular sheet.

This talk reports on a joint work with Michiko Maeda, from the same department as the author.

posters

On the flame structure
in Multi-temperature Mixture Theory

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We study the simple case of stationary one-dimensional flame propagation, modeled by the stechiometric formula $A \rightarrow B$ [1]. To this aim we consider a binary mixture where the constituent A prevails before the flame while B outnumbers A behind the flame. For the mathematical description of the problem, we refer to Mixture Theory and compare the predictions obtained by multi-temperature mixture balance laws [2], [3] with those (known in literature [4], [5], [6]) obtained with single-temperature equations. Also the possible role played by the viscosity is analyzed and discussed.

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Some stability results in the rotating Bénard problem

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We study the classical Bénard system, with and without rotation [1], in a variety of boundary conditions, both for the velocity field and the temperature field. For the temperature field we consider fixed boundary temperatures (perfectly conducting boundaries), fixed heat fluxes (also known as "insulating" boundary conditions) [2], and mixed, or Newton- Robin, boundary conditions. A range of stability estimates [3], with linear instability methods and energy methods, are presented, in rotating and nonrotating systems [4]. Some known linear results for Newton-Robin boundary conditions are confirmed by new energy estimates. Nonlinear energy estimates for the rotating system with one or two *rigid* boundaries are given, for any value of the Prandtl number, and a wide range of rotation speeds. Our initial approach is in the Boussinesq approximation, but we will extend our studies to the general case of compressible fluids, including also magnetic field effects [5,6,7].

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An interfield parallel method with user-controllable numerical dissipation for heterogeneous structural dynamic systems

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This contribution reports on a joint work with O.S. Bursi, A. Bonelli and P. Pegon. A novel partitioned algorithm able to solve ODEs arising from transient structural dynamics is presented. The spatial domain is partitioned into a set of disconnected subdomains owing to computational or physical considerations; and continuity conditions of the velocity at the interface are modelled using a dual Schur formulation, where Lagrange multipliers represent reaction forces. Interface equations along with subdomain equations lead to a system of DAEs for which an interfield parallel procedure is developed. The algorithm first solves interface Lagrange multipliers, that are subsequently used to advance the solution in subdomains. The proposed coupling algorithm that enables arbitrary Generalized-*alpha* schemes [1, 2] to be coupled with different time steps in each subdomain is an extension of a method originally proposed by Pegon and Magonette [3]. Thus, subcycling to deal with stiff and nonstiff subsystems is allowed. In detail, the paper presents the convergence analysis of the interfield parallel scheme for a linear single-degree-of-freedom system as a multi-degree-of-freedom system is too difficult to analyse mathematically. However, the insight gained from the analysis of this coupled problem and the conclusions drawn are confirmed by means of numerical experiments on a four-degrees-of-freedom system.

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Three flow regimes of a viscous jet falling onto a moving surface under gravity

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A thin jet of a viscous Newtonian fluid falling from a nozzle onto a moving surface can fall in three different regimes, which are characterized by convexity of the jet's shape. In the first one the shape of the jet is convex and the jet is tangent to the surface. In the second regime the fluid flows down vertically. And in the last regime, which occurs when the flow velocity at the nozzle is large, the jet's shape is concave, comparable to a ballistic trajectory. Then, the fluid flow at the nozzle is aligned with the nozzle orientation.

The jet model incorporates inertia, viscosity and gravity. The correct boundary conditions for the stationary jet and the parameters region for each flow regime are obtained by studying the characteristics of the equation of motion for a dynamic jet. The theoretical predictions of the parameter regions for the three flow regimes correspond with experiments.

For each flow regime we prove existence and investigate uniqueness. A jet solution might not be unique if the nozzle does not point down vertically. In this case up to three stationary solutions are possible, which leads to instabilities, also observed in the experiments.

NEWTON-PRODUCT INTEGRATION FOR A STEFAN PROBLEM WITH KINETICS

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This contribution reports on a joint work with B. Babayar Razligi and M.R. Mokhtarzadeh. We reduce the Stefan problem with kinetics to a system of nonlinear Volterra integral equations of second kind and apply Newton's method to linearize it. We present product integration solution of the linear form. Sufficient conditions for convergence of the numerical method are given and their applicability is illustrated with examples.

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VIBRATIONS OF MICROLAYERED FUNCTIONALLY GRADED MEDIA

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Composites with continuously varying properties are called *functionally graded materials* (*FGM*), cf. [6]. In this note we analyse composites with a laminated structure on a micro level. However, on a macro level these composites can be treated as made of a functionally graded material.

In these structures a distribution of components is known. Despite of a geometry of microstructure cannot be described exactly, thermo-mechanical phenomena for these composites can be investigated within micromechanical models with idealised geometries. FGM-type media are analysed using modified approaches, which were proposed for macroscopically homogeneous composites, e. g. periodic composites (laminates). Some of these modelling techniques are mentioned in the book [5]. Between these approaches we have to mention those based on the asymptotic *homogenization* proposed and developed for periodic composites and structures. Unfortunately, averaged equations of models based on this technique neglect the effect of the microstructure size.

An alternative approach to analyse thermo-mechanical problems for functionally graded materials is a generalization of *the tolerance averaging technique*, proposed to describe non-stationary problems for periodic composites and structures, cf. [7]. For FGM-type media the tolerance averaging technique leads from equations with functional, highly-oscillating, locally-periodic and non-continuous coefficients to a system of differential equations with slowly-varying coefficients. Averaged models based on this technique take into account the effect of the microstructure size on the overall behaviour of a medium.

This approach is applied to analyse various problems for FGM-type composites in a series of papers, e. g. for an elastic response in [4], [6]; for a heat conduction in [1], [3]. Averaged models of laminates with functionally graded structure are shown in [2], where considerations are restricted to the macrostructural model, neglecting the effect of the microstructure size.

The first aim of this contribution is to present averaged equations of tolerance model, which describe the above effect in various problems of those laminates. The second aim is to apply obtained equations to analyse vibrations of a thick layer made of two linear-elastic materials distributed in laminas with varying thicknesses. The distribution of lamina thicknesses is extrapolated by a smooth, slowly-varying cell distribution function.

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On the sharp interface limit of a two-scale reaction-diffusion system

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We discuss the fast-reaction limit of a two-scale reaction-diffusion model. If the reaction constant a tends to infinity, then a two-scale PDE system with a free boundary in the local cell problems is obtained. Moreover, we show that the same two-scale free-boundary problem is obtained if we first pass to the fast-reaction limit $a \to \infty$ and then take the homogenization limit $\varepsilon \to 0$ that is behind the derivation of the two-scale model. Here ε is the typical size of the microstructure.

On the heat conduction in functionally graded infinite hollow cylinder

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This contribution reports on a joint work with B. Michalak and deals with a heat conduction in infinite hollow cylinder with apparent properties smoothly varying along the radial direction. The aim of this contribution is the analysis stationary and nonstationary heat transfer in the two-phase hollow cylinder with a deterministic microstructure. This microstructure is periodic along the angular axis and has slowly varying effective (macroscopic) properties in the radial direction. Since apparent properties in the radial direction can characterize a smooth passage from one component material to the other, thus we deal here with a special class of the functionally graded materials, FGM, cf. Suresh, Mortensen (1998).
The exact equation of Fourier heat transfer comprise highly-oscillating and non-continuous coefficients. A formulation of macroscopic models of composite conductors with a deterministic microheterogeneous structure can be based on the non-uniform homogenization cf. Jikov at al.(1994). However, the homogenization technique leads to the model equations independent of the microstructure size on the overall response of the FGM-conductor. The proposed modeling procedure is based on the tolerance averaging technique of the Fourier heat conduction equation, cf. Woźniak, Wierzbicki (2000), and general approach to the description of longitudinally graded stratified media can be found in [Michalak at al. 2007]. This model takes into account the effect of microstructure size on the overall heat transfer behaviour.
The obtained averaged model equations will be applied to analysis stationary and non-stationary problem of heat transfer in the circular microheterogeneous hollow cylinder. Since the proposed model equations have smooth and slowly varying functional coefficients then in most cases solutions to specific problems of the heat transfer in conductor under consideration have to be obtained using numerical methods. . In this contribution we shall use finite difference method to derive the solution of averaged model equations.

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TOLERANCE MODELLING OF HEAT CONDUCTION IN LAMINATES WITH FUNCTIONALLY GRADED STRUCTURE

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This presentation reports on a joint work with Jarosław Jêdrysiak. The object of our considerations is a two-component composite made of conductors, which are non-periodically distributed in the form of micro-laminas along the thickness of the layer. It is assumed that the macroscopic properties of this laminated composite vary continuously across laminas. This kind of materials is called *functionally graded materials* (*FGM*), cf. [8].

In order to describe the behaviour of FGM-type composites some methods can be used, which were proposed and discussed in [8]. Between these methods, we have to mention those based on *the asymptotic homogenization* proposed for periodic composites and structures, [2]. For analysing the heat transfer problems it can be also used the method proposed in the framework of *models with micro-local parameters*, [4]. Unfortunately, the above models usually neglect *the effect of microstructure size* on the overall behaviour of laminates. Another way to solve the problem is *the higher-order theory* for functionally graded materials presented in [1].

It is possible to consider *the effect of microstructure size* by using *the tolerance averaging technique*, presented for periodic composites in [10]. In the last years *the modified tolerance averaging technique* was applied for problems of FGM-type structures, e. g. elastodynamics [7, 9] and heat conduction in [5, 3 and 6]. This approach leads from equations of those structures with functional, highly-oscillating, locally-periodic and non-continuous coefficients to the system of differential equations with slowly-varying coefficients, describing *the effect of microstructure size* on the overall behaviour of the composite with a microstructure. The aim of the paper is to compare results of one-direction heat conduction in the FGMtype laminate across laminas calculated by *the tolerance model*, [3], and *the higher-order theory*, proposed in [1].

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Müller's K vector in thermoelasticity

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The concept of the K vector first proposed by I. Müller made revolutionary changes in irreversible thermodynamics. It may be important also in the theory of thermoelasticity. The well known theories of thermoelasticity are based on thermal expansion, and the recent improvements are looked for in the theory of heat conduction. The reason is that heat conduction is accounted with scalar and vector variables while elasticity with second order tensors and there is no direct coupling between second order tensors and vectors or scalars in linear order if the material is isotropic. The deviations from the present theories urge new pathways for research. Such a new track can be opened by Onsager's thermodynamics supplemented with dynamic degrees of freedom. This theory is usually referred to as extended thermodynamics. The key moment is in the general form of the entropy current out of local equilibrium, which leads to the formal introduction of the transport of the dynamic degrees of freedom. The skeleton of the possible theories is based on the introduction of one or more vectorial dynamic variables. They can be coupled to the current density of the heat flow, while their 'diffusion' intensities are second order tensors coupled directly in linear order to the stress tensor even if the material is isotropic. The possibilities are demonstrated on an example with one dynamic degree of freedom. The new theory may explain why a thin coat of mortar can prevent the disintegration of the rock inside a tunnel.

The dynamic modeling and analysis of certain functionally graded plates

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This presentation reports on a joint work with B. Michalak. The subject of an analysis are thin plates with apparent properties smoothly varying along the preferred direction. The aim of this contribution is to formulate and investigate an averaged model describing the dynamic behaviour of a plate with inhomogeneous microstructure which is periodic along a certain direction and have slowly varying effective properties in the perpendicular direction. Since effective properties of this composite plate are graded in space then we deal with special class of the functionally graded materials, FGM, cf. Suresh, Mortensen (1998).

The exact equations describing of the dynamics behaviour of the FGM-plates comprise highly-oscillating and non-continuous coefficients. The modeling problem is how to describe microheterogeneous plate by certain averaged equations with functional but smooth and slowly varying coefficients. For the above problem we can apply homogenization technique for equations with non-uniformly oscillating coefficients, cf. Jikov at al.(1994). However, the averaged model obtained by using this method neglects the effect of the microstructure size on the overall response of the FGM-plate. The proposed approach is based on the tolerance averaging of equations of motion for thin elastic plates and is a generalization of the tolerance averaging technique for composites with periodic microstructure, cf. Woźniak, Wierzbicki (2000).

The aim of this contribution is two-fold. First, to formulate a non-asymptotic model of the FGM-plate under consideration. This model takes into account the effect of the microstructure size on the dynamic behaviour of the FGM-plate. Second, to investigate a free-vibration problem in the framework of non-asymptotic model.

The obtained averaged model equations will be applied to analysis a free-vibration problem for the annular plates. Since the proposed model equations have smooth and slowly varying functional coefficients solution to eigenvalues problem for circular plates will be obtained using finite difference method.

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