

## Mathematical Continuum Mechanics

20.08.–26.08.2000

### Introduction

This workshop was organized by J.M. Ball (Oxford), R.D. James (Minneapolis) and S. Müller (Leipzig) and focused on recent developments at the interface of nonlinear analysis and continuum mechanics. It led to a lively exchange between mathematicians (who constituted the largest group), physicists and engineers. Topics included

Mathematical problems arising in nonlinear elasticity, in particular including phase transitions, microstructure and mathematical concepts to capture these (weak convergence, quasiconvexity, Young measures, ... )

Mathematical tools to pass from atomistic to continuum models

Thin films and the derivation of two-dimensional limiting theories for thin three-dimensional objects

General concepts of continuum mechanics to model complex materials

The meeting also included a very lively discussion session on the future role of continuum mechanics and theory in general at a time where in parts of the applied sciences ‘theory’ often is almost synonymous to ‘large scale numerical simulation’.

# Abstracts

## Electromechanical behavior of ferroelectric ceramics

Kaushik Bhattacharya

The talk describes problems in the calculus of variations and homogenized theory motivated by a continuum mechanical model of ferroelectric materials. Ferroelectrics are crystalline solids that are spontaneously polarized and distorted below the Curie temperature; symmetry breaking at this temperature implies that the crystal may be polarized in one of many crystallographically equivalent directions. The electromechanical behavior is modeled using a variational principle, where the functional consist of a multiwell Devonshire-type potential, an electromechanical loading potential and a nonlocal electric field energy. The functional is not weakly lower semicontinuous and energy minimization automatically predicts experimentally observed domain patterns. The model is used to identify a novel electromechanical load path which yields large electrostriction; experimental tests stimulated by this theory have demonstrated five times the electrostriction of commonly used materials. A homogenized functional that describes the effective of polycrystals (ceramics) is derived using the notion of  $\Gamma$ -convergence, and used to understand the anomalous behavior at morphotropic phase boundaries.

## Fast singular limits of mechanical systems

Folkmar Bornemann

Elimination of fast scales amounts, e.g. in molecular dynamics, for establishing the limit of mechanical systems with a strong constraining potential:

$$\mathcal{L}_\epsilon = \frac{1}{2}\langle \dot{x}, \dot{x} \rangle - V(x) - \epsilon^{-2}\mathcal{U}(x).$$

Here  $N = \mathcal{U}^{-1}(0)$  is assumed to be nondegenerate critical. Two questions are considered: First, is there a limit Lagrangian  $\mathcal{L}_0$  on  $TN$ , second, when is this Lagrangian the Lagrangian of holonomic constraints  $\mathcal{L}_{\text{hol}} = \frac{1}{2}\langle \dot{x}, \dot{x} \rangle - V|_N$  on  $TN$ . In general it turns out that under mild resonance condition we get  $\mathcal{L}_0 = \mathcal{L}_{\text{hol}} + \mathcal{U}_0$ , where  $\mathcal{U}_0$  is a Born-Oppenheimer type of potential, which can explicitly be given. The method of proof we use is the method of weak convergence, where we mainly use a suitable generalization of the Riemann-Lebesgue-Lemma.

## **Extension of the Monge-Kantorovich problem to classical Electrodynamics**

Yann Brenier

We extend to the framework of classical Electrodynamics the Monge-Kantorovich problem which originally comes from Continuum Mechanics and has become very popular in the last ten years in the field of Nonlinear PDEs, especially because of its connection with the Monge-Ampère equation (and also Porous Medium equations, Euler equation of incompressible fluids etc...).

The first step of the construction is to revisit the Monge-Kantorovich (MK) considering geodesics and probability measures as in the MK problem (in its new formulation), we consider extremal surfaces in the 5-dimensional Minkowski space. Next, we consider generalized surfaces (which can be also described with the concepts of Cartesian currents, as in Giaquinta-Modica-Soucek book) and the corresponding action (that shares some similarity with the Born-Infeld action of nonlinear electromagnetism). This leads to some nonlinear Euler-Maxwell equations from which the classical Euler-Maxwell (relativistic and pressureless) can be recovered from a 3 point discretization of the 5<sup>th</sup> variable.

## **Rigorous bounds for the Föppl-von Kármán theory of isotropically compressed plates**

Sergio Conti

with H. Ben Belgacem, A. DeSimone, S. Müller.

We study the Föppl-von Kármán theory for isotropically compressed thin plates in a geometrically linear setting, which is commonly used to model weak buckling of thin films. We consider generic smooth domains with clamped boundary conditions, and obtain rigorous upper and lower bounds on the minimum energy linear in the plate thickness  $\sigma$ . This energy is much lower than previous estimates based on certain dimensional reductions of the problem, which had lead to energies of order  $1 + \sigma$  (scalar approximation) or  $\sigma^{2/3}$  (two-component approximation).

## **Soft Ferromagnetic Films**

Antonio DeSimone

In joint work with R.V. Kohn, S. Müller, and F. Otto, a two-dimensional variational model for the response of soft ferromagnetic films to in-plane applied fields has been derived from three-dimensional micromagnetics via a Gamma-convergence argument. Domain patterns emerge from the competition between the aligning effect of the applied field and the bias towards divergence-free patterns due to dipolar interactions.

A numerical scheme has been derived and used to compare the predictions of the theory with experimental results.

## Some remarks on metastability in martensite under load

Alain Forclaz

A few years ago, interesting biaxial loading experiments were performed by C. Chu and R.D. James. A mathematical treatment of these was then initiated by J.M. Ball and R.D. James. In those experiments, it is observed that an homogeneous deformation  $y_1(x) = U_1x$  is the stable state for small loads while  $y_2(x) = U_2x$  is stable for large loads. Crucially, it has been proved by Ball and James that for a certain intermediate range of loads,  $y_1(x) = U_1x$  remains metastable (i.e., is a local - as oppose to global - minimizer of the energy). It is easy to get an upper bound for when metastability finishes. However, it was also observed that this bound (the Schmid Law) may not be sharp, but that required some geometric restriction. In this talk, I focus on this last point and give a precise statement of what these geometric restrictions are.

## One dimensional lattice waves: rigorous continuum limit via a renormalization group approach

Gero Friesecke

The speaker discussed recent progress in the understanding of the long-time dynamics of Fermi-Pasta-Ulam (FPU) chains, i.e., 1D infinite chains of nonlinear oscillators with ‘generic’ anharmonic nearest-neighbour interaction,

$$H = \sum_{j=-\infty}^{\infty} (p_j^2/2 + V(q_{j+1} - q_j)).$$

These are the perhaps simplest prototypes of non-integrable Hamiltonian systems of infinitely many particles where Fermi, Pasta and Ulam’s fundamental (1947) question can be investigated as to whether and how thermalization (i.e., energy transport from coherent modes and macroscopic scales to microscopic, radiative modes) occurs.

While it has been clear for some time that these systems support exact solitary waves (G.F., J.A.D. Wattis, Commun. Math. Phys. **161**, 391-418, 1994), it has recently been shown in joint work with Robert L. Pego, University of Maryland, that at near-sonic wavespeed such waves are (i) unique and rigorously approximated by a KdV continuum limit (G.F., R.L. Pego, Nonlinearity **12**, 1601-1627, 1999), (ii) stable globally in time in the sense of ‘start close, stay close’ (G.F., R.L. Pego, to appear). This is to our knowledge the first result that establishes the large time behaviour of an open set of initial data in infinite-D phase space, and proves that thermalization cannot hold for generic initial data.

The precise statement on passage to a continuum limit for near-sonic solitary waves is as follows:

Theorem. Given any interaction potential  $V$  satisfying the generic conditions  $V(0) = V'(0) = 0$ ,  $V''(0) > 0$ ,  $V'''(0) \neq 0$ , and given any wavespeed  $c$  bigger than, but sufficiently

close to, the speed of sound  $c_S = \sqrt{V''(0)}$ , the following hold.

(i) The Hamiltonian system admits a unique single-pulse solitary wave solution  $q_{j+1}(t) - q_j(t) = r_c(j - ct)$  of speed  $c$ . (Single-pulse means the derivative of the profile  $r_c(z)$  vanishes only at a single point.)

(ii) As  $\epsilon := \sqrt{24(c/c_S - 1)} \rightarrow 0$ , the sequence of renormalized profiles  $\epsilon^{-2}r_c(\epsilon^{-1}\cdot)$  converges strongly in  $H^1(\mathbb{R})$  to a nonzero limit  $r$ .

(iii) The limit solves the Korteweg-de-Vries travelling wave equation

$$-r_x + r_{xxx} + 12(V'''(0)/V''(0))r r_x = 0.$$

Hence, by uniqueness of nontrivial solutions to this equation, the limit is given explicitly by  $r = (V''(0)/V'''(0))((1/2)\operatorname{sech}(x/2))^2$ .

The proof of (iii), i.e. rigorous passage to the limit assuming the scaling laws implicit in the compactness result (ii), can be understood in a clear and simple way using the renormalization group framework introduced by G.F. and R.L. Pego (see above reference), in which the KdV equation emerges naturally as a fixed point of the renormalization group. This framework also leads to a simple proof of the existence (though not the uniqueness) result (i), by applying the implicit function theorem with the renormalization parameter  $\epsilon$  as a parameter to show that the well known solitary wave solution to the continuum limit equation persists into the discrete system. The proof of the compactness result (ii), which in particular implies uniqueness and which identifies the correct scaling laws as  $\epsilon \rightarrow 0$ , is deeper, and requires an understanding of the lattice equation on all frequency scales. This has been achieved via a careful study of a certain naturally arising lattice Fourier multiplier, leading to, among other things, a new Harnack inequality for nonlinear differential-difference equations.

## On induced microstructures occurring in models of finite-strain elastoplasticity

Klaus Hackl

We derive a novel variational principle for a time-discretized model of the flow theory of elastoplasticity at finite strains. Within a single time-step the functional

$$\mathcal{I}_{\mathbf{P}_0, p_0}(\boldsymbol{\phi}, \mathbf{P}, p) = \int_{\Omega} (\Psi(\mathbf{F}\mathbf{P}, p) + J^*(\Delta(\mathbf{P}_0, \mathbf{P}), p - p_0)) \, d\mathbf{x} - \ell(\boldsymbol{\phi})$$

has to be minimized with respect to the total deformation  $\mathbf{F}$  and the plastic quantities  $\mathbf{P}$ ,  $p$  as independent variables for given initial values  $\mathbf{P}_0$ ,  $p_0$ , where  $\ell$  is the potential of external forces and  $\Delta(\mathbf{P}_0, \mathbf{P})$  denotes a discretized rate of evolution. We assume that  $\Psi$  is polyconvex and  $J^*$  convex. Elimination of  $\mathbf{P}$  and  $p$  leads to the reduced energy density

$$\Psi_{\mathbf{P}_0, p_0}^{\text{red}}(\mathbf{F}) = \min \left\{ \Psi(\mathbf{F}\mathbf{P}, p) + J^*(\Delta(\mathbf{P}_0, \mathbf{P}), p - p_0) \mid (\mathbf{P}, p) \right\}$$

which can be further investigated for its convexity properties. This allows to study the occurrence of microstructures much in the same way as it is done when considering phase transitions.

Finite element calculations indeed show layered microstructures. The results are, however, mesh-dependent. To overcome this effect a  $R_1$ -convexification of the potential  $W = \Psi_{\mathbf{P}_0, p_0}^{\text{red}}$  defined by

$$\begin{aligned} R_1 W(\mathbf{F}) \\ = \inf \{ (1 - \lambda)W(\mathbf{F} - \lambda \mathbf{a} \otimes \mathbf{b}) + \lambda W(\mathbf{F} + (1 - \lambda) \mathbf{a} \otimes \mathbf{b}) \mid 0 \leq \lambda \leq 1, \quad |\mathbf{a}| = 1 \} \end{aligned}$$

is performed numerically using a gradient-line-search algorithm. The results obtained using the relaxed potential are essentially mesh-independent.

A specific example based on a model of crystal-elastoplasticity with a single slip-system is discussed.

*Reference:* A. Mielke, K. Hackl, C. Carstensen: *Nonconvex Potentials and Microstructures in Finite-Strain Plasticity*. Manuscript, in preparation.

## Multiphase Flow in Porous Media

Rudolf Hilfer

The commonly accepted microscopic and macroscopic equations for immiscible displacement of two incompressible Newtonian fluids in a rigid porous medium are critically examined. A mathematical connection between the microscopic and the macroscopic equations appears unlikely because the latter equations are incomplete with regard to predicting changes in residual saturations. A novel system of 10 coupled equations is presented. The basic physical ideas are firstly to distinguish connected and a disconnected (trapped) sub-phase within each fluid phase and secondly to introduce energy balance laws including interfacial energies. As a consequence the specific internal surface area appears as a new variable. The mass, momentum and energy balance equations are based on continuum mixture theory and the pairwise character of interfacial energies is explicitly taken into account. The constitution assumptions follow those commonly accepted for single phase flow and include a mass exchange between connected and disconnected subphases that is taken from experimental capillary desaturation curves. The approach obviates the need for a capillary pressure function. Capillarity enters instead through the energy equations. One finds a generalized Darcy law with relative permeabilities  $k_w^r(S_w, A_w) \sim (S_w - S_{w_i}^*)^3 A_w^{-2}$  of Brooks-Corey type that depend also on specific internal surface area. The irreducible water saturation  $S_{w_i}^*$  is determined as part of the solution in the same way as the water saturation  $S_w$  and the specific internal surface area of the water  $A_w$ . The change of the relative permeability  $k_w^r$  with wettability conditions is also found to be in qualitative agreement with experiment.

## The 2-Well problem in 3 dimensions

Bernd Kirchheim

We discuss properties of generalized convex hulls of the set  $K = SO(3) \cup SO(3)H$  with  $\det H > 0$ . The question is motivated by the consideration of energy minimizing configurations in shape memory alloys.

If  $K$  does not contain any rank-1 connection, we show that the quasiconvex hull of  $K$  is trivial if  $H$  belongs to a certain (large) neighbourhood of the identity. It turns out that the polyconvex hull of  $K$  can be nontrivial if  $H$  is sufficiently far from Id, while the (functional) rank-one convex hull is always trivial.

This is joint work with G. Dolzmann, S. Müller, V. Šverák.

## Some Mathematical Theories on Liquid Crystals

Chun Liu

Liquid crystal materials are, in fact, different intermediate phases between isotropic fluid and crystalline solid. The understanding of such materials is the first step in studying polymers and other more complicated structured fluids. From the fluid aspect of the material, liquid crystals can be described by the conservation laws: mass, linear momentum and energy. It also requires the special constitutive equations on the stress tensor and the balance laws for the order parameters. These are also responsible for the non-Newtonian features of the materials. From the solid point of the view, liquid crystals can store elastic energy due to the order parameters (e.g. the orientational director for nematic and the layer parameter for smectic). The coupling between the fluid properties and the solid behaviors gives many difficulties in dealing with such systems. In this talk, I will go over some of the theories and approaches that we used in treating these coupled systems. We will discuss the interaction between the fluid velocity and the parameter configurations, the relations between the stability and uniqueness to the higher order energy laws, as well as some analytical and modeling open problems.

## A mathematical model for a sphalerite-chalcopyrite phase change

Stephan Luckhaus

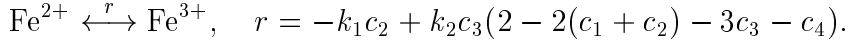
with K. Bente, Institut für Mineralogie, Universität Leipzig.

The model is describing a phase change in a system of ZnS-FeS, CuFeS<sub>2</sub> which is diffusion induced. The phase change corresponds to a symmetry breaking of the lattice induced by the periodic (non random) distribution of Cu and Fe on metal ion sites.

For the description of the diffusion process, the concentrations of  $\text{Zn}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Fe}^{3+}$  and  $\text{Cu}^+$  are needed. The overall model is of Stefan type:

$$\begin{aligned}\partial_t c_i &= \nabla(L_{ij}\nabla\mu_j) + r_i, \quad \text{where } 1 \leq i, j \leq 4 \\ \mu_j &= \frac{\partial}{\partial c_j} f(c), \quad f(c) = \min\{\alpha f_1(c_\alpha) + (1 - \alpha)f_2(\bar{c}_\alpha) \mid 0 \leq \alpha \leq 1, c = \alpha c_\alpha + (1 - \alpha)\bar{c}_\alpha\}\end{aligned}$$

and  $f_1, f_2$  are free energies for sphalerite and chalcopyrite. The reaction rate is the rate of oxidation of iron



That is the mass action law (with Arrhenius kinetics). One observation is that the diffusion equation can be written as a system of 4 equations

$$\partial_t c_i = \nabla \cdot J_i + r_i \quad (\text{conservation law})$$

and one inequality

$$\partial_t f \leq \nabla(J_i \mu_i) - Q_J(J) - Q_J^*(\nabla\mu) - Q_r(r) - Q_r^*(\mu) \quad (\text{entropy production law})$$

where \* denotes the Legendre transform.

$$Q_J(J) = \frac{1}{2} J \cdot L^{-1} \cdot J, \quad Q_J^*(\nabla\mu) = \frac{1}{2} \nabla\mu \cdot L \cdot \nabla\mu$$

and  $Q_r$  contains a logarithmic expression.

Independent diffusion processes are combined by adding corresponding  $Q$  s. Therefore it is natural to split  $Q_J$  as

$$Q_{\text{I}}(J_1, J_2 + J_3, J_4) + Q_{\text{II}}(J_2 - J_3)$$

where  $Q_{\text{II}}$  and  $Q_r$  are small corresponding to the fastest processes.

Singular perturbation arguments lead then finally to one elliptic equation for  $c_2 - c_3$  and a system of three diffusion equations for the metal ion movement.

## Gradient systems with wiggly energies and related averaging problems

Govind Menon

We study a two-dimensional generalization of a model for the kinetics of martensitic phase transitions proposed by Abeyaratne, Chu and James. We derive homogenized equations for the macroscopic motion in certain regions of phase space, but these equations typically do not have unique solutions. Generically most of the phase space breaks into a countable number of domains, in the interior of which the homogenized dynamics are rectilinear.



These domains have a Cantor-like structure originating in bifurcations of two parameter families of circle diffeomorphisms. Consequently, the homogenized equations vary on all scales. V.P. Smyshlyaev has studied this problem independently, and some of our results are similar.

## **Shape Memory Alloys - Phenomenon - Simulation - Applications**

Ingo Müller

Shape memory alloys exhibit a strong dependence of their load-deformation curves upon temperature. Thus at low temperature they are quasiplastic; their hysteresis loop contains the origin and the deformations are due to conversion of one variant of martensite into another one. At high temperature the load-deformation behaviour is pseudoelastic with hysteresis loop in the first and third quadrant. Yield and recovery in this case are due to an austenitic martensitic phase transition. A model is constructed which simulates this behaviour. The model is based on rate law for the phase fractions and the transition probabilities are those of an activated process akin to chemical reactions. Adjusting four parameter by simple diagnostic experiments one obtains a predictive theory of the load-deformation-temperature behavior of specific shape memory alloys. The model is tested in a feedback control experiment on a loaded wire and it is found that there is very good agreement between theory and experiment. Application of the theory include the automatic adaptation of the profile of an airplane wing to the extent, and changing flight conditions. Apart from feedback control the theory can also be used for online optimal control of the wing shape. The most recent application has been to the self-adjustment of the winglets of an airplane for the purpose of reducing the drag at constant lift.

## **Ostwald ripening in thin films**

Barbara Niethammer

We rigorously derive a mean-field model for Ostwald ripening in two-dimensional systems which arise in the growth of thin metallic films. This extends the classical LSW-theory in two ways. First, it shows that an LSW-type model is valid also in two dimensions, even though the formal derivation seems less convincing than in three dimensions. Second, it clarifies the regime of validity and provides an inhomogeneous extension.

## **Thin viscous films**

Felix Otto

The capillarity-driven spreading of a thin droplet of a viscous liquid on a solid plane is modelled by the lubrication approximation, an evolution equation for the film height  $h$ .

However, as a consequence of the no-slip boundary condition for the liquid at the solid plane, logarithmic divergences in the viscous dissipation rate occur if the support of  $h$  changes.

This well-known singularity is removed by relaxing the no-slip condition, thereby introducing a microscopic lengthscale  $b$ . Matched asymptotics suggests a relationship (Tanner's law) between the speed of the contact line (the boundary of the support of  $h$ ) and the macroscopic contact angle (the slope of  $h$  near the boundary of its support), modulo a logarithm involving  $b$ . This dynamic contact angle condition, which balances viscous forces and surface tension, is quite different from the static contact angle condition (Young's law), which balances just the surface tensions.

Tanner's law predicts a specific scaling for the spreading of the droplet. In a joint work with L. Giacomelli, we rigorously derive the scaling of the spreading, which is consistent with the one predicted based on Tanner's law, including the logarithmic terms. Mathematically speaking, this amounts to estimates of appropriate integral quantities of the evolution equation, which comes in form of a nonlinear parabolic equation of fourth order.

## **A mathematical model for diffusion-induced grain-boundary motion**

Oliver Penrose

with J.W. Cahn, C. Elliott, P. Fife.

If a thin film of one metal, say Fe, is placed in the vapour of another metal, say Zn, the boundaries between the crystal grains are often observed to move. Since the Zn atoms cannot diffuse directly into the Fe crystal, they dissolve in the Fe indirectly by diffusing in along the grain boundary which then moves aside and leaves Ni atoms dissolved in the newly formed part of the growing crystal grain.

Our continuum model consists of two P.D.E.'s, one a diffusion-type equation for the concentration field, the other a Cahn-Allen type equation for a "crystallinity" field which is +1 in the growing grain, -1 in the shrinking grain, and takes intermediate values in the grain boundary. For realistic parameter values, the P.D.E.'s can be reduced using a shape-interface approximation to a pair of ODE's. By solving these one can predict the speed and cross-sectional shape of the moving grain boundary. An interesting feature is that the model predicts two completely different types of geometry for the moving grain boundary, one connecting the two sides of the specimen, the other trailing back to infinity inside it.

## **Self-similar singular solutions of the complex Ginzburg-Landau equation**

Petr Plecháč

In the joint work with V. Šverák (University of Minnesota) we studied self-similar singular solutions to the complex Ginzburg-Landau equation. In this talk we address the

open problem of existence of singularities for the complex Ginzburg-Landau equation. Using a combination of rigorous results and numerical computations we describe a countable family of self-similar singularities. Our analysis includes the super-critical non-linear Schrödinger equation as a special case, and most of the described singularities are new even in that situation. We also consider the problem of stability of these singularities.

## On Ferroelastic Microstructures

Ekhard K.H. Salje

The theoretically predicted divergence at  $T \rightarrow T_C$  of the width of a twin wall (rank-1 connected twins) in a 2<sup>nd</sup> order transition was observed experimentally in  $\text{LaAlO}_3$ . Typical wall thicknesses at  $T \ll T_C$  are some nanometers with corresponding wall energies of  $\approx 10^{-2} \text{J/m}^2$ . The results are fully compatible with LG potentials of the type

$$G = \int dr^3 \left\{ \frac{1}{2} A \Theta_S \left( \coth \frac{\Theta_S}{T} - \coth \frac{\Theta_S}{T_C} \right) Q^2 + \frac{1}{4} B Q^4 + \frac{1}{2} g (\nabla Q)^2 \right\}$$

where  $Q$  is the structural order parameter (e.g.  $Q = \nabla u$ ). The atomic origin of  $G$  is discussed.

Fast diffusion along twin walls was shown for Na and O diffusion in twinned  $\text{Na}_x\text{WO}_{3-x}$ . Superconducting twin walls were generated. Complex microstructures are strain dominated, both in displacive and ferroelastic old systems. The dominant coarsening mechanism is the formation and retraction of needle domains. Local theories for the analysis of needle trajectories were briefly discussed.

## On the Geometric Structure of Cauchy's Theory of Stresses

Reuven Segev

A generalization of Cauchy's theory for the existence of stresses to the geometry of differentiable manifolds is presented using the language of differential forms. Body forces and surface forces are defined in terms of the power densities they produce when acting on generalized velocity fields. The velocity fields are sections of a vector bundle  $W$  over the  $m$ -dimensional material manifold  $S$ . Thus, a body force on a body  $R$  is an  $W^*$ -valued,  $m$ -form on  $R$  and a surface force is a  $W^*$ -valued,  $(m-1)$ -form on  $\partial R$ .

The balance law is written in terms of the total power expanded by forces and it is viewed as a boundedness or regularity assumption on the force functionals for the various bodies. The normal to the boundary is replaced by the tangent space equipped with the outer orientation induced by outwards pointing vectors.

In the resulting Cauchy's theorem stresses are modeled as  $m-1$ , covector valued forms. A stress induces a surface force by restriction to the tangent space to the boundary, while

the outer orientation of the tangent space is taken into account. This operation, to which we refer as inclined restriction, uses a sign rule based on an orientation of the material manifold.

The special cases of volume manifolds and Riemannian manifolds are discussed. In the case of a volume manifold, it is shown how a tensor can represent a stress form using the volume element. Finally, the classical Cauchy formula is recovered for Riemannian manifolds.

The above construction is used in the case where  $W$  is the trivial line bundle,  $S$  is interpreted as the space manifold so a typical  $R$  is interpreted as a control region. This situation models the balance of a certain scalar property in space. It is shown that without any additional geometrical structure this setting induces body points and material structure associated with the given scalar property.

## **Mathematical problems in geometrically linear theory of phase equilibrium in solids**

Gregory Seregin

We discuss recent results on existence, relaxation and regularity for variational problems describing phase equilibrium in solids in geometrically linear setting.

## **Anisotropic Lagrangian Averaged Navier-Stokes Equations**

Steve Shkoller

We develop a new Lagrangian averaging procedure for the incompressible Navier-Stokes (NS) equations. The method is based on “fuzzifying” the Lagrangian flow map by composing the exact flow with near-identity volume preserving diffeomorphisms  $\xi^\alpha$ , and then averaging the kinetic energy of the fuzzy flow  $\eta^\alpha$  over all possible perturbations  $\xi^\alpha$ . Performing asymptotic expansions about  $\alpha = 0$  in the variational principle, averaging and computing the first variation yields a new model of fluid turbulence, which we call the anisotropic Lagrangian Averaged Navier-Stokes (LANS) equations; those equations capture the large scale flow of the NS equations (for spatial scales greater than  $\alpha > 0$ ), while averaging over spatial scales smaller than  $\alpha$ . The LANS model is a dynamically coupled system of equations for the Lagrangian mean velocity  $U$  and the covariance tensor  $F$ . The mean  $U$  is the first term in the asymptotic expansion; our theory also provides an auxiliary linear PDE, a corrector, whose solution gives the second term in the asymptotic expansion. After presenting the derivation, we state our theorem on the global well-posedness of 3D classical solutions on *domains with boundary* with  $u = 0$  BCs and prove the regular limits of zero viscosity.

## Patterned Single and Double Layer Shape Memory Films

Manfred Wuttig

Stresses in films can be controlled by patterning. While planar films are in a state of biaxial stress thin strips with a high aspect ratio (height to width) are in a state of uniaxial stress on a substrate. We have recently prepared NiTi films on Si with aspect ratios ranging from  $10^{-2}$  to 0.6. The films are deposited at room temperature and subsequently annealed at  $500^\circ\text{C}$  for crystallization. The magnitude of the thermoelastic stresses which developed during cooling back to room temperature was  $E/(1-\gamma)\partial\alpha\Delta T$  ( $\partial\alpha =$  difference of coefficients of thermal expansivity of NiTi and Si) and  $E\partial\alpha\Delta T$  for low and high aspect ratios.

The martensitic transformation can be controlled by stresses. We have used the thermoelastic stress to engineer a double layer film consisting of the rhombohedral and tetragonal NiTi phases. The damping of this double film is 10 times larger than the damping of the individual components strongly suggesting an interactive damping mechanism. Details of this mechanism are presently unknown.

## Non-Lipschitz minimizers of smooth uniformly convex functionals

Xiaodong Yan

with Vladimír Šverák.

We consider variational integrals of the form

$$I(u) = \int_{\Omega} f(Du(x))dx, \quad (1)$$

where  $\Omega$  is a bounded open set with smooth boundary in  $\mathbf{R}^n$ ,  $u: \Omega \rightarrow \mathbf{R}^m$ ,  $Du$  is the gradient matrix of  $u$  and  $f: M^{m \times n} \rightarrow \mathbf{R}$  is a smooth uniformly convex function (i.e. there exists a constant  $\nu > 0$ , such that for all  $\xi \in M^{m \times n}$ ,  $X \in M^{m \times n}$ , the inequality  $f_{p_{\alpha}^i p_{\beta}^j}(X)\xi_{\alpha}^i \xi_{\beta}^j \geq \nu|\xi|^2$  holds.) with uniformly bounded second derivatives. We shall consider the problem of regularity of minimizers of  $I$ . By a minimizer we mean a mapping  $u \in W^{1,2}(\Omega, \mathbf{R}^m)$  such that for any smooth mapping  $\phi: \Omega \rightarrow \mathbf{R}^m$  compactly supported in  $\Omega$  the inequality  $I(u + \phi) \geq I(u)$  holds. When  $f$  is uniformly convex with uniformly bounded second derivatives, it is not difficult to see that  $u$  is a minimizer of  $I$  if and only if  $u$  is a weak solution of the *Euler-Lagrange* equation of  $I$ , i.e.  $u$  is a weak solution of

$$\partial_{\alpha} f_{p_{\alpha}^i}(Du(x)) = 0, \quad i = 1, \dots, m. \quad (2)$$

(Here and in what follows we use the summation convention.)

It is well known that when  $n = 2, m \geq 1$  or  $n \geq 2, m = 1$   $f$  is a smooth uniformly convex function with uniformly bounded second derivatives every minimizer of  $I(u)$  is smooth.

Here we constructed counterexamples showing, among other things, that when  $m > 1$  in general for  $n \geq 3$  we cannot expect Lipschitz continuity of the minimizer of a smooth uniformly convex functional. Moreover, for  $n = 5$  we find a locally unbounded solution to (2). We recall that  $n = 5$  is the first possible dimension where such an example is possible. (When  $n \leq 4$  each minimizer must be Hölder continuous, since it belongs to  $W^{2,2+\delta}$  for some  $\delta > 0$ .) We also construct a completely new example for  $n = 4, m = 3$ . The important new feature in this example is the low dimension of the target space. The construction also gives a non-Lipschitz minimizer in this case. The mapping used in that example is derived from the Hopf fibration  $S^3 \rightarrow S^2$ . In addition, as a byproduct of our methods, we found an example (with  $n = m = 3$ ) of non-uniqueness of weak solutions of a type of elliptic systems in the spaces  $W^{1,p}$  with  $1 < p < 2$ .

A precise statement of our results is given in the following theorem ( $B_1^n$  denotes the unit ball in  $\mathbf{R}^n$ ):

**Theorem 1.** *i) Let  $u^\epsilon : B_1^n \rightarrow \mathbf{R}^m$  be given by  $u_{ij}^\epsilon = \frac{x_i x_j}{|x|^{1+\epsilon}} - \frac{1}{n}|x|^{1-\epsilon}\delta_{ij}$ , where  $m = \frac{n(n+1)}{2} - 1$ . Then for  $0 \leq \epsilon < \frac{n+1-\sqrt{\frac{3(n+1)}{n-1}}}{\sqrt{\frac{3(n+1)}{n-1}+1}}$ , there exists a smooth uniformly convex function  $f^\epsilon : M^{m \times n} \rightarrow \mathbf{R}$  such that  $|D^2 f^\epsilon| \leq c$  in  $M^{m \times n}$  and*

$$\operatorname{div} \nabla f^\epsilon(\nabla u^\epsilon) = 0 \quad \text{in } \mathbf{R}^n.$$

*ii) Let  $v^\epsilon : B_1^4 \rightarrow \mathbf{R}^3$  be given by  $v^\epsilon(z, w) = \left( \frac{\Re(\bar{z}w)}{r^{\epsilon+1}}, \frac{\Im(\bar{z}w)}{r^{\epsilon+1}}, \frac{|w|^2 - |z|^2}{2r^{\epsilon+1}} \right)$ . Where  $z = x_1 + ix_2, w = x_3 + ix_4$ . For  $0 \leq \epsilon < \sqrt{7} - 2$ , there exists a smooth uniformly convex function  $f^\epsilon : M^{3 \times 4} \rightarrow \mathbf{R}$  such that  $|D^2 f^\epsilon| \leq c$  in  $M^{3 \times 4}$  and*

$$\operatorname{div} \nabla f^\epsilon(\nabla v^\epsilon) = 0 \quad \text{in } \mathbf{R}^4.$$

*iii) Let  $w^\epsilon : B_1^3 \rightarrow \mathbf{R}^3$  be given by  $w^\epsilon(x) = \frac{x}{|x|^{1+\epsilon}}$ . For  $\frac{3}{2} < \epsilon < 3$ , there exists a smooth uniformly convex function  $f^\epsilon : M^{3 \times 3} \rightarrow \mathbf{R}$  such that  $|D^2 f^\epsilon| \leq c$  in  $M^{3 \times 3}$  and*

$$\operatorname{div} \nabla f^\epsilon(\nabla w^\epsilon) = 0 \quad \text{in } \mathbf{R}^3.$$

## Mountain pass solutions for a two-well energy

Kewei Zhang

Under small dead-load perturbations, and the natural boundary value condition (Neumann condition), we establish the existence of an unstable critical point (mountain pass point) for a variational integral in the form  $I_\epsilon(u) = \int_\Omega W(Du(x)) + \epsilon f(x) \cdot u(x) dx$  for  $u \in W^{1,2}(\Omega, \mathbf{R}^N)$  with a two-well structure. The integrand we consider is the explicit quasiconvex relaxation  $W(X) = Q \operatorname{dist}^2(X, \{A, B\})$  of the squared distance function due to Kohn. We show that

for sufficiently small  $\epsilon > 0$ , the energy  $I_\epsilon$  has three critical points: a global minimizer, a local minimizer and a mountain pass point. We introduce the notion of the Weak Palais-Smale condition (WPS) to deal with the lack of compactness of the functional  $I_\epsilon$ .

## E-mail addresses

Giovanni Alberti	alberti@dm.unipi.it
Gregoire Allaire	allaire@ann.jussieu.fr
John M. Ball	ball@maths.ox.ac.uk
Hafedh Ben Belgacem	hafedh.belgacem@mis.mpg.de
Albrecht Bertram	albrecht.bertram@mb.uni-magdeburg.de
Kaushik Bhattacharya	bhatta@caltech.edu
Folkmar A. Bornemann	bornemann@mathematik.tu-muenchen.de
Yann Brenier	brenier@ann.jussieu.fr
Carsten Carstensen	cc@numerik.uni-kiel.de
Sergio Conti	conti@mis.mpg.de
Elaine Crooks	crooks@maths.ox.ac.uk
Antonio DeSimone	desimone@mis.mpg.de
Georg Dolzmann	dolzmann@mis.mpg.de
Wolf-Patrick Düll	duell@iam.uni-bonn.de
Alain Forclaz	forclaz@maths.ox.ac.uk
Gero Friesecke	gf@maths.ox.ac.uk
Klaus Hackl	hackl@am.bi.ruhr-uni-bochum.de
Rudolf Hilfer	hilfer@ica1.uni-stuttgart.de
Viet Ha Hoang	H.V.Hoang@damtp.cam.ac.uk
Richard D. James	james@aem.umn.edu
Bernd Kirchheim	bk@apoll.mis.mpg.de
Chun Liu	liu@math.psu.edu
Stephan Luckhaus	luckhaus@mathematik.uni-leipzig.de
Govind Menon	govind@cfm.brown.edu
Alexander Mielke	mielke@mathematik.uni-stuttgart.de
Ingo Müller	im@thermodynamik.tu-berlin.de
Stefan Müller	sm@mis.mpg.de
Barbara Niethammer	barbara.niethammer@iam.uni-bonn.de
Felix Otto	otto@iam.uni-bonn.de
Roberto Paroni	paroni@maths.ox.ac.uk
Oliver Penrose	oliver@ma.hw.ac.uk
Petr Plecháč	plechac@math.udel.edu
Marc Oliver Rieger	rieger@mis.mpg.de
Raffaella Rizzoni	rizzoni@ing.unife.it
Ekhard K.H. Salje	es10002@esc.cam.ac.uk
Anja Schlömerkemper	schloem@mis.mpg.de
Reuven Segev	rsegev@bgumail.bgu.ac.il
Gregory A. Seregin	seregin@pdmi.ras.ru, seregin@math.uni-sb.de
Steve Shkoller	shkoller@math.ucdavis.edu
Florian Theil	theil@maths.ox.ac.uk
Manfred Wuttig	wuttig@eng.umd.edu
Xiaodong Yan	xiayan@math.umn.edu
Kewei Zhang	k.zhang@sus16x.ac.uk
Johannes Zimmer	zimmer@mathematik.tu-muenchen.de



## Participants

Prof. Dr. Giovanni Alberti  
Dipartimento di Matematica  
Universita di Pisa  
Via Buonarroti, 2  
I-56127 Pisa

Prof. Dr. Kaushik Bhattacharya  
Dept. of Applied Mechanics  
104-44  
California Inst. of Technology  
Pasadena , CA 91125  
USA

Prof. Dr. Gregoire Allaire  
Laboratoire d'Analyse Numerique,  
Tour 55-65  
Universite P. et M. Curie(Paris VI)  
Boite Courrier 187  
F-75252 Paris Cedex 05

Prof. Dr. Folkmar A. Bornemann  
Lehrstuhl f. Numerische Mathematik  
und Wissenschaftliches Rechnen  
Technische Universität München  
80290 München

Prof. Dr. John M. Ball  
Mathematical Institute  
Oxford University  
24-29, St. Giles  
GB-Oxford OX1 3LB

Prof. Dr. Yann Brenier  
Laboratoire d'Analyse Numerique  
Tour 55  
Universite Pierre et Marie Curie  
4, Place Jussieu  
F-75005 Paris

Dr. Hafedh Ben Belgacem  
Max-Planck-Institut für Mathematik  
in den Naturwissenschaften  
Inselstr. 22-26  
04103 Leipzig

Prof. Dr. Carsten Carstensen  
Mathematisches Seminar  
Universität Kiel  
Ludewig-Meyn-Str. 4  
24118 Kiel

Prof. Dr. Albrecht Bertram  
Institut für Mechanik  
Otto-von-Guericke-Universität  
Magdeburg  
Postfach 4120  
39016 Magdeburg

Dr. Sergio Conti  
Max-Planck-Institut für Mathematik  
in den Naturwissenschaften  
Inselstr. 22-26  
04103 Leipzig

Dr. Elaine Crooks  
Mathematical Institute  
Oxford University  
24–29, St. Giles  
GB-Oxford OX1 3LB

Prof. Dr. Klaus Hackl  
Institut für Mechanik  
Ruhruniversität Bochum  
Universitätsstr. 150  
44801 Bochum

Prof. Dr. Antonio DeSimone  
Max-Planck-Institut für Mathematik  
in den Naturwissenschaften  
Inselstr. 22–26  
04103 Leipzig

Dr. Rudolf Hilfer  
Institut für Computeranwendungen  
Numerik für Höchstleistungsrechner  
Universität Stuttgart  
Pfaffenwaldring 27  
70569 Stuttgart

Dr. Georg Dolzmann  
Max-Planck-Institut für Mathematik  
in den Naturwissenschaften  
Inselstr. 22–26  
04103 Leipzig

Prof. Dr. Viet Ha Hoang  
Dept. of Applied Mathematics and  
Theoretical Physics  
University of Cambridge  
Silver Street  
GB-Cambridge , CB3 9EW

Wolf-Patrick Düll  
Institut für Angewandte Mathematik  
Universität Bonn  
Wegelerstr. 10  
53115 Bonn

Prof. Dr. Richard D. James  
Department of Aerospace Engineering  
and Mechanics  
University of Minnesota  
110 Union Street S. E.  
Minneapolis , MN 55455  
USA

Alain Forclaz  
Mathematical Institute  
Oxford University  
24–29, St. Giles  
GB-Oxford OX1 3LB

Prof. Dr. Gero Friesecke  
Mathematical Institute  
Oxford University  
24–29, St. Giles  
GB-Oxford OX1 3LB

Dr. Bernd Kirchheim  
Max-Planck-Institut für Mathematik  
in den Naturwissenschaften  
Inselstr. 22–26  
04103 Leipzig

Prof. Dr. Chun Liu  
Department of Mathematics  
Pennsylvania State University  
218 McAllister Building  
University Park , PA 16802  
USA

Dr. Barbara Niethammer  
Institut für Angewandte Mathematik  
Universität Bonn  
Wegelerstr. 6  
53115 Bonn

Prof. Dr. Stephan Luckhaus  
Fakultät für Mathematik/Informatik  
Universität Leipzig  
Augustusplatz 10  
04109 Leipzig

Prof. Dr. Felix Otto  
Institut für Angewandte Mathematik  
Universität Bonn  
Wegelerstr. 10  
53115 Bonn

Govind Menon  
Division of Applied Mathematics  
Brown University  
Box F  
Providence , RI 02912  
USA

Prof. Dr. Roberto Paroni  
Mathematical Institute  
Oxford University  
24–29, St. Giles  
GB-Oxford OX1 3LB

Prof. Dr. Alexander Mielke  
Mathematisches Institut A  
Universität Stuttgart  
Postfach 801140  
70569 Stuttgart

Prof. Dr. Oliver Penrose  
Dept. of Mathematics  
Heriot-Watt University  
Riccarton-Currie  
GB-Edinburgh , EH14 4AS

Prof. Dr. Ingo Müller  
FB 6 - Inst. für Verfahrenstechnik  
Schr. HF 2 - Thermodynamik  
TU Berlin  
Straße des 17. Juni 135  
10623 Berlin

Prof. Dr. Petr Plechac  
Department of Mathematical Sciences  
University of Delaware  
501 Ewing Hall  
Newark , DE 19716–2553  
USA

Prof. Dr. Stefan Müller  
Max-Planck-Institut für Mathematik  
in den Naturwissenschaften  
Inselstr. 22–26  
04103 Leipzig

Marc Oliver Rieger  
Max-Planck-Institut für Mathematik  
in den Naturwissenschaften  
Inselstr. 22–26  
04103 Leipzig

Dr. Raffaella Rizzoni  
Dip. di Matematica  
Universita di Ferrara  
Via Machiavelli 35  
I-44100 Ferrara

Dr. Florian Theil  
Mathematical Institute  
Oxford University  
24–29, St. Giles  
GB-Oxford OX1 3LB

Prof. Dr. Ekhard K.H. Salje  
Dept. of Earth Sciences  
Univ. of Cambridge  
Downing Street  
GB-Cambridge CB2 3EQ

Prof. Dr. Manfred Wuttig  
Dept. of Chemical & Nuclear Eng.  
University of Maryland  
College Park , MD 20742–2111  
USA

Anja Schlömerkemper  
Max-Planck-Institut für Mathematik  
in den Naturwissenschaften  
Inselstr. 22–26  
04103 Leipzig

Dr. Xiaodong Yan  
School of Mathematics  
University of Minnesota  
127 Vincent Hall  
206 Church Street S. E.  
Minneapolis , MN 55455  
USA

Prof. Dr. Reuven Segev  
Dept. of Mechanical Engineering  
Ben-Gurion Univ. of the Negev  
84105 Beer-Sheva  
ISRAEL

Prof. Dr. Kewei Zhang  
School of Mathematical and  
Physical Sciences  
University of Sussex  
GB-Brighton BN1 9QH

Prof. Dr. Gregory A. Seregin  
Steklov Mathematical Institute  
POMI  
Lomi, Fontanka 27  
St. Petersburg 191011  
RUSSIA

Johannes Zimmer  
Zentrum Mathematik  
TU München  
Arcisstr. 21  
80333 München

Prof. Dr. Steve Shkoller  
Dept. of Mathematics  
University of California  
Davis , CA 95616-8633  
USA