Weierstraß–Institut
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Contributions to Continuum Theories

Anniversary Volume for Krzysztof Wilmański

collected by Bettina Albers

Report No. 18

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Preface

On March 1, 2000, Krzysztof Wilmański will celebrate his 60th birthday. This collection of research papers is dedicated to him on this occasion.

Krzysztof Wilmański's work is distinguished and marked by deep mathematical, physical and mechanical understanding. He has set high standards in research and teaching, and many colleagues and students have benefited from his extensive knowledge. His influential and lasting contributions to continuum mechanics and thermodynamics comprise topics like phase transitions, porous bodies and granular media.

Krzysztof Wilmański has a special ability for interdisciplinary research. His readiness to discuss new mathematical concepts from the physical point of view has been of great influence for many researchers from different fields, in particular for mathematicians, including myself. This way he has for instance contributed considerably to the development of modern mathematical models for phase transition and hysteresis phenomena, and as the head of the research group "Continuum Mechanics" he plays an important role in the interdisciplinary research at the Weierstrass Institute for Applied Analysis and Stochastics (WIAS).

Krzysztof Wilmański's personal qualities of commitment, modesty, and integrity leave a lasting impression on his colleagues, students, and friends. This volume reflects their appreciation, gratitude, and friendship.

Berlin, January 2000 J. Sprekels (Director of WIAS)

Curriculum Vitae of Krzysztof Wilmański

[1940] March 1; born in Lodz, Poland.

[1962] MSc at Civil Engineering Department, Technical University of Lodz, Poland; diploma work on *Elastic-plastic thermal stresses in a thin ring.*

[1965] graduated at the Technical University of Lodz (Poland). PhD-work: *Some two dimensional problems of fibrous materials.* Field: Continuous Models of Discrete Systems.

[1966 – 86] Associate Professor and Professor in the Institute of Fundamental Technological Research, Polish Academy of Sciences, Warsaw, Poland. Since 1970 the head of the Research Group: "Continuum Thermodynamics". Main fields of interest: axiomatic and kinetic foundations of continuum thermodynamics, theory of mixtures, phase transformations in solids. Works with Prof. Henryk Zorski.

[1969 – 70] Postgraduate at the Johns Hopkins University, Baltimore (USA). Works on axiomatic and kinetic foundations of continuum thermodynamics with Prof. J. Ericksen and Prof. C. Truesdell (both Johns Hopkins University).

[1970] Habilitation in 1970 in the Polish Academy of Sciences, Warsaw (Poland). Work: *Dynamics of Bodies with Microstructure.* Field: Nonlocal Continuum Mechanics.

[1971] M. T. Huber Prize of the Polish Academy of Science for the work on axiomatic foundations of thermodynamics.

[1972 – 74] Visiting Professor at the College of Engineering, University of Baghdad, Iraq.

[1979] Nomination to the Professor (title) by the State Counsil of Poland.

[1984] Fellow at "Wissenschaftskolleg zu Berlin", Institute for Advanced Studies. Works on martensitic phase transformations (SMA), non-newtonian fluids, acoustic waves in continua with Prof. Ingo Müller (TU Berlin, Germany) and Prof. Ronald Rivlin (Lehigh, USA).

[1985 – 86] Research Grant to the Technical University of Berlin, Hermann-Föttinger-Institut. Work on a model of crystalizing polymers with Prof. Ingo Müller (TU Berlin).

[1986 – 87] Visiting Professor at the University of Paderborn, Germany. Work on a nonlocal thermodynamic model of plasmas and electrolytes with Prof. J. Schröter.

[1987 – 90] Research Grant to the Technical University of Hamburg-Harburg, Germany. Work on crystal plasticity and the evolution of textures with Prof. O. Mahrenholtz.

[1990 – 92] Research Grant to the Technical University of Berlin, Germany. Work on the martensitic phase transformations with Prof. Ingo Müller.

[1992 – 96] Lecturer at the University of Essen, Department of Civil Engieering. Work on thermodynamic models of porous materials.

[1995] Habilitation (*Venia legendi*) at the University of Essen, Germany.

[1996–] Tenure at the Weierstrass Instutute for Applied Analysis and Stochastics, Berlin, Germany. Head of the Research Group "Continuum Mechanics" in WIAS (Berlin).

[1998] Habilitation (*Venia legendi*) at the Technical University of Berlin, Germany.

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On Adsorption and Diffusion in Porous Media

Abstract. The paper contains a macroscopic continuum model of adsorption in porous materials consisting of three components. We consider the flow of a fluid/adsorbate mixture through channels of a solid component. The fluid serves as carrier for an adsorbate whose mass balance equation contains a source term. This term consists of two parts: first a Langmuir contribution which is connected with bare sites on internal surfaces and describes the Langmuir isotherm in equilibrium. The second one is due to changes of the internal surface driven by the source of porosity which is a part of the balance equation for porosity. We clearly state the range of applicability of the model. A simple numerical example which describes the transport of pollutants in soils illustrates the coupling of adsorption and diffusion. The results show that after a certain time arises a maximum in the rate of adsorption as a function of fluid/adsorbate velocity.

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Shock Waves in Grad's 13-Moment Theory Revisited - A View from Extended Thermodynamics -

Abstract. Grad applied his 13-Moment theory to the problem of the shock wave structure and reported the results in his elaborated paper "The Profile of a Steady Plane Shock Wave" [1]. An indepth study of this paper is worthwhile for anyone trying to solve the problem of the shock wave structure with higher Moment theories or Extended Thermodynamics: Many of the problems encounterd with more moments are anticipated by the relatively simple 13 moment case.
Thus we follow Grad in calculating the direction field of the 13-moment case for several Mach numbers together with the corresponding shock solutions. The results, especially the singular points arising in the analysis, are discussed from the viewpoint of extended thermodynamics.

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Stress-Softening in Combined Triaxial Stretch and Simple Shear of a Rectangular Solid

Abstract. Stress-softening effects of the combined triaxial stretch and simple shear deformation of a rectangular block are studied for a general isotropic, incompressible stress-softening material called a Mullins material. It is shown that the stress response to a specified triaxial deformation of a Mullins material preconditioned in a superimposed cyclic simple shear is smaller than its virgin material response to the same triaxial stretch. This result includes the special case of stress-softening of a rod in simple extension preconditioned by a superimposed cyclic simple shear. It is also shown that the stress response to a specified simple shear deformation of a Mullins material that is preconditioned further in a superimposed cyclic triaxial stretch is smaller than its virgin material response to the same amount of shear. The problem of stress-softening due to preconditioning of the block by a superimposed cyclic simple extension is included. Specific results are illustrated for a Mooney-Rivlin parent material model with exponential stress-softening.

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Weakly Nonlocal Effects in Mechanics

Abstract. We use the term 'weakly nonlocal' to specify relatively short–range effects accounted for functionals which can be approximated using an endistancing theorem of Coleman and Noll. We remark that certain corollaries of that theorem may mislead one into attributing the rôle of stress to a tensor entering the approximate expansion.

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Global Existence for the Conserved Phase Field Model with Memory and Quadratic Nonlinearity

Abstract. A nonlinear system for the heat diffusion inside a material subject to phase changes is considered. A thermal memory effect is assumed in the heat conduction law; moreover, on account of thermodynamical considerations, a linear growth is allowed for the latent heat density. The resulting problem couples a second order integrodifferential equation, derived from the balance of energy, with a fourth order parabolic inclusion which rules the evolution of an order parameter χ. Homogeneous Neumann boundary conditions guarantee that the space average of χ is conserved in time. Global existence of solutions is proved in a variational setting.

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On the Austenite $\rightarrow$ Ferrite Phase Transition in Steel

Abstract. We investigate jump conditions at moving interface boundaries. A comparison of two models, viz. the singular surface model and the phase field model is carried out.
This work grew out of an intense discussion with the materials scientist Yvonne van Leeuwen, who studies the phase transition in steel between austenite and ferrite. The current investigation is the starting point of a series of studies to relate the motion of the austenite / ferrite interface to measurable diagrams of the temporal evolution of the ferrite phase fraction.

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Surface Waves in a Porous Medium

Abstract. The paper concerns surface waves at an interface separating a saturated porous medium and a liquid. Existence and peculiarities of surface wave are investigated on the base of the mathematical model which combines approaches of M.Biot [1,2] and K.Wilmanski [3]. Three types of surface waves are proven to be possible: true Stonely surface wave propagating almost without dispersion, leaky slow pseudo-Stonely wave, and leaky generalized Rayleigh wave.

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About Non-Spherically Symmetric Deformations of an Incompressible Neo-Hookean Sphere

Abstract. A class of non-spherically symmetric deformations of a neo-Hookean incompressible elastic ball is considered. It is shown that the only possible solutions to the equilibrium equations are the trivial solution, the cavitated radially symmetric solution and the deformation of radial inflation and polar stretching. These are the same solutions as found by Polignone-Warne and Warne [6] for a smaller class of deformations. This fact shows once again that the radial deformations are the only deformations, at least within the class considered, which may support a formation of a cavity in the center of an incompressible, isotropic, elastic sphere.

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A Note on Wrinkling and Saturated Elasticity

Abstract. When any given hyperelastic constitutive law is supplemented with a saturation condition, the right Cauchy-Green strain tensor is shown to abide by an additive decomposition law governed by a normality rule. The situation is exemplified by the wrinkling of anisotropic elastic membranes.

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A Minimization Problem in the X-ray Theory

Abstract. My purpose is to elaborate some features of a continuum theory of X-ray observations of crystals, relating to an energy minimization problem. The problem is similar to one commonly used in thermoelasticity theory to analyze phenomena relating to phase transitions and twinning, but there are some subtle differences.

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On the Method of Active Reduction of Forced Vibrations

Abstract. In the paper an iterative method of reduction of vibrations of mechanical systems is presented. The method is based on linerization of the system in each step of iteration and on experimental identification. Convergence of the procedure is demonstrated in some examples.

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Impact of Air Shock Wave on Obstacle Covered by Porous Screen

Abstract. Some features of the reflection of air shock waves from a rigid wall covered by a porous layer have been investigated numerically. The mathematical two velocity model with two stress tensors constructed by methods of the mechanics of multiphase media has been applied for the investigation of wave processes in saturated porous media. The algorithm for numerical realisation of the model was based on the modified version of the Laks - Wendroff two - step scheme. The processes of passing the boundary between gas and porous medium by a wave of step - type and the reflection from a rigid wall covered by the porous material have been considered; the influence of the parameters of the porous medium and the wave on the process of the reflection has been analysed; the comparison of the calculated results with the experiment data of other authors has been made.

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Three-dimensional Wind-induced Baroclinic Circulation in Rectangular Basins

Abstract. We present results of various circulation scenarios for the wind-induced currents in two vertically stratified rectangular basins of constant depth with different sizes; these are obtained with the aid of a semi-spectral semi-implicit finite difference code developed in [4, 11]. Our focus is to see whether the code allows reproduction of the many well-known processes exhibited in stratified waters of a lake basin on the rotating Earth. Often, the internal dynamics exhibits Kelvin and Poincaré-type oscillations, whose periods depend upon the stratification and the geometry of the basin and which persist for a long time, the attenuation being the result of the turbulent dissipation mechanisms. It is shown that the numerical dissipation of our code can be sufficiently restricted that such wave dynamics obtained with it is realistically persistent for typical time scales of physical limnology. By solving the eigenvalue problem of the linearized shallow water equations of two-layered closed rectangular basins, the interpretation of the oscillations as Kelvin and Poincaré-type waves is corroborated.

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Lagrange Multipliers in Nonequilibrium Thermodynamics

Abstract. The role of Lagrange multipliers in several formulations of extended thermodynamics is compared, to outline some points of contact between them. They are given an explicit physical interpretation and some open problems are pointed out.

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On the Mass Flux through a Permeable Boundary of a Porous Material

Abstract. The aim of the present paper is to show which constants of the present macroscopic continuum model influence essentially the mass transport through the boundary of the considered control volume. The base for this analysis is a new class of models of two-component continua characterized by the balance equation for porosity. One of such models is used to describe a special physical problem, namely the consolidation phenomenon. The initial-boundary value problem with regard to the physical features of the consolidation is formulated and some constitutive relations required for the consistent description of the porous boundary are proposed. Regarding these constitutive relations an example of one-dimensional structure for the purpose of a study of some constants of the model is calculated and the numerical results are discussed.

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Hypoplasticity – A New Paradigma for Plasticity

Abstract. This paper contains a systematic introduction to hypoplasticity, explains its mathematical structure, its capabilities, shows how to calibrate hypoplastic models and gives a review on its applications.

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A Thermodynamically Consistent Hysteresis Model of Thermovisco-Elastoplasticity

Abstract. We propose a thermodynamic interpretation and give a survey of results for a model of the uniaxial behavior of thermovisco-elastoplastic materials for which the total stress σ contains, in addition to elastic, viscous and thermic contributions, a plastic component $\sigma^p(x,t) = \mathcal{P}[\varepsilon(x,\cdot),\theta(x,t)](t)$. Here, ε and θ are the fields of strain and absolute temperature, respectively, and $\{\mathcal{P}[\cdot,\theta]\}_{\theta>0}$ denotes a family of (rate-independent) hysteresis operators of Prandtl-Ishlinskii type, parametrized by the absolute temperature. We show that the momentum and energy balance equations governing the space-time evolution of the material coupled with suitable initial and boundary conditions admit a unique global strong solution and the corresponding process is compatible with the second principle of thermodynamics.

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The Scaling of Time and Space in Micro-Macro Transitions

Abstract. We consider two kind of time-space scalings for the solutions of Riemannian initial value problems that arise in the context of micro-macro transitions. The observed scaling properties are not restricted to the Riemann solutions, but in this case they have a very nice formulation.
The first kind of scaling leads to the description of pure wave phenomena and is obtained for a micro-macro transition in a one-dimensional atomic chain consisting of N atoms, if N tends to infinity. On the micro scale we have a multi-particle system that is determined by Newtons equations. Then the macroscopic quantities mass density, momentum density and energy density are obtained as mean values in terms of the so called window function in time and space. As a consequence of this wave scaling there occur only states of local equilibrium in the atomic chain, and in addition we will see that there is no unique description of local equilibrium. For special microscopic distribution functions of the atomic velocities and distances in the chain the local equilibrium property will lead to different explicit hyperbolic systems of symmetric type (see [5], [6], [8]) and specific entropies on the macro scale by rigorous micro-macro transitions, starting from Newtons equations of motion for the multi-particle system, see [3].
The second kind of time-space scaling describes pure diffusion in three space dimensions and is illustrated for the solution of the kinetic Euler scheme proposed in [1], [2], [4], [7] with a contact discontinuity in the Riemannian initial data (i.e. the pressure is constant at the beginning). On the micro scale we describe the kinetic evolution of a phase density in a similar way as using the Boltzmann equation. The macroscopic fields are the moments of mass, momentum and energy of this phase density. If the number of time steps with a constant relaxation time τ_M in the kinetic scheme tends to infinity we observe the same scaling invariance of the macroscopic fields as for the usual heat equation. Then we obtain a parabolic system of nonlinear diffusion equations for the macroscopic quantities. This scaling invariance was observed by applying the kinetic Euler scheme for a large number of time steps and must be essentially used in order to derive these diffusion equations.

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Autonomous Underwater Vehicle for Seismic Offshore Petroleum Exploration

Abstract. A preliminary design of autonomous underwater vehicle for seismic offshore petroleum exploration was performed in 1995 by the team of Mechanical Engineering students, of University of British Columbia under the supervision of the author. The paper describes the main features of the system and its advantages. The proposed AUV is the only vehicle capable of surveying Arctic and Antarctic Ocean basins where surface ice currently limits the extent to which vessels can perform seismic surveys.

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On Acoustic Waves in Compressible Porous Media

Abstract. In this paper propagation and attenuation of acoustic waves in compressible porous media are presented. The basic formulation of Bowen's model is adopted to describe the saturated porous media composed of a linear elastic compressible skeleton and a compressible fluid. In particular, the porosity change is modified to associate with the divergence of velocities of solid and fluid rather than their displacements as in Bowen's model. The modified governing field equations are then used to study the propagation condition of acoustic waves in two-component porous materials. It is shown that two types of waves are realizable in the media. Finally, in the context of homogeneous weak discontinuity, the evolution of wave amplitudes is analyzed.

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Thermoelasticity of Inhomogeneous Solids and Finite-Volume Computations

Abstract. Basic elements of a thermodynamically admissible finite-volume numerical scheme for inhomogeneous thermoelasticity are presented together with illustrations. Directions to include a proper treatment of the irreversible progress of thermomechanical phase-transition fronts are given. This involves ideas of the recently developed theory of material inhomogeneities.

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Stability of a Spherical Droplet in Solution Growing by Diffusion

Abstract. Two constituents in two phases require two conditions on the chemical potentials at the phase interface. These conditions are exploited here in a manner similar to the analysis of Mullins & Sekerka [1] who had only one interfacial condition. As a result it turns out that a spherical droplet in solution has a greater radius of stability than previously calculated.

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Studies on Shear-Induced Strain Fields in Cubic Materials

Abstract. An approximate analytical 2-D solution for the strain field components , and occurring in a cubic material due to a coherently bonded shear eigenstrained inclusion of cylindrical geometry was obtained by means of Continuous Fourier Transforms (CFT). A numerical model based on the Discrete Fourier Transform (DFT) was used in order to test the validity of the results. For the case where the cylindrical inclusion and the surrounding media are elastically homogeneous and the orientation of their principal crystal axes are the same, a correlation between the analytical and numerical models is demonstrated for silver, a strongly anisotropic material. Moreover, the strain fields within the inclusion are shown to be homogeneous-isotropic. Finally, an expression for the closed-form strain energy of two cylindrical inclusions at arbitrary radius and angle was derived, and then used to determine the minimum energy configuration for the system.

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Regularization Methods of Plastic Flow Processes via Constitutive Postulates

Abstract. The main objective of the paper is the development of the elasto–viscoplastic regularization procedure valid for a broad class of thermodynamic plastic flow processes in damaged solids. The initial–boundary value problem (the evolution problem) is formulated and its well posedness is discussed. The regularized evolution problem based on an elastic–viscoplastic model of a material is examined. The numerical solution of the regularized evolution problem is investigated by the application of the finite difference method. An approximation scheme is formulated. The Lax–Richtmyer equivalence theorem is proposed and its validity for an approximation scheme is discussed. In numerical example it has been shown that the satisfaction of the stability criterion in the form Courant–Friedrichs–Lewy condition leads to the convergence of an approximation scheme.

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Second-Gradient Constraints in Second-Grade Materials

Abstract. In this note we consider materials whose deformations are constrained to obey an algebraic restriction on (some of) their first N gradients, the N-th being included. We briefly discuss the idea that such materials should be studied within a theory of materials of grade N whose mechanical response should not necessarily depend on all the deformation gradients from the first to the N-th. As an example, we sketch the case of a second-gradient constraint in a hyperelastic material whose stored energy depends only on the first deformation gradient.

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Maximum of Entropy Density in Equilibrium and Minimax Principle for an Hyperbolic system of Balance Laws

Abstract. In this paper we first discuss the properties of an equilibrium state for a general hyperbolic system of balance laws compatible with an entropy principle and concave entropy density. Then, under a natural dissipative condition, we prove that the density of entropy is maximum in the equilibrium state. In this manner the difference between the entropy density in equilibrium and the entropy density in a generic state becomes an alternative natural measure - instead of the entropy production - of the distance from a generic state to the equilibrium one. We discuss the problem of non-controllable boundary conditions in stationary processes and in the case of moment system associated with the Boltzmann equation in the BGK approximation we compare the results using the minimax principle of entropy production to those obtained by the one using this new distance from equilibrium.

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The Rank 1 Convex Hull of Two Isotropic Wells

Abstract. The rank 1 convex hull of a set consisting of two isotropic wells in dimension 2×2 is evaluated. The hull is shown to coincide with the polyconvex (and hence also with the quasiconvex) hull. If the two wells are incompatible (i.e., contain no rank 1 connection), the hull consists of the union of the hulls of the two wells, while if the wells are rank 1 connected then the hull is strictly larger than the union of the hulls of the two wells. Combining this result with recent results by Dacorogna & Marcellini on the Cauchy–Dirichlet problem for first order nonlinear systems, an attainment result is derived for functions with values in the two wells.

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Quantum Effects of Magnetic Fluxes in Glasses

Abstract. Dielectric low-temperature properties of glasses are derived within a generalized tunneling model, considering the motion of charged particles on a closed path in a double-well potential. The presence of a magnetic induction field violates the time reversal invariance due to the Aharonov-Bohm phase and leads to flux periodic energy levels. At ultra-low temperature, this electromagnetic flux effect is strongly enhanced by dipole-dipole interaction between tunneling systems and becomes measurable.

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Positive and Negative Entropy Productions and Phase Densities for Approximate Solutions of the Boltzmann Equation

Abstract. Approximate solutions of the Boltzmann equation like the Chapman-Enskog expansion or the Grad moment method yield a phase density which may become negative in contradiction to its definition. This, however, is no problem, if the approximate solutions are considered in their proper range of applicability. Other authors showed that the entropy production of the Burnett (second-order Chapman-Enskog) phase density may become negative, in contradiction to Boltzmann's H-theorem. Simple arguments show that this failure is related to the negativity of the phase density, and poses no problem in the proper range of applicability.

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Remarks on Relativistic M.H.D. with Finite Electrical Conductivity

Abstract. Starting from the *method of generators* a system of conservation laws with a convex extension is proposed for relativistic magneto-hydrodynamics with finite electrical conductivity, at thermal equilibrium. The system includes the usual balance laws of mass conservation, energy-momentum balance, Maxwell equations, charge conservation and a new covariant balance law for the conduction electric current J_C^α (*generalized Ohm's law*) and the electrical conductivity σ. The new laws, together with the charge conservation law, are formally similar to the the equations governing a second fluid at thermal equilibrium. The test of convexity of negative entropy density is provided.

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Lattices with next to nearest neighbor interaction: surface relaxation and size effect

ABSTRACT. A relation between continuum theory of elasticity and its crystal lattice prototypes is often discussed in terms of pair-wise interaction potentials restricted to the nearest neighbors (NN). Certain phenomena, however, like wetting or surface relaxation are due to the interaction of at least next to nearest neighbors (NNN). The corresponding effects cannot be neglected when one deals with particularly thin films or studies formation of new surfaces near the tip of the opening crack.

In this paper, we revisit the simplest linear one-dimensional lattice with NNN interactions. We assume that the effective springs, describing NN and NNN interactions have different reference lengths which introduces a mismatch or pre-stress and results in either bulk modulations or surface relaxation in an unloaded body. Depending on the magnitude of the ratio of NN and NNN elastic moduli, we obtain three types of equilibrium solutions: homogenous with monotone boundary layers at the free surfaces, homogenous with oscillatory boundary layers and inhomogeneous, describing commensurate and incommensurate non-Bravais lattices. For a finite body with the prescribed (double) forces at the boundary we explicitly find displacement fields and calculate the total energy of the lattice. In the case when the crystal is large comparing to the thickness of exponential boundary layers, we obtain a finite form expression for the surface energy as a function of pre-stress. For sufficiently small crystals we demonstrate a characteristic size effect originating from the overlapping of surface boundary layers. The latter results are particularly relevant for the description of sub nano-scale films.

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Why Should We Teach Continuous Media Physics

ABSTRACT. The knowledge of basic facts from continuous media physics is essential for understanding of many everyday life phenomena. It is also very important for those doing science in various branches of biology, medicine, economy etc. In this talk few examples thought as arguments in favor of teaching continuous media physics, are being discussed.

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Ferromagnetism And Hysteresis Operators

Abstract. Processes in *space-distributed* ferromagnetic systems are described by coupling the Maxwell equations with suitable constitutive relations. Even when the form of the latter relations has been established for nondistributed systems, the formulation of such a P.D.E. model raises nontrivial questions.

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Snelson Tensegrity Structures

Abstract. Tensegrity structures were first constructed by the artist Kenneth Snelson in 1948. This type of structure was named and popularized by Buckminster Fuller as possible architectural constructs. Since the mid-seventies, generalized versions of these constructs, namely structures some of whose elements cannot sustain compression, have been studied by both engineers and mathematicians. With I. J. Oppenheim [1, 2, 3], the author has begun a study of the structures which are of the type built by Snelson. Here we present some results which help to characterize the equilibria of such constructs, and discuss a technique for describing the evolution of the positions.

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Model of Local Rigidity in the Theory of Peptide Chain

Abstract. The peptide chain is one of the most important biological structures. In this paper it is treated as kinematic chain, the peptide units being regarded as rigid bodies. We begin with a very simple static problem, in which the choice of variables entering the interaction energy follows from a more general theory. Exact solutions are presented for some simple energies and their stability examined. In the case of long chains loaded by a force on its ends, deterministic chaos may occur. A brief account of the continuum theory is given emphasizing its origins in the discrete theory.