Mathematisches Forschungsinstitut Oberwolfach

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Thermodynamic Constitutive Theory

December 12th – December 23rd, 2000

The conference was organized by W. Bürger (Karlsruhe) and I. Müller (Berlin) and it attracted 35 scientists from 9 countries. Thirty two scientific lectures were presented and as well as one entertaining after-dinner-lecture on surprising physical phenomena in the world of toys.

Thermodynamics with its basic conservation laws, invariance principles and its entropy principle provides a universal tool for the determination of constitutive properties in all phases of a body. Indeed, it governs the transition between the phases as well as the choice of boundary values at the phase boundaries. Accordingly the scope of the conference included solids, liquids and gases. Indeed, this sequence of phases provided the guideline through the program: We have started with thermodynamic properties of plastic deformation, damage in solids, and shape memory, proceeded with the onset of convection in liquids and gases, and finished with the description of rarefied gases in the range of large Knudsen numbers.

In the formal sessions and during the lively informal group discussions over wine and beer in the evenings three topics were mostly debated, sometimes passionately:

- the necessity to take compressibility into account in the proper treatment of the onset of convection,
- the determination of boundary values for non-controllable variables in extended thermodynamics,
- the role of the Eshelby tensor in the determination of phase equilibrium between pre-stressed solids.

Doubtless these discussions will continue by mail and in future meetings between the participants. The present conference may have served the good purpose, however, to identify the problems and to familize various proponents with each other's lines of arguments.

The staff of the institute with their commendable, – and by now finely-tuned – efficiency made the stay pleasant and memorable.

The meeting ended on Friday, December 22nd at lunch-time. A group of 12 participants stayed until the next morning.

Abstracts

A model for evolving microstructures formed by phase transitions

H.-D. Alber

Starting from the second law of thermodynamics a mathematical model for evolving phase transitions in nickel based superalloys is developed. In these alloys the matrix phase γ deforms viscoplastically, whereas the precipitates γ' deform purely elastically. The viscoplastic behaviour is modeled using internal variables. The second law of thermodynamics requires that the normal velocity $v(x,t)$ of the phase interface and the expression $n(x,t) \cdot [\sigma(x,t)]n(x,t)$ must have the same sign. Here $[\sigma]$ denotes the jump of the Eshelby tensor at the interface, and $n(x,t) \in R^3$ denotes a unit normal vector to the interface. The evolution equation

$$v(x,t) = c\left(n(x,t) \cdot [\sigma(x,t)]n(x,t)\right)$$

satisfies this restriction, if the function c fulfills the condition $c(s)s \geq 0$ for all s.

In several steps, this evolution equation for the phase interface is transformed into a distribution partial differential equation for the characteristic function S of the γ'-phase. If the characteristic function S is replaced by a smooth function S approximating the characteristic function, this evolution equation takes the form

$$S_t = -c\Psi_s\left(\varepsilon\left(\bigtriangledown_x u\right), S, z\left|\bigtriangledown_x S\right|\right),$$

a Hamiltion-Jacobi equation for S. Here c is a positive constant, is the strain tensor, z is the vector of internal variables and Ψ is the free energy.

Phase diagrams - heat of mixing and interfacial energy

J. Ansorg

The form of phase diagrams is affected by intermolecular energies between the components but also by interfacial energies between the phases. The first are responsible for phenomena like azeotropy and miscibility gaps, while the latter deform domains of the phase diagrams, especially the miscibility gap.

In a qualitative model for binary mixtures an interfacial energy is introduced, and the influence of the interfacial energy on phase diagrams of ideal mixtures, eutectica and peritectica is exhibited.

The shock tube experiment in extended thermodynamics

J. Au

Results of investigations of the shock tube experiment with Extended Thermodynamics (ET) are presented. ET provides dissipative field equations for monoatomic gases which are symmetric hyperbolic.

The start-up phase of the idealized shock tube experiment is calculated with ET of many moments. For small times more and more moments have to be taken into account for a physically valid description.

In the limit of $t \to 0$ the solutions of ET converge to the corresponding solution of the collisionless Boltzmann equation.

Numerically efficient discrete kinetic models

H. Babovsky

We introduce a class of kinetic Discrete Velocity Models which are based on two concepts:

(i) Reducible kinetic schemes; these can be transformed into a system decoupling into a small nonlinear and a large linear part and can be easily analyzed and calculated;

(ii) Hierarchies built up of reducible schemes.

These kinetic models are efficiently solvable and are intended to shed some light on a couple of open problems in the domain between Rarefied Gas Dynamics and Fluid Dynamics.

Onset of Bénard convection in gases - Navier-Stokes Fourier and 13 moments

E. Barbera

The aim of the talk was the illustration of the onset of Bénard convection in gases. In order to describe the onset of convection two different models for the gas are used: The classical Navier-Stokes-Fourier theory and extended thermodynamics with thirteen moments. In both cases a linear stability analysis was performed. The critical Rayleigh number, a parameter that measures the appearence of the convection in the Bénard problem, was computed in terms of the Knudsen number, a parameter which expresses the degree of rarefaction of the gas. The results obtained by use of the two theories were illustrated and compared. It turns out that the 13 moment theory predicts a smaller range of stability.

Relativistic gas: Moment equations and maximum wave velocity

G. Boillat

For a rarefied relativistic gas we consider the N-moment equations associated with the relativistic Boltzmann-Chernikov eqation and we require the compatibility with the entropy principle, thus obtaining a closed symmetric hyperbolic system. This interesting form permits one to deduce a lower and upper bound for the maximum velocity of a wave propagating in a classical monatomic gas or a degenerate gas of fermions or bosons. We prove that, with N increasing, this velocity tends to the speed of light. This argument first appeared in an article by G. Boillat & T. Ruggeri, J. Math. Phys. Dec. 1999.

Effects of compressibility on the Rayleigh-Bénard problem

A. Bormann

The Rayleigh-Bénard problem usually is investigated by applying the Boussinesq approximation for the calculation of the critical temperature difference that brings convection movement into the system. Unfortunately the Boussinesq approximation ignores compressibility and, – by assuming thermal expansion at the same time – is precarious from a thermodynamic point of view. In order to overcome these drawbacks a linear stability analysis has been performed on the basis of the compressible Navier-Stokes-Fourier equations. This procedure results in a critical Rayleigh number that, in contrast to the Boussinesq approximation, is no longer constant, but depends strongly on the layer thickness. The effect of compressibility can be accounted for by adding a term to the Boussinesq Rayleigh

number. The two parts of this new Rayleigh number represent two mechanisms that are responsible for the onset of convection a) friction due to viscosity and b) compression of the fluid due to hydrostatic pressure. This ansatz is verified and confirmed by the numerical linear stability analysis for a N-S-F fluid.

Boundary data for a stationary heat conduction problem in radial symmetry

F. Brini

Two different problems related to Extended Thermodynamics with 14 moments are presented. First of all the hyperbolicity of the system is investigated in order to choose "good initial" or boundary data and to check the admissibility of the solutions. Secondly we consider the problems related to the choice of boundary data which cannot be controlled (moments of order higher than 13). Some hints and suggestions for the solution of this problem may be obtained from the consideration of heat conduction in radial symmetry.

Evening lecture on: Some entertaining experiments

W. Bürger

A PINHOLE MAGNIFIER without a collecting lens is essentially a small hole of, say, $0.6mm$ in an aluminium foil. It is able to magnify small objects 8-fold. RESCUE WHISTLES for cases of emergency on sea (and also the Metropolitan whistles of the bobbies in London) are double pipes, emitting, in addition to two neighbouring notes, their difference sound. It is of low pitch not found in the acoustic spectrum but invented by the ear.

PIETER BREUGEL'S WIND WHEELS documented on his famous painting "children's games" (1560) must have (as we proved) elastic vanes. The rotor turns always in the same sense of rotation irrespective of whether the child pushes or pulls. Are you able to make a LOOPING WITH A GLASS? Fill the glass with water and put it on a tablet fixed to long strings ($1m$), so you can swing it over your head without waves to appear on its surface. Be, however, cautions to overcome the critical range of angular speeds in which the string becomes slack! FOLDING GEARS are intelligent mechanisms not only to make Origami figures move (e.g. dogs barking, or cranes flapping) but also for nanotechnology. Moreover, they may be a better solution for unfolding large maps or the huge solar sails which are needed for space ships driven by the pressure of the sun's radiation. SANTA CLAUS ON THE STRING who is able to move upwards by a sophisticated stick-slip mechanism whishes you MERRY CHRISTMAS!

On the scaling behaviour of micro-macro-transitions

W. Dreyer

Joint work with M. Kunik

We start from a $1D$ atomic chain consisting of N atoms that evolve in time accordingly to Newton's equations of motion, and we solve various Riemannian initial value problems. Newton's equations and the solutions obtained are used to establish macroscopic limit equations which are PDE's for macroscopic fields.

The macroscopic limit consists of conservation laws, – which follow from the microscopic equations rigorously – , and of closure relations, which are completely determined by the distributions of the microscopic motion.

We have observed several different types of microscopic motion and several types of macroscopic limits.

The macroscopic limits are established by calculating a sequence of increasing space time regions, generated by increasing numbers of atoms. The sequence of macroscopic solutions induces a sequence of macroscopic fields which all are mapped, through rescaling, to a representative space time region.

There are special Riemannian initial data and corresponding special types of rescaling so that the macroscopic limit equations either form nonlinear hyperbolic or parabolic systems.

Reactions to internal constraints: Workless (non dissipative) or non-workless (dissipative)?

M. Fremond

Consider a point sliding with velocity U on a plane with normal $\vec{N}$: The reaction to the impenetrability condition $-R\vec{N}$ is such that $RU = 0$, but thermodynamics require only that $RU \geq 0$. The question arises whether there are situations for which $RU > 0$ holds, i.e. where the reaction to the impenetrability condition is dissipative or not workless. We show that this is possible, if the evolution is non-smooth: i.e. if there is a collision between the point and the plane.

The equation of motion is $m(\vec{U}^+ - \vec{U}^-) = -\vec{P}^d - \vec{P}^{reac}$, where $\vec{P}^d$ is the dissipative percussion and $\vec{P}^{reac} = P^{reac}\vec{N}$, $P^{reac} \in \partial I(U_N^+)$. ($U_N$ is the normal velocity, $\vec{U} \cdot \vec{N}$ and ∂I is the subdifferential set of the indication function of R^+). If contact persists after the collision ($U_N^+ = 0$), the work of the reaction force is equal to $\vec{P}^{reac} \cdot (\vec{U}^+ + \vec{U}^-) = \vec{P}^{reac}\vec{U}_N > 0$. Closed form solutions can be computed for $\vec{P}^d = k\ (U_N^+ + U_N^-)\vec{N}$.

The kinematic quantity $\vec{U}^+ - \vec{U}^-$ used to describe the collision appears to be the best one from the theroretical point of view. Experiments have been performed with small triangles and rectangles colliding in a plane: They show that the best way to describe $\vec{P}^d$ depending on $\vec{U}^-$ and $\vec{U}^+$is $\vec{P}^d(\vec{U}^+ + \vec{U}^-)$. The experiments show that the tangential percussion $\vec{P}_T^d$ satisfies a Coulomb law $\vec{P}_T = -P_N\ \Phi(\vec{U}_T^+ + \vec{U}_T^-)$ and $\vec{P}_N = P_N(\vec{U}_N^+ + \vec{U}_N^-)$ ($\vec{U}_T$ is the tangential velocity).

Moving fronts in transparent equations

K. P. Hadeler

For the $1D$ transport equation with two velocities "optimal" conditions are given for the existence of moving front solutions via reduction to the parabolic case. These results carry over to reaction telegraph equations and Cattaneo systems. H. Schretlick has extended such results to transport equations in several space dismensions.

Aspects of thermodynamics of damaged solids

G. Herrmann

Conservative (or conventional) thermodynamics of irreversible processes is employed to establish a novel theory of elastic bodies prone to damage. Such a body is regarded as a thermodynamic system characterized by a set of extensive variables that can be defined in both equilibrium and non-equilibrium states, and assigned approximately the same values in both the physical and the abstract state space, (i.e. the Gibbsian phase space of constrained equilibrium). The local state approximation is applied by assigning to

the entropy and temperature in physical space local values which can be calculated in the Gibbsian phase space. This leads to an explicit expression for the entropy production. The rate (or evolution) equations for the damage are then postulated in such a way as to conform to the second part of the second law of thermodynamics. The resulting theory captures many features of real material behaviour such as loading-unloading paths, quasiductility, dependence on loading − or straining − rates, transition from brittle to ductile behaviour, dependence on size and shape of the structural element, as well as special modeling of the influence of microstructure associated with toughening mechanisms.

Kinetic solutions of the Boltzmann-Peierls-equation (BPE)

M. Herrmann

Joint with W. Dreyer & M. Kunik

The Boltzmann-Peierls-equation (BPE) describes the evolution of the phase density $f(t;x;k)$ of a phonon gas. The corresponding entropy density is given by the entropy of a Bose-gas. The collision operator is the sum of two collision operators $S = S_R + S_N$.

S_R and S_N correspond to different kinds of interactions and can be derived from the Maximum-Entropy-Principle (MEP). The main results are

1. We derive a reduced kinetic equation that has a simpler structure than the BPE.
2. The MEP can always be applied to the reduced equation. The resulting moment systems are equivalent to moment systems of the BPE.
3. There exists a consistent kinetic approach. We derive kinetic schemes for the kinetic equation as well as for the moment systems. All schemes have the same formal structure.

Transport equations in mathematical biology

T. Hillen

Reaction transport equations are models for spatial spread and interactions of biological species. Relevant model parameters can be estimated from individual behaviour (e.g. mean run length, turn angle distribution, reproduction rate etc.).

I study reduction methods to obtain simpler models from the full kinetic equation. Here I focus on two approaches

i) the parabolic scaling method, which leads to reaction-advection-diffusion equations, and

ii) the moment closure method to obtain hyperbolic models.

I illustrate the relations between these methods and I will apply the resulting models to the chemotaxis problems. Chemotaxis is the active orientation of animals on chemical signals. This may lead to aggregation and pattern formation.

The inverse problem from the Bayesian point of view

J. Honerkamp

Preisach-type model of stress-strain hysteresis of shape memory alloys at various temperature

Y. Huo

The stress-strain relations of shape memory alloys (SMA) show hysteresis and can have very different shapes for samples with different compositions, different heat treatment and different testing temperatures. Preisach-type models of hysteresis are a good mathematical method to account for the complexity of the stress-strain hysteresis of SMAs, provided that the distribution function can be determined by experiments. Two methods are introduced to determine the distribution functions. One requires the differentation of the experimental strain-stress curves which induces large numerical errors and difficulties. The other one is based on a normal distribution function with six parameters to be identified by experiments. This method gives a better procedure for the numerical simulation and provides some physical meaning for the distribution function.

Maximum entropy moment systems and Galilean invariance

M. Junk

Starting from the Boltzmann equation of gas dynamics, a system of moment equations is derived based on the Maximum Entropy closure. The resulting system is Galilean invariant, if the space of moment functions is invariant under arbitrary rotations and translations. Since any finite dimensional function space with this property consists of polynomials, a problem arises if Galilean invariance is required for ME-systems involving polynomial moments of degree larger than two: The domain of definition of these systems is not convex and has equilibrium states on its boundary. As a consequence, linearization around equilibrium states is not justified and no local existence results are available for equilibrium initial values. Without the requirement of Galilean invariance, the situation can be quite different. This is demonstrated for a moment system based on the semiconductor Boltzmann equation in connection with Kane's dispersion relation.

Aspects of mechanics in material space

R. Kienzler

The common and well-known mechanics in physical space or Newtonian mechanics describes stress, displace-ment and motion of objects in the physical space in which they find themselves. Mechanics in material space or mechanics in configurational space or Eshelbian mechanics describes the motion of objects relative to the material in which they are embedded. Far-reaching analogies between these two mechanical viewpoints exist. For example, physical as well as material forces are introduced via the gradient of a potential energy. Notions like free-body diagrams, trajectories, stability of equilibrium etc. are introduced in material space. In the talk examples are discussed like the interaction of a circular hole and a dislocation in plane elastostatics, application in strength-of-materials type of theories. Also some new findings in elasto-dynamics are described.

Aspects of uniqueness in nonlinear elastostatics and related constitutive assumptions

R. J. Knops

Joint work with C. Trimarco (Pisa) and H.T. Williams (Jaguar, Coventry)

Failure of uniqueness in many counter-examples suggests that only simple problems might be expected to possess a unique solution. A proof is outlined for uniqueness of the stress in the null-traction boundary value prob-lem for homogeneous nonlinear elasticity on a star-shaped region subject to certain convexity assumptions on the complementary stored energy which is postulated to exist a priori. These assumptions are analogous to those of quasi-convexity and rank − one convexity usually adopted for the strain energy function. An important dis-tinc-tion, however, is that a complementary energy is defined on functions (the stress distribution, whereas strain energy is defined on the gradients of functions (deformation gradients). [The differencen can be partly remedied by expressing the equilibrium stresses as the curl of a second order tensor]. The assumptions intro-duced for the complementary energy are termed para-convexity and rank $(n-1)$-convexity and an identity similar to that derived by Green, Hill and several others is employed to obtain a contradiction from which the uniqueness result follows.

Finally, it was shown that para-convexity implies rank $(n-1)$-convexity. The reverse implication remains open, although J. Kristiansen appears to have established equivalence for 2-dimensions.

H-Theorem, model equations and wave propagation in a relativistic gas

G. H. Kremer

One of the aims of this report is to introduce the following theorems, which are valid for a relativistic ideal gas:

1) A summational invariant is a linear combination of the momentum four-vector;

2) The function $H(t)$ tends to its equilibrium value when $t \to \infty$;

3) The one-particle distribution function tends to its equilibrium value when $t \to \infty$.

The next objective is to show that the Anderson and Witting model equation leads to different results concerning the transport coefficients of a relativistic gas, when the method of Chapman-Enskog or the method of moments of Grad are applied as closures of the Boltzmann equation.

The last objective is to analyse the behaviour of the phase velocity and of the absorption coefficient when the relativistic gas is described by a five-, thirteen- and fourteen-field equation. In the case of a five-field theory the constitutive equations of Navier-Stokes-Fourier and Burnett are used. The limiting cases of a non-relativistic and ultra-relativistic gas are also analysed.

Plastic spin and evolution of an anisotropic yield condition

H. Lippmann

Joint work with H. P. Truong Qui

The local average of the rotation of the grains in a polycrystalline material may be expressed in terms of the continuum mechanical concept of the "plastic spin" representing, according to the author's opinion, a special event of the more general concept of the COSSERAT continuum. The present contribution aims at the experimental confirmation of the existence of the plastic spin. While in the past isotropic materials have been examined using X-ray techniques, and averaging individual grain rotations over meso-volumes, this time an experimental approach by BOEHLER & KOSS, (1991/1992) has been adapted to do this task. The same approach was also applied by KIM & YIN, (1997) without knowledge of the previous work by BOEHLER & KOSS. It is based on the determination of the plastic yield locus of pre-rolled sheet metal stretched in various directions with respect to the rolling direction. The present authors have identified the parameters of a theoretical approach, super-imposing isotropic and kinematic hardening to local rigid-body rotation with the aid of small-strain tests of aluminium sheets. They obtained a fair to good agreement, however they found out that the special, linear PRAGER approach to kinematic hardening cannot hold true. A pretty large plastic spin was observed even for small strain, and this was confirmed by comparison with results of BUNGE & NIELS, (1997) obtained by direct observations. Moreover it is shown that the initial orthotropy of the sheet metal is destroyed at small "off-axes " stretchings (i.e., neither in the pre-rolling direction nor in the transversal direction) thus confirming a corresponding statement by BOEHLER & KOSS, however contradicting an opposite statement by KIM & YIN. (All authors agree that at large strains orthotropy is (re-) established in the direction of stretching).

The Chapman-Enskog expansion for semiconductor Boltzmann-Poisson systems

A. Majorana

In this talk we consider the Boltzmann equation describing the carrier transport in a semiconductor. A modified Chapman-Enskog method is used in order to find approximate solutions in the weakly non-homogeneous case. These solutions allow us to calculate the mobility and diffusion coefficients as functions of the electric field. The integral-differential equations derived by means of the above-mentioned method are numerically solved using a combination of the box method and finite-difference operators. The Kane model for the electron band structure is assumed. The numerical values of the mobility and diffusivity in a silicon device are compared with experimental data. The Einstein relation is also recovered.

Thermodynamics and wave propagation in pre-stressed solids

A. Morro

The equation of motion and the constitutive equation are considered for a pre-stressed anisotropic solid with memory in the linear approximation for the incremental stress and strain. Hence, by exploiting the second law of thermodynamics, the Fourier sine transform of the stress-strain kernel is shown to be negative definite. With a view to wave propagation problems, the attempt is made to frame the governing equations in a state-variable formulation. Although the equation of motion does not involve exactly the (Cauchy)

stress, it follows that the restriction of thermodynamic character is crucial to obtain the state-variable formulation. Next, in connection with time-harmonic waves, the solution is determined, in terms of the propagation matrix, for propagation in planarly-stratified layers. Further, the reflection and transmission matrices of multilayers are derived.

Computer modeling of microstructural changes in solids by continuum theory and phase field models

W. Müller

Joint work with W. Dreyer

A model based on continuum theory is presented that is capable of handling the problem of phase separation and coarsening as observed in tin-lead based eutectic solders. The equations of equilibrium of forces are solved on a first step together with Hooke's law to determine the local stresses and strains on a heterogeneous body (the representative volume element of the material). In a second step these stresses are used in an extended diffusion equation together with the expressions for Fick's law and the Cahn-Hilliard interface term to determine the field of the concentration as a function of time and position. This procedure is repeated to generate computer simula-tions of the microstructural evolution. The simulations are quantitative based on experimental coefficients ob-tained from the literature.

Some problems for non-linearly thermoelastic crystalline solids

M. Pitteri

The presentation focusses on the problem of phase transitions in non-simple lattices, a topic for which a well-developed theory still does not exist, although various special models are available. The research presented is part of the activities of the TMR research project "Phase Transitions in Crystalline Solids", funded by the European Community.

Through a simple example, in which the algebraic complexities are reduced to the bare essentials (the example is a diatomic 2-lattice with constituent simple lattices that are primitive tetragonal, the whole 2-lattice being tetragonal itself.) By means of a kinematic description of multilattices proposed by the author in 1984-1985 it is shown how the configuration space can be represented for 'small but finite' deformations, by means of $R^6 \times R^3$, on which the tetragonal holohedry acts orthogonally and independently in the two factor spaces. It is shown that also in this case generic bifurcations occur provided the tensor of moduli (second-order derivatives of the free energy density with respect to the configurational parameter) has irreducible-invariant proper spaces, one of which is the kernel of the tensor itself. This requires the transition to be either (purely) configurational (the center atom follows the deformation of the skeleton) or structural (the center atom displaces itself either along the tetragonal axis or orthogonal to it). Among other things, the analysis suggests that the belief of Landau, that the skeleton of a crystal should not be "generically" more symmetric than the whole crystal, may not always hold. For, in this case, the simplest potential that allows for a structural transition along which the central atom moves orthogonally with respect to the tetragonal axis, leaves the skeleton having tetragonal symmetry, while the crystal class of the 2-lattice is a subgroup of the orthorhombic holohedry.

A binary mixture of Euler fluids: Second sound and diffusion

T. Ruggeri

In the present paper we prove by a change of variables that the differential system of a binary mixture of Euler fluids can be written as the system of a single fluid with heat conduction. In this manner a natural generalization of the Cattaneo equation arises, and we find a simple justification of the "thermal inertia" introduced in previous papers for the second sound phenomena in crystals. This presentation permits to verify that the second sound is a common characteristic of low temperatures. Critical temperatures for the $He\ II$ in which the shock front changes behaviour are also determined by imposing the breakdown of the genuine non-linearity of the hyperbolic system.

Dynamic properties of shape memory alloys

S. Seelecke

In recent years, shape memory alloys have attracted increasing attention due to their unusual dynamic properties. The hysteretic phase transformations constitute an intrinsic dissipation mechanism resulting in a damping capacity, which is orders of magnitude larger than in conventional metals. Currently, potential applications are investigated in the context of seismic isolation or mitigation of wind-induced hazards of structures like buildings or bridges.

This presentation focuses on the simulation of the rotational vibration of a rigid mass suspended by a thin-walled shape memory tube. An extended version of the Müller-Achenbach model is employed to calculate the free and forced vibration behaviour of the mass.

Depending on the temperature, shape memory alloys exhibit either quasiplastic or pseudoelastic behaviour, which differ considerably with respect to their damping characteristics. Furthermore, the forced vibration case reveals a strong amplitude dependence of the system response, which is an interesting nonlinear effect due to the hysteresis.

Finally, it is shown that, for pseudoelasticity, it is of crucial importance to include the balance of energy in the simulation to account for the strong thermomechanical coupling due to the latent heats of phase transformation.

Convection in porous media

B. Straughan

The problem is considered where water lies in a porous plane layer with boundaries $z = 0$ and $z = d$, the z-axis being vertical. The bottom boundary is held at temperature $0°C$ while the top is held at $T_n \geq 4°C$. The permeability in the porous medium is transversely isotropic with the isotropy axis inclined at angle β to the horizontal. It is shown that bifurcation into convection is of Hopf type. A sharp nonlinear stability bound is derived which is very close to the threshold of linear instability.

Boundary conditions for moment equations via kinetic schemes

H. Struchtrup

The Navier-Stokes-Fourier equations fail to describe flows in rarefied gases with Knudsen numbers above 0.01. In this case one may consider Grad's moment equations – which approximate the Boltzmann equation – for the description of the gas. A numerical scheme

– called "kinetic schemes" – permits the solution of boundary value problems for the Grad moment equation for the first time. Here, kinetic schemes are considered for the calculation of stationary heat transfer in the Grad moment system with up to 430 moments. The results exhibit temperature jumps at the walls with adjacent boundary layers. For given temperatures and a given Knudsen number, the result changes with the number of moments, and it converges if the number of moments is increased.

Wave propagation and related phenomena in crystal solids at finite temperatures

M. Sugiyama

Thermomechanical properties of waves propagating in anharmonic crystal lattices are studied and discussed, and the related phenomena such as dynamic fracture and collision phenomena are briefly mentioned The contents of the talk is as follows:

1. Introduction
2. Basis equations
3. Linear analysis
4. Continuum approximation of the evolution equations
5. Shock waves
6. Other related topics
7. Evolution equations for 3-dimensional anharmonic lattices.

The Maxwell energy-stress tensor: From electrostatics to continuum mechanics

C. Trimarco

The Maxwell energy-stress tensor of electrostatics was revisited and re-proposed in elasticity by Eshelby, in 1951. The two tensors share the following feature: Both account for the presence of an inhomogeneity. In electrostatics the /inhomogeneity/ is the electric charge whereas, in elasticity, it is the material /defect/ of a body. Despite the close similarity of the two tensors, they definitely differ from one another as they describe distinct physical phenomena. An Eshelby-like tensor is here proposed for electrostatics. This tensor identically vanishes outside the body, whereas the Maxwell stress tensor is defined everywhere in space.

Determination of boundary conditions for plane harmonic waves

W. Weiss

Plane harmonic waves may be created in a tube filled with a gas and with a loudspeaker on one end. If the frequency is very high, theories like Euler or Navier-Stokes-Fourier are not sufficient to describe the waves satisfactorily. From the kinetic theory one may derive field equations for many variables (e.g. Grad's 20 moment system). Such systems should be able to describe the waves up to high frequencies. However, more boundary conditions are needed than one can control in the experiment. It is shown that the minimization of the entropy production is a method to determine the remaining boundary values. Results are given for the 20 moment theory and for different frequencies.

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