Reasearch group on *Phase Transitions and Plastic Flow Localization Phenomena*

IMAR Participants: C. Faciu, M. Suliciu, D. Polisevschi, A. Capatana
Romanian Cooperations: Bucharest University (through a joint scientific seminar), "Ovidius" University Constanta.
International Cooperations:
France: Universities of Metz and Saint Etienne
Workpackages involved: A1, B2, C5.
Doctoral research: Dr.-Ing. Andreas Heckmann from the Institute of Materials, Faculty of Mechanical Engineering of Ruhr-University Bochum has been accepted for one month visit at IMAR as a Ph.D student in July 2002. His topic of interest was "Microstructure and fatigue of shape memory alloys". Andreas Heckmann performed in Germany laboratory experiments. He measured the way the phase transformation is endothermic and how the material is subjected to self heating during the transformation. These aspects have been compared with the prediction of the model developed by C. Faciu and M. Mihailescu-Suliciu. In 2003 Andreas Heckmann has obtained his doctor degree at the University of Bochum with the thesis "Mikrostruktur und Ermüdung von NiTi-Form-gedächtnislegierungen" (Microstructure and fatigue of NiTi-shape memory alloys) being directed by Prof. Em. E. Hornbogen.

Scientific Objectives:

1. Mathematical models for describing the behaviour of Shape Memory Alloys.
2. the multiple-scale convergence method in connection with the microperiodic domains composed of two connected phases.
3. contact problem with friction between a linearly elastic body and a rigid foundation.

Main Scientific Results:

1. C. Faciu and M. Mihailescu-Suliciu: *On a rate-type thermo-mechanical model for shape memory bars. Strain-controlled problems*. 6p, Proceedings of the Workshop on Shape Memory Alloys, September 3 - 6, 2001, Warsaw, Poland, organized by the Institute of Fundamental Technological Research, Polish Academy of Sciences and Center of Excellence "Advanced Materials and Structures" (AMAS).
2. C. Faciu and M. Mihailescu-Suliciu: *On modelling phase propagation in SMAs by a Maxwellian thermo-visco-elastic approach*, Int. J. Solids Structures, 39 (2002) 3811-3830.
3. C. Faciu and M. Mihailescu-Suliciu: *On a rate-type thermo-mechanical model for shape memory bars. Stress-controlled problems.* Zeitschrift fur angewandte Mathematik und Physik ZAMP, 53 (2002) 1014-1025.
4. C. Vallee, D. Fortune, C. Brouby and W. Pietraskiewicz: *Calculus of the square root of a positive definite symmetrical linear mapping by solely determining a rotation* in Proceedings of the 5th International Seminar on "Geometry, Continua and Microstructure", Eds. S. Cleja-Tigoiu and V. Tigoiu, Editura Academiei, Bucharest, Romania, 2002.
5. D. Polisevski: *Basic homogenization results for a biconnected ε-periodic structure*}, Applicable Analysis, 82(4), 301-309, 2003.
6. C. Faciu} and M. Mihailescu-Suliciu: *On modelling exothermic/endothermic phase transformations in shape memory alloys*, in Current Topics in Continuum Mechanics, Vol. II, p. 41-85, Ed. Lazar Dragos, Editura Academiei, Bucharest, 2003.
7. C. Faciu and M. Mihailescu-Suliciu: *Shape Memory Effect: A Maxwellian rate-type constitutive approach*, In Proceedings of NATO Advanced Research Workshop, "New Trends in Phase Transformations and their Applications to Smart Structures", April 23 -26, 2003, Metz, France - to appear Kluwer Academic Publishers.

Research Activity:

- Shape memory alloys (SMA) and their two unusual characteristics: the pseudo-elastic hysteresis and the shape memory effect have received sustained attention in recent years. The shape memory effect is the material's ability to recover at zero stress large mechanically-induced strains (up to 8%) by moderate increases in temperature (aprox. 10-20 ^{0}C). Pseudo-elasticity refers to the materials's ability in a somewhat higher temperature regime to be strained significantly (to strains higher than 6%) and to return to its unstrained configuration upon unloading via a hysteresis loop. The underlying mechanism is a reversible transformation between two solid state phases called *austenite (A)* and *martensite (M)* often occurring near room temperature. The transformation can be stress-induced or temperature-induced causing a strong thermo-mechanical coupling in the material behavior. These properties have been discovered half a century ago, but the interest in these alloys has recently increased and stems in part from their applicability as elements in active structure.
- C. Faciu and M. Mihailescu-Suliciu have proposed a Maxwellian thermo-viscoelastic approach to the problem of phase transformation in shape memory alloys bars. The equilibrium stress-strain-temperature response of this model is a non-monotone stress-strain relation for certain ranges of temperature. The corresponding free-energy function, which depends on stress, strain and temperature is a non-convex function. Each domain of convexity of the equilibrium free energy is identified with a phase (or variant of phase) of the material. The model has been published in the International Journal of Solids and Structures and its predictions for strain- stress- and temperature-controlled experiments have been also published and presented at international scientific meetings (see references below). The numerical simulations successfully capture the nucleation and evolution of transformation fronts. A very good agreement with the laboratory experiments performed by Shaw & Kyriakides at the University of Texas at Austin (*On the nucleation and propagation of phase transformation fronts in a NiTi alloy*, Acta Materialia 45, 683-700, 1997) has been obtained. The number of nucleation events and kinetics of transformation fronts were found to be sensitive to the imposed loading rate due to the release/absorbtion of latent heat. It was also shown that the pseudo-elastic hysteresis in their strain-stress curves increases when the imposed rate is increased. The prediction of the model for a loading strain-controlled experiment (austenitic - martensitic phase transformation) is illustrated by the evolution of strain and temperature fields in the bar (see Example1 or Example2:
  http:// www.imar.ro/~cfaciu/example1,
  http://www.imar.ro/~cfaciu/example2).
  The shape memory effect is illustrated by the animated representation in Example3 (http://www.imar.ro/~cfaciu/example3).
- C. Faciu and A. Molinari from the University of Metz have investigated from theoretical point of view the impact problem of two shape memory alloy bars in an isothermal setting. A paper entitled "Impact-induced phase transitions in elastic versus rate-type viscoelastic bars" is almost finished. The constitutive relations of the shape memory alloy bars are based on a non-monotone elastic stress-strain relation, or on a Maxwellian rate-type viscoelastic constitutive equation. The partial differential equation system which governs the motion of the bars is of mixed hyperbolic-elliptic type for the elastic system, or of hyperbolic type for the viscoelastic one. For the elastic system we solved analytically the Riemann and Goursat problems as initial and boundary value problems. The main theoretical difficulty is related with the non-uniqueness of the solutions due to the non-convexity of the free energy function. We have determined the wave structure and estimated the velocity of the propagating phase boundary for both forward and reverse transformations. For the hyperbolic viscoelastic system the same problem has been solved numerically.
  Since the laboratory LPMM of the University of Metz is very well equipped with gas canon, Hopkinson bars and VISAR interferometry system for free surface velocity measurements, we have discussed with Dr. Alexis Rusinek, which is responsible of the laboratory experiments at LPMM, the possibility to realize effectively such kind of experiments. One has envisaged this

type of experiments as a controlled mean for estimating the velocity of propagating phase boundary. Thus, one controls the impact velocity of the projectile and one measures the time of contact between the flyer and target as well as the velocity-time profile at the free end of the target.

- Another topic of interest is the modelling of the behavior of some austenitic steels which can be transformed in martensite phase by plastic deformation (transformed induced plasticity - TRIP). Discussions with Prof. Alain Molinari and Dr. Alexis Rusinek lead to progresses in the modelling of the dynamic response of TRIP steels. A free energy function has been constructed which allows to account for strain hardening, temperature and rate dependence and to describe the role of the plastic deformation on phase transformation. This constitutive formulation will be used later to analyze the dynamic response of TRIP steels under various loading rates. Of particular importance is the interpretation of shock experiments. It will be explored later how to consider this problem for TRIP steels. This problem is of particular importance since TRIP steels are used by the automotive industry as structural components to absorbs shock during car crashes.
- Dan Polisevski (IMAR) has continued the study of the multiple-scale convergence method in connection with the microperiodic domains composed of two connected phases.
- Anca Capatana (IMAR) and Frederic Lebon have investigated an unilateral contact problem with friction between a linearly elastic body and a rigid foundation. The contact is modelled by Signorini's law and a nonlocal version of Coulomb's friction law. We are concerned with a number of questions for this problem. First, dual formulations has been considered. It is known that contact problems with friction cannot be formulated as extremum problems hence usually duality approaches do not apply to such problems. We have used Mosco-Capuzzo-Dolcetta-Matzeu duality theory to obtain a dual quasi-variational inequality which is a problem for the stress on the contact surface only. Next the internal approximation of these problems by using equilibrium finite element methods has been considered. Error estimates on stress formulations have recently been obtained. In a future work the convergence proof will be addressed. At the same time one will consider various finite element methods of dual formulations in order to obtain numerical validations of the results.

Presentation of the results at scientific meetings:

1. *C. Faciu*: IUTAM Symposium on Material Instabilities and the Effect of Microstructure, Austin, Texas, Mai 7-11, 2001 with the contribution: *A rate-type thermo-viscoelastic approach for shape memory alloys.*
2. *C. Faciu and M. Mihailescu-Suliciu*: Workshop on Shape Memory Alloys, Institute of Fundamental Technological Research, Polish Academy of Sciences, September 3 - 6, 2001, Warsaw, Poland with the contribution: *On a rate-type thermo-mechanical model for shape memory bars. Strain-controlled problems.*
3. *C. Vallee*: The 25th National Conference of Solids Mechanics, September 20 - 23, 2001, Constanta, Romania with the contribution: *Choice of invariants - Nonlinear isotropic law - Convex potentials.*
4. *C. Vallee*: 5th International Seminar on "Geometry, Continua and Microstructure"}, September 26 - 28, 2001, Sinaia, Romania with the contribution: *Calculus of the square root of a positive definite symmetrical linear mapping by solely determining a rotation.*
5. *C. Faciu and M. Mihailescu-Suliciu*: NATO Advanced Research Workshop, New Trends in Phase Transformations and their Applications to Smart Structures, April 23 -26, 2002, Metz, France with the contribution: *Non-equilibrium thermodynamics of pseudoelasticity and shape memory effect*
6. *D. Polisevski*: The International Conference "Analysis and Optimization of Differential Systems", September 2002, Constanta, Romania with the contribution: *Basic homogenization results for a biconnected ε-periodic structure*.
7. *C. Faciu*: Sudoesteuropa-Tagung "Wissenschaftsdialog in Sudoesteuropa zum Thema Neue Technologien"}, Zagreb, Croatia, October 18-20, 2002, organized by the Alexander von Humboldt Foundation with the contribution: *On modelling shape memory alloys - a continuum rate-type approach.*}
8. *C. Faciu and M. Mihailescu-Suliciu*: 5th EUROMECH Solid Mechanics Conference, Thessaloniki, Grece, August 17-22, 2003 with the contribution: *On describing thermo-mechanical instabilities accompanying phase transition phenomena.*}
9. *C. Faciu and M. Mihailescu-Suliciu*: 5th Congress of Romanian Mathematicians, June 22-28, 2003, Pitesti, Romania with the contribution: *On modelling thermo-mechanical interactions accompanying reversible phase transformations.*
10. *C. Faciu and M. Mihailescu-Suliciu*: The International Conference "New Trends in Continuum Mechanics", September 8-12, 2003, Constanta, Romania with the contribution: *Initiation and propagation of thermo-mechanical instabilities in thin shape memory bars. A linear stability analysis.*
11. *A. Capatana and F. Lebon*: The International Conference "New Trends in Continuum Mechanics", September 8-12, 2003, Constanta, Romania with the contribution: *Remarks on the equilibrium finite element method for frictional contact problems.*}

EURROMMAT Conferences organized at IMAR:

1. Mario Ahues and Alain Largillier, (Universite Jean Monnet, Saint Etienne, France) - October 29, 2001: *Approximate inverses in astrophysics: numerical approximation of the integral transfer equation.*
2. Andrzej Ziolkowski, (Polish Academy of Sciences, Institute of Fundamental Technological Research, Warsaw, Poland) - November 5, 2001: *Thermo-mechanical behavior of shape memory alloys. Part I: Experimental evidence.*
3. Andrzej Ziolkowski, (Polish Academy of Sciences, Institute of Fundamental Technological Research, Warsaw, Poland) - November 12, 2001: *Thermo-mechanical behavior of shape memory alloys. Part II: Modelling.*
4. Alain Molinari, (Laboratoire de Physique et Mecanique des Materiaux, Universite de Metz, France) - Mai 20, 2002: *Modeling of viscoplastic porous media with applications to stability of sintering and dynamic damage. Part I: Modeling of viscoplastic porous materials*

5. Alain Molinari, (Laboratoire de Physique et Mecanique des Materiaux, Universite de Metz, France) - Mai 20, 2002: *Modeling of viscoplastic porous media with applications to stability of sintering and dynamic damage. Part II: Micro-macro transition for porous materials under high strain rate.*
6. Frederic Lebon, (Laboratoire Mecanique Materiaux Structures, Universite Claude Bernard Lyon 1, France) - 10, 2002: *Analysis of soft thin layers*}
7. Andreas Heckmann, (Institute of Materials, Faculty of Mechanical Engineering, Ruhr-University Bochum, Germany) - July 7, 2002: *Microstructure and pseudo-elastic low cycle high amplitude fatigue of NiTi.*
8. Frederic Lebon, (Laboratoire Mecanique Materiaux Structures, Universite Claude Bernard Lyon 1, France) - July 27, 2002: *Primal and dual algorithms for multilateral contact with friction problems.*
9. Frederic Lebon, (Laboratoire Mecanique Materiaux Structures, Universite Claude Bernard Lyon 1, France) - July 10, 2003: *Modelling of soft thin layers: on two classes of non-linear behavior*:
    - *Part I: Non-associated plasticity (Mohr-Coulomb, Drucker-Prager).*
    - *Part II: Non-convex energies.*
10. Alexis Rusinek, (Laboratoire de Physique et Mecanique des Materiaux, Universite de Metz, France) - October 2, 2003: *On the behavior of sheet metal at high strain rates and the effect of adiabatic heating. Part I: New experimental methods for sheet steel based on Hopkinson bar. Part II: Modelling: analytical and numerical results.*
11. Alain Molinari, (Laboratoire de Physique et Mecanique des Materiaux, Universite de Metz, France) - October 30, 2003: *The structure of steady plastic shock waves in metals.*

Conferences and seminaries of the Romanian participants:

1. C. Faciu: *A continuum approach for exothermic-endothermic phase propagation in SMAs*, Technische Universitaet Munchen, Germany, October 14, 2002.
2. C. Faciu: *On modelling phase propagation in SMAs - a thermoviscoelastic approach*, CAESAR - Center of Advanced European Studies and Research, Bonn, Germany, November 5, 2002.
3. D. Polisevski: *Specific methods of homogenization*, Centre pour le Developpement du Calcul Scientifique Parallele de l'Institut Scientifique et Technique des Ingenieurs de l'Universite Claude Bernard de Lyon, in the seminar "Modelisation et Calcul Scientifique", November 2002, Lyon, France.
4. A. Capatana: *Some optimal control problems*, Universite Claude Bernard Lyon 1, Lyon, France in the seminar "Numerical analysis and partial differential equations", April 2003.

Lecture Series:

1. Doina Cioranescu (Univ. Paris 6): 4 lectures on *Non Newtonian Fluids: Differential Type Fluids*, at IMAR in November 2001.

Organization of:

- **The International Conference *"New Trends in Continuum Mechanics"*, Constanta, Romania – September 8 -12, 2003.** Organized by the "Simion Stoilow" Institute of Mathematics of the Romanian Academy and the "Ovidius" University, Constanta. *(Annex 22)*

Main Topics:

Modelling in dolid and fluid mechanics; thermodynamics and heat transfer; fractura mechanics and damage; soil and rock mechanics; non-Newtonian and electrorheological fluids; optimal control problems; problems in porous media; shock waves and related topics; phase transition and strain localization; random materials and smart materials; turbulence and related topics; gasdynamic interactions; computing methods in mechanics;.

A minisymposium on "Homogenization and applications to mechanics of continuous media".

Scientific Programme:

BACROIX B.*, R.BRENNER, O.CASTELNAU, Ph. GERBER, H.NOUIRA : Prediction of the heterogeneity of stored energy in rolled polycristalline copper using various homogeneization techniques - Comparison with experimental data.

BADEA A.*, BOURGEAT A. : Geological pattern recognition.

BADEA LORI : On a multilevel method for the minimization of non-quadratic functionals.

BIRSAN MIRCEA : A bending theory of porous thermoelastic plates .

BONTCHEVA N.*, PETZOV G. : Grain size evolution and phase transformation during metal forming processes.

BRAESCU L.*, BALINT A.M., BALINT ST. : On the stability of the shape of a a LiNb0-{3} bar grown from the melt in a vacuum by E.F.G. Method.

CAPATINA A.*, LEBON F. : Remarks on the equilibrium finite element method for frictional contact problems

CARABINEANU ADRIAN : The study of the self-propulsion by the integral equations method

CHANG QIANSHUN : Efficient algebraic multigrid algorithms and their applications

CHASHECHKIN D. YULI : Mathematical and laboratory modelling of stratified flows

CIORANESCU DOINA : Homogenization of nonlinear elastomers

CLEJA-TIGOIU SANDA : Material symmetry in finite elasto-plasticity with continuum

COCOU M.*, SCARELLA G. : A dynamic contact problem for a cracked viscoelastic body; modelling and approximation

CRACIUN E.M.*, BAESU E., DUSZA J.: Stress concentration in prestressed fiber reinforced composite containing two collinear cracks supposed to be under antiplane shear loadings

CRISTESCU DAN NICOLAIE : A closed form solution for falling cylinder viscometers

DAMLAMIAN ALAIN : Iterated homogenization for domains with isolated holes

DUMITRACHE ALEXANDRU : An interactive computing method for steady and unsteady flows

ENE HORIA : Flow in fracturated porous media

FORTUNE D., VALLEE C.*, BAN M., MENSAH-DOMPKIN L., G. de SAXCE : Unicity of the bipotential modelling a standard-implicit material

FRUNZULICA F.*, CIUTA T.: Static and vibration analysis of wing structures using equivalent plate model

FRUNZULICA F.*, ANDREI I.: Computational mesh generation : past, present and future

IONESCU R.I.*, CAMPILLO M. : Initiation of instability on a fault system under slip dependent friction

JIROVEANU D.*, SOLER J. : Numerical aspects on a splitting model of bubbles by a turbulent flow field

KASLIK E.*, BALINT A.M., BIRAUAS S., BALINT ST. : On the controlability of the roll rate of the ALFLEX reentry vehicle during its final approach and landing phase

KASLIK E., BALINT A.M., BALINT ST.*: Gradual approximation of the domain of attraction by gradual extension of the "embryo" of the transformed optimal Lyapunov function

KASLIK E., BALINT A.M.*, BIRAUAS S., BALINT ST. : Approximation of the domain of attraction of an asymptotically stable fixed point of a first order analytical system of difference equations

LUCA I.*, FANG C., HUTTER K. : On thermodynamics of turbulent motions in a granular material

LUPU MIRCEA : Optimization method for maximal drag airfoils in the case of nonlinear problems in hydro-aerodynamics

MADAY YVON : Some elements for the modelisation and the numerical simulation of the respiration tree

MARINA VASILE : Reading the possibilities to decode the microstructure characteristics from macroexperience

MARINESCU D.*, GRUNFELD C.P. : Convergent numerical scheme for generalized nonlinear Boltzmann models

MARINOSCHI GABRIELA : On a nonlinear boundary value problem related to infiltration in unsaturated media

MATEI BASARAB : Non-linear subdivision schemes with applications to ENO interpolation

NEGREANU MIHAELA : Discrete inequalities

PANASENKO GRIGORY : Asymptotic decomposition of a domain in Continuum Mechanics

PASA GELU : Variable permeability for Saffman-Taylor instability

PERADZINSKI ZBIGNIEW : Generalized (weak) solutions in collisionless fluids

PEREZ EUGENIA MARIA : On the local problems for vibrating membranes with concentrated masses

PIECHOR KAZIMIERZ : On the hydrodynamic limit of the Enskog equation with square-well potential in the case of weak attractive forces

POLISEVSCHI D.*, SCHILTZ-BUNOIU R. : Heat conduction through a first order jump interface

POPESCU MIHAI : On the optimal control of bilinear systems

RADUCANU RAZVAN : Over the mortar finite element method in linear elasticity

SBURLAN S.*, SBURLAN C.: A coincidence degree for bifurcation problems with applications in mechanics of continua

SELESCU RICHARD : Conical motions and the related ones. Part I .The general properties of the conical flows

SELESCU RICHARD : Conical motions and the related ones. Part II. The "tronconical" flow

SIMION NICOLAE : Models of heat propagation in solid bodies

SIMIONESCU-PANAIT OLIVIAN : Propagation of attenuated waves in isotropic solids subject to initial electro-mechanical fields

SOCOLESCU DAN : On Leray problems for the stationary respectively non-stationary motions of a viscous incompressible fluid

STAVRE RUXANDRA : Boundary control of a non-stationary magneto-hydrodynamic flow

STOIA-DJESKA MARIUS : Adjoint sensitivity analysis for unsteady inviscid flows with shock waves

TEODORESCU P.P.,BADEA T., MUNTEANU L., ONISORU J.*: On the wave propagation in composite materials with a negative stiffness phase
TEODORESCU P.P., MUNTEANU L., CHIROIU V.*: On the wave propagation in chiral media
TIMOFTE CLAUDIA : Homogenization results for reactive transport through porous media
TIGOIU V.*,C.CIPU : Flow of some viscoelastic fluids in a falling cylinder viscometer and the evaluation of shear viscosity
URSESCU A.*, K.HUTTER : Channel flow of electrorheological fluids under inhomogeneous electric fields
URSESCU A.*, C.DASCALU : Thermally conductive elliptic hole in an anisotropic solid
VERNESCU BOGDAN : Effective properties and waves in electrorheological and magnetorheological fluids