Annual Report
2005

Chair of Applied Mechanics
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1 Preface

The present booklet reports on the activities of the Chair of Applied Mechanics at the University of Kaiserslautern. Although the external budget conditions become increasingly more tied, the Chair of Applied Mechanics was fortunately developing in a very satisfactory manner during the year 2005.
This success is exclusively due to the hard work and never ending enthusiasm of all the members of the Chair of Applied Mechanics. This report is intended to shed a spotlight on the current status of affairs of Applied Mechanics at the University of Kaiserslautern and should convince the reader about the high degree of dedication and ambition of all the members of this group.

Paul Steinmann

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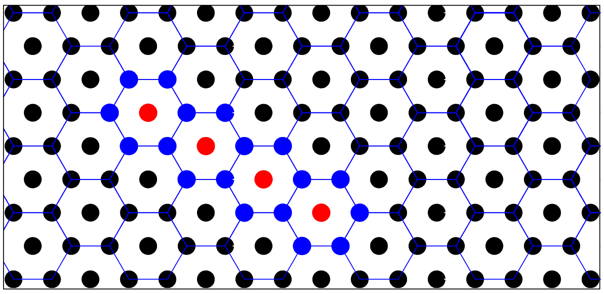
Hexagonal lattice model

Tadesse Abdi, Paul Steinmann

We intended to develop a model that has periodic structure. The atoms in a crystal are in a regular repeating pattern with the important consequence of this repetition being the fundamental property of a crystal lattice such as symmetry and periodicity. These properties dictate the lattice to have a profound influence on the behavior of a material. In the light of these we consider a crystal which is a collection of identical unit cells stacked to fill the surface with the interatomic attractions taking the responsibility of cohesion and the Lennard Jones pair potential used for the description of the interaction. This model is used to compute stress in discrete atomic systems, where the notion of stress can be seen from the stand point of the interatomic forces arising from interactions between neighboring atoms in the collection. For the computation of stress we employed the virial stress theorem



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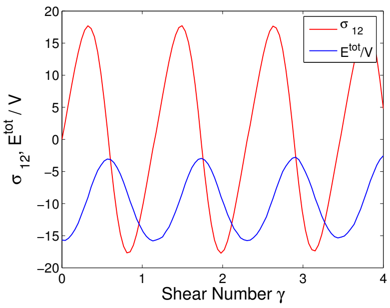


The figure on the left depicts the hexagonal lattice while the one on the right reveals the comparison of energy per volume of the lattice with the shear component of the stress.

Reference:

J. A. Zimmermann, E.B.Well III J.J. Hoyt, R.E.Jones, P.A. Klein and D.J. Bammann: Calculation of stress in atomic simulation, *Modelling Simul. Mater. Sci. Eng.* 2004; **12** 319–332

Computational constitutive modelling of rate-dependent domain switching effects in ferroelectric materials

Arunachalakasi Arockiarajan, Andreas Menzel

In recent years, piezoelectric and ferroelectric materials have widely been used for the design of smart materials and intelligent systems. The behaviour of ferroelectric materials are almost linear under the action of low electric fields or low mechanical stresses, but exhibits strong non-linear response under high electric fields or mechanical stresses. This work starts with developing a micromechanical model for ferroelectric materials. The microstructure of piezoelectric ceramics shows that it contains many grains. For the simulation, a bulk piezoceramic material is considered and each grain is represented by one finite element. Reduction in free energy of individual domains is adopted as a criterion for the initiation of domain switching processes. Intergranular effects are incorporated into the developed framework via a phenomenologically motivated probabilistic approach by relating the actual energy level to a critical energy level. Consequently, a rate-dependent polarisation framework is proposed at various frequencies. The reduction in free energy of a grain is used as a criterion for the onset of the domain switching processes. Nucleation in new grains and propagation of the domain walls during domain switching is modelled by a linear kinetics theory [1]. The macroscopic response of the bulk material is predicted by classical volume-averaging techniques. The second part of this work is focused on ferroelastic domain switching which refers to the reorientation of domains under purely mechanical loading. Rate-dependent domain switching effects are captured for various frequencies and mechanical loading amplitudes by means of the developed volume fraction concept which relates the particular time interval to the switching portion. The final part of this work deals with ferroelectric and ferroelastic domain switching and refers to the reorientation of domains under coupled electromechanical loading. If the free energy for combined electromechanical loading exceeds the critical energy barrier, elements are allowed to switch [2]. Secondly, additional mechanical loads in axial and lateral direction are applied to the specimen, see figure 1. Rate-dependent domain switching effects are captured for various frequencies and mechanical loading amplitudes by means of the developed kinetics theory.

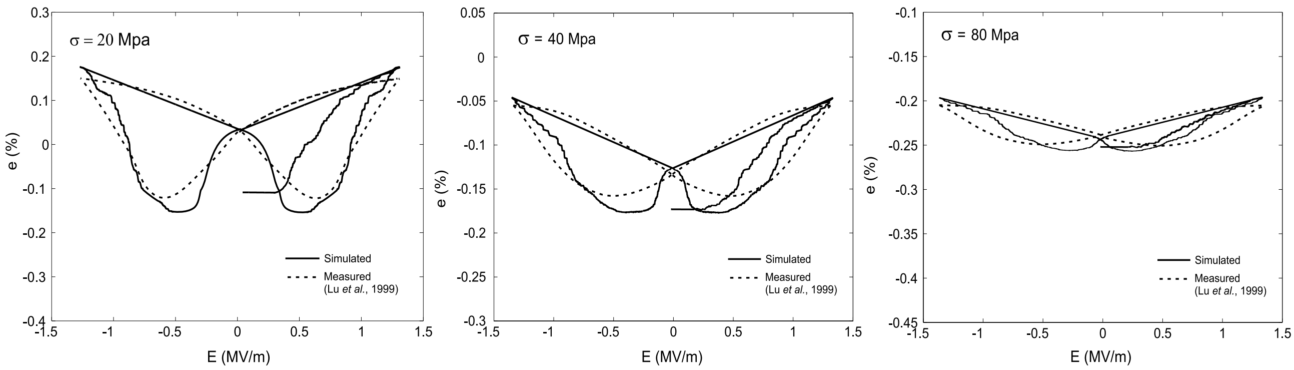


Figure 1: Butterfly curves for different axial compressive stresses σ.

References

[1] A. Arockiarajan, B. Delibas, A. Menzel and W. Seemann, Studies on rate dependent switching effects of piezoelectric materials using a finite element model, *Comput. Mater. Sci.*, 2005, available online.

[2] A. Arockiarajan, B. Delibas, A. Menzel and W. Seemann, Micromechanical modeling of switching effects in piezoelectric materials – a robust coupled finite element approach, submitted for publ.

Modeling of non-classical thermoelasticity

Swantje Bargmann, Paul Steinmann

Due to experimental observations of thermal waves in solids non-classical theories of thermoelasticity were developed in recent years. A very promising theory was developed by Green and Naghdi. The classcial theory (type I) is fully embedded in their approach. An outstanding property of their thermal theory of type II besides the modeling of thermal wave propagation at finite speed is that it conserves energy. We investigate type III, a combination of type I and II, as well. The natural extension of a rigid heat conductor leads to deformable elastic continua. Consequently each of the three heat equations is coupled with the balance of momentum. We suggest a discretization based on Galerkin finite elements for the spatial as well as for the temporal discretization of the equations. The linear theory of thermoelasticity is applied to an isotropic and homogeneous elastic-deformable continuum.

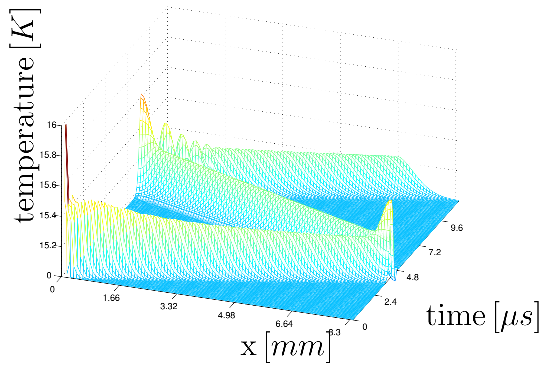


Figure 1: Stabilized heat flow in NaF according to type II. Undamped wave propagation according to dissipationless theory is acknowledged.

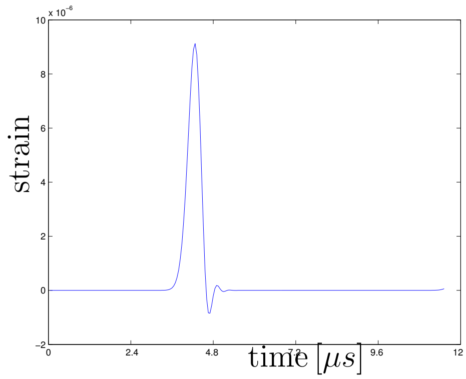


Figure 2: Strain vs. time at the right end of the bar ($x = 8.3$mm), type II.

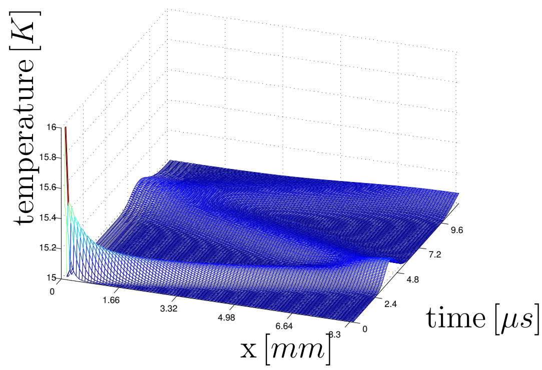


Figure 3: Heat flow in NaF according to type III. Energy dissipation is permitted. The model is stable, consequently, no stabilization is necessary.

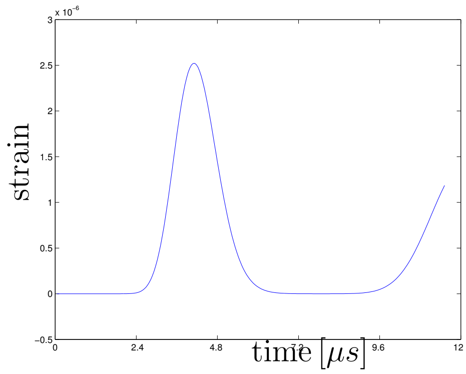


Figure 4: Strain vs. time at the right end of the bar ($x = 8.3$mm), type III.

Interaction of process and machine during high–performance–grinding

Robin Ching, Andreas Menzel, Paul Steinmann

This research project is a joint co-operation with the Institute of Manufacturing Engineering and Production Management (FBK) at the University of Kaiserslautern. The main goal of the entire project is to develop a comprehensive simulation tool that accounts for both, the grinding process and the influence of the grinding machine. The modelling of the grinding process itself is thereby performed with the help of a so–called kinematic simulation (KSIM). This tool is embedded into a finite element formulation (FEM) which enables the incorporation of essential machine properties. As a key modelling concept, the KSIM delivers a force signal (F or T) which serves as input for the FEM. Based on this, the FEM recomputes representative displacements (δ) which act as a new input signal for the KSIM. This iteration technique is repeated until specific stop criteria are satisfied and in general allows interpretation as a staggered algorithm, compare figures 1 and 2. Apart from focusing on efficient implementation strategies, future research will also place emphasis on the comparison on simulation results with experimental data to validate the proposed model.

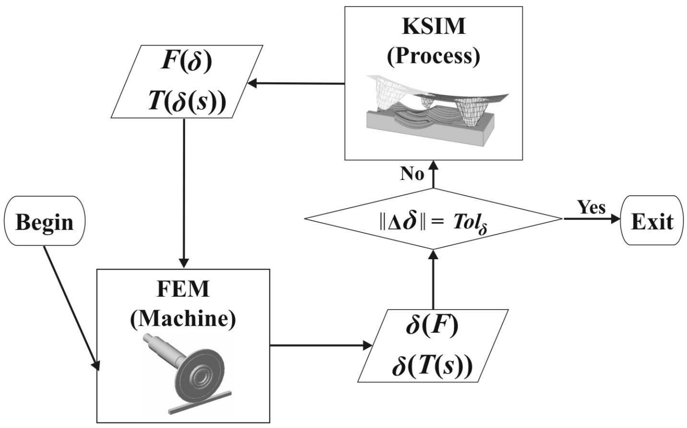


Figure 1: Flow chart of the proposed staggered algorithm – starting with FEM.

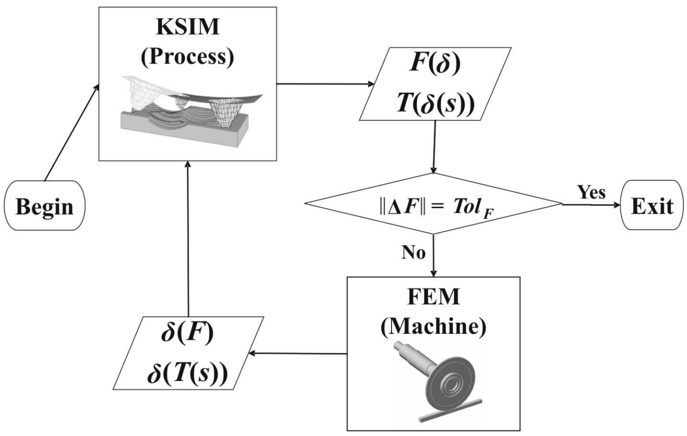


Figure 2: Flow chart of the proposed staggered algorithm – starting with KSIM.

References

[1] P. Herzenstiel, C.Y. Ching, S. Ricker, A. Menzel, P. Steinmann, and J.C. Aurich. Interaction of process and machine during high performance grinding – towards a comprehensive simulation concept. submitted for publication, 2005.

Meshless Methods in Engineering Computations

Alexandru Constantiniu, Paul Steinmann

Trying to overcome some of the FEMs drawbacks, numerous meshless methods have been developed in the last years.
Continuing the work of closing the bridge between classical FEM and standard meshless methods, a novel meshless finite element method is proposed.

Adaptive Delaunay Tessellation

Mesh generation algorithm.

- Generate arbitrary distributed nodes in the domain
- Build a Delaunay tesselation
- Check the relative position of each circumcenter of a polytope
- Create extended polytopes by uniting the initial ones

A unique mixture of polytopes is obtained, adapted to the distributed nodes. The computation time is bounded and bad-shaped elements are avoided.

Rational Barycentric Coordinates

A new intuitive geometric interpretation of barycentric coordinates was recently presented. It computes rational coordinates of minimal degree and combines simplicity with computational convenience.
Properties.

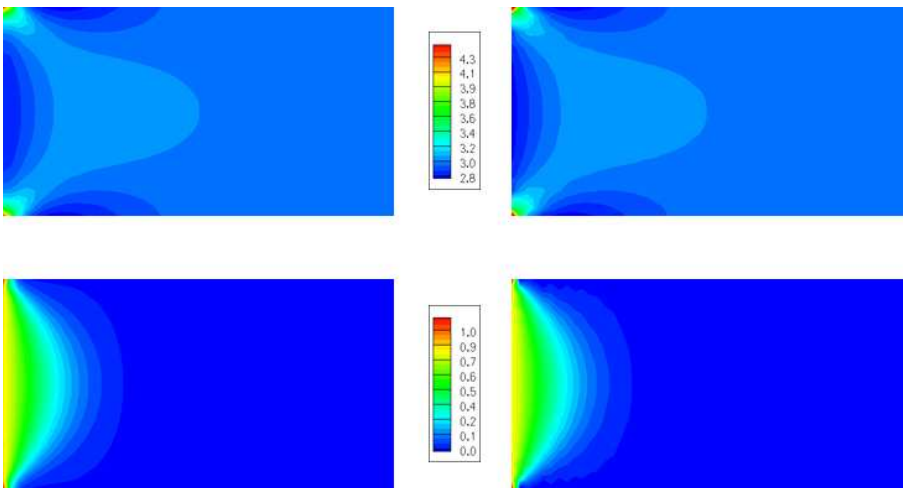
- are non-negative for all x in P
- form a partition of unity
- have linear precision
- are smooth in x
- restricting the coordinates to one facet of P yields the same coordinates as defining them directly on the facet

Stabilized Nodal Integration

Numerical integration is performed as the sum of integrals over the representative area around the nodes. Strains are smoothed at the nodal points via a spatial averaging. A boundary integration of a representative nodal domain is required for computing the smoothed gradient matrix elements and a two-point trapezoidal rule is used for each boundary segment.

Numerical results

We consider a thin rectangular plate subjected to a uniformly distributed load and compare the results with FEM.

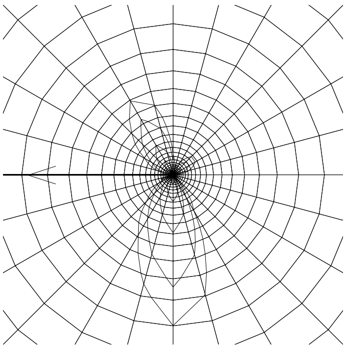


Material forces in computational single-slip crystal-plasticity

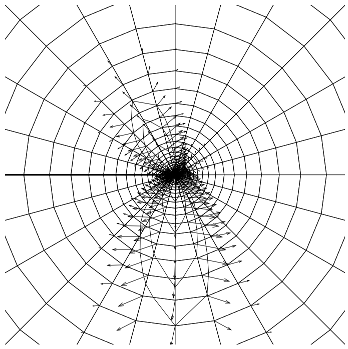
Ralf Denzer, Andreas Menzel, Paul Steinmann

In this contribution we elaborate the material force method with application to standard dissipative materials, in particular crystal-(elasto)plasticity. It thereby turns out that material heterogeneities caused by the gradient of the corresponding slip parameters induce additional material volume forces. As a result, we observe that these forces contribute to computations of typical boundary value problems as e.g. the calculations of the J-integral in fracture mechanics. Their impact on numerical results is discussed by means of a straight traction free crack under mode I loading conditions whereby, special emphasis is placed on different orientations of the underlying crystalline microstructure.

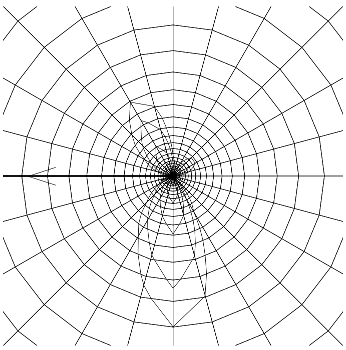
For one orientation of a single slip system which is defined by an angle $\alpha = 15°$ relative to the crack faces the resulting discrete material forces and the hardening parameter κ are depict below. The discrete material surface forces F^h_{sur} consists of a volume part F^h_{vol} and a internal part F^h_{int}.



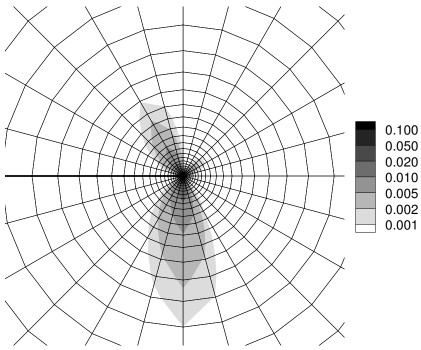
$F^h_{int} \times 0.5$



$F^h_{vol} \times 0.5$



$F^h_{sur} \times 0.5$



κ

References

[1] A. Menzel, R. Denzer, P. Steinmann. Material forces in computational single-slip crystal-plasticity. *Comp. Mat. Sci.*, **32**(2005), 446-454.

Horizontal Coupling in Continuum-Atomistics

Aitor Elizondo, Paul Steinmann

The main objective of this work is to present a new multi–scale algorithm to investigate the mechanical behavior of a monoatomic solid for different cases of deformation, combining a mixed continuum–atomistic aproach. The basic idea is that the simulation focused exclusively on atomistic level is restricted, due to computational costs, only in a small critical regions of a structure where it is necessary, as near defects such vacancies, dislocations, cracks, while continuum aproach is used to describe deformation away from the complex behavior. On the one hand, molecular dynamics method is applied as atomistic framework. It is a numerical simulation technique where the time evolution of a set of atoms are followed in order to describe physical and mechanical properties. On the other hand, finite element method is applied as continuum technique based on the so–called Cauchy–Born rule, which provides an elegant formulation for linking the deformation between continuum and atomistic models.

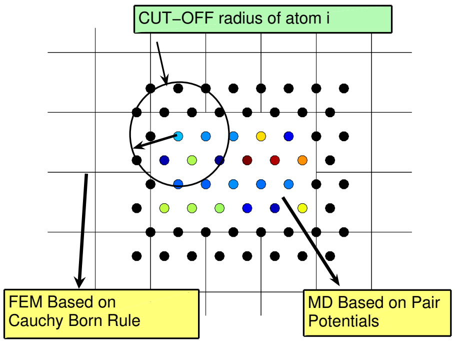


Fig. 1. Coupling between molecular dynamics and finite element method.

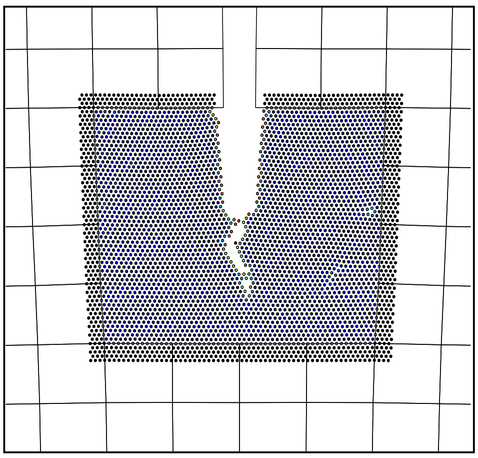


Fig. 2. Eaxample of application of the coupling method.

Modeling and simulation of polymeric materials

Paul Fischer, Ellen Kuhl

Polymer chains have many conformations of nearly equal energy. Perturbing the chains away from their equilibrium conformations typically generates entropic forces that oppose these perturbations. This is the basis for entropy based elasticity. Since the number of different configurations which a long chain molecule may assume is very large, the treatment of each of them individually would be a complex, maybe even unmanagable, task. Long chain molecules are thus commonly described by statistical mechanics, a concept which was originally developed in the context of entropic rubber elasticity.

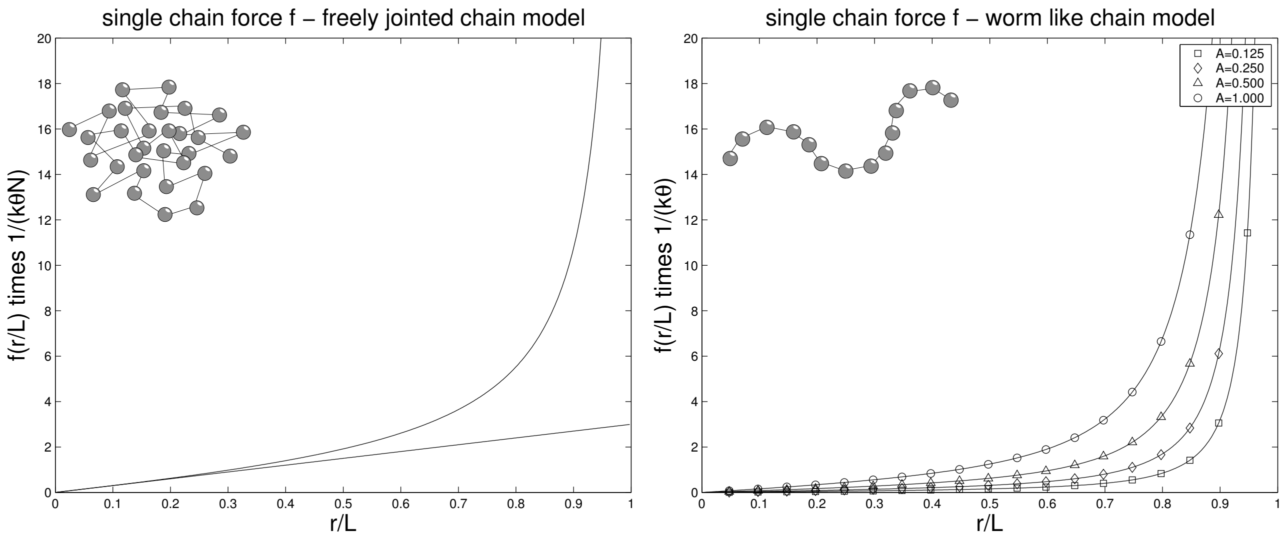


Figure 1: Force elongation response of the freely jointed chain and the wormlike chain model

Figure 1, left, depicts the force elongation behavior of a Gaussian and an inverse Langevin freely jointed chain. The two curves clearly monitor the deviation of Gaussian and the inverse Langevin statistics in the large strain regime, for which the linear force elongation behavior of Gaussian statistics is no longer appropriate. The inverse Langevin freely jointed chain model, however, nicely captures the characteristic locking behavior as the chain approaches its full extension. Figure 1, right, displays the force elongation response of the so-called wormlike chain model, a model which has been used preferably in the context of biomechanics. The wormlike chain model offers the additional freedom of a second parameter, the persistence length, which can obviously be used to fit the shape of the force elongation curve appropriately.
From the standpoint of polymer structures, rubber consists of a complex three-dimensional network of polymer chains laterally attached to one another at occasional points along their lengths. To account not only for the behavior of the individual chains as such, but also for the characteristic cross-link effects of the network structure, a number of different chain network models have been proposed over the past. The main goal of this project is the systematic elaboration and comparison of different individual chain models in combination with appropriate chain network models to simulate the behavior of polymeric structures.

References

[1] E. Kuhl, K. Garikipati, E.M. Arruda, K. Grosh. Remodeling of biological tissue: Mechanically induced reorientation of a transversely isotropic chain network. *J. Mech. Phys. Solids*, Vol. 53, pp. 1552–1573, 2005.

On Material Forces within the Extended Finite Element Method

Jürgen Glaser, Paul Steinmann

The combination of the Material Force Method (MFM), leading to a singular material force at the crack tip which is interpreted as the driving force for crack propagation and the Extended Finite Element Method (X-FEM) which allows the modelling of a discontinuity independently from the FE mesh forms an elegant tool to assess fracture mechanics problems.
The X-FEM models a discontinuity by the introduction of discontinuous shape functions $\overline{N}^j$ and additional nodal degrees of freedom (DOFs) such that the introduction of the MFM within the framework of the X-FEM leads to two types of discrete material node point forces, those at standard (eq. 1) and those at enriched DOFs (eq. 2).

$$\mathfrak{F}_h^{sur,I} =: \mathbf{A}_{e=1}^{n_{el}} \int_{\mathcal{B}_0^e} \Sigma^t \cdot \nabla_X N^i dV \tag{1}$$

$$\overline{\mathfrak{F}}_h^{sur,J} =: \mathbf{A}_{e=1}^{n_{el}} \int_{\mathcal{B}_0^e} \Sigma^t \cdot \nabla_X \overline{N}^j dV \tag{2}$$

In the sense of an energetic pairing the discrete resulting material (surface) force at standard DOFs $\mathfrak{F}_h^{sur,J}$ acting on the crack tip, which is closely related to the J-integral of fracture mechanics, describes the tendency of a crack to change its lenght, i.e. to propagate (figure 1). The amount of that force, which is the same in classical FEM, is equal to the J-integral. A corresponding energetic pairing for the material forces stemming from the enriched DOFs $\overline{\mathfrak{F}}_h^{sur,J}$ has to connect these additional forces to a variation of the material enriched DOFs. The nature of these additional material forces still has to be discussed in detail.

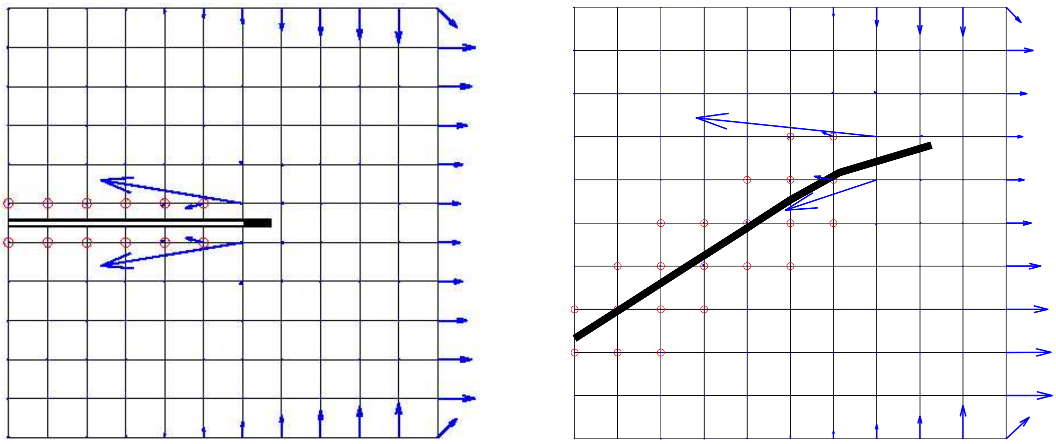


Figure 1: Material forces at standard DOFs $\mathfrak{F}_h^{sur}$ with corresponding virtual crack propagation for crack under 0° and 30° respectively

For the X-FEM the total nodal displacements are formed by a sum of the calculated standard and enriched DOFs in the sense of the X-FEM approximation . For the so calculated displacements as well as for the material forces at standard DOFs $\mathfrak{F}^{sur,I}$ and especially for the J-integral we find a good coincidence with the results of a standard FEM approximation with a mesh adapted to the crack geometry. In comparison to standard FEM, where a singular material standard force $\mathfrak{F}^{sur,I}$ is located at a node at the crack tip, the X-FEM produces distributed material forces on the nodes around the crack tip. Figure 1 shows an example of the material standard forces $\mathfrak{F}^{sur,I}$ for a crack under 0° and 30° respectively as well as the directions of crack propagation predicted by the resulting material force vectors at the crack tip. For quasi-static crack growth the above described method calculates suitable crack paths.

Theory and Implementation of Time-Dependent Fibre Reorientation in Transversely Isotropic Materials

Grieta Himpel, Andreas Menzel, Ellen Kuhl, Paul Steinmann

Transversely isotropic materials are commonly described by one characteristic direction $\boldsymbol{n}^A$in the material configuration, which generally is assumed to be constant. However for some applications it makes sense to consider a reorientation of the characteristic direction, as for instance the orientation of biological materials adapts to the mechanical loading, see e.g. [1]. Other examples are piezoelectric materials, which change their electric polarisation due to an electric or mechanical loading, as described in [2], and liquid crystals changing their orientation on account of an electric field, see [3]. Furthermore simulations with a reorientation of the characteristic direction can be used in the context of optimisation of composites. In this contribution we restrict ourselves to the modelling of hyper-elasticity and assume a time dependent reorientation of the characteristic direction due to the maximum principal strain direction $\boldsymbol{n}_3^C$, see for instance [4]. Thereby we concentrate on the numerical implementation into a finite element code. The example in figure 1 shows a transverse isotropic strip unter tension with (a) fixed and (b) reorientating characteristic direction under constant displacement loading.

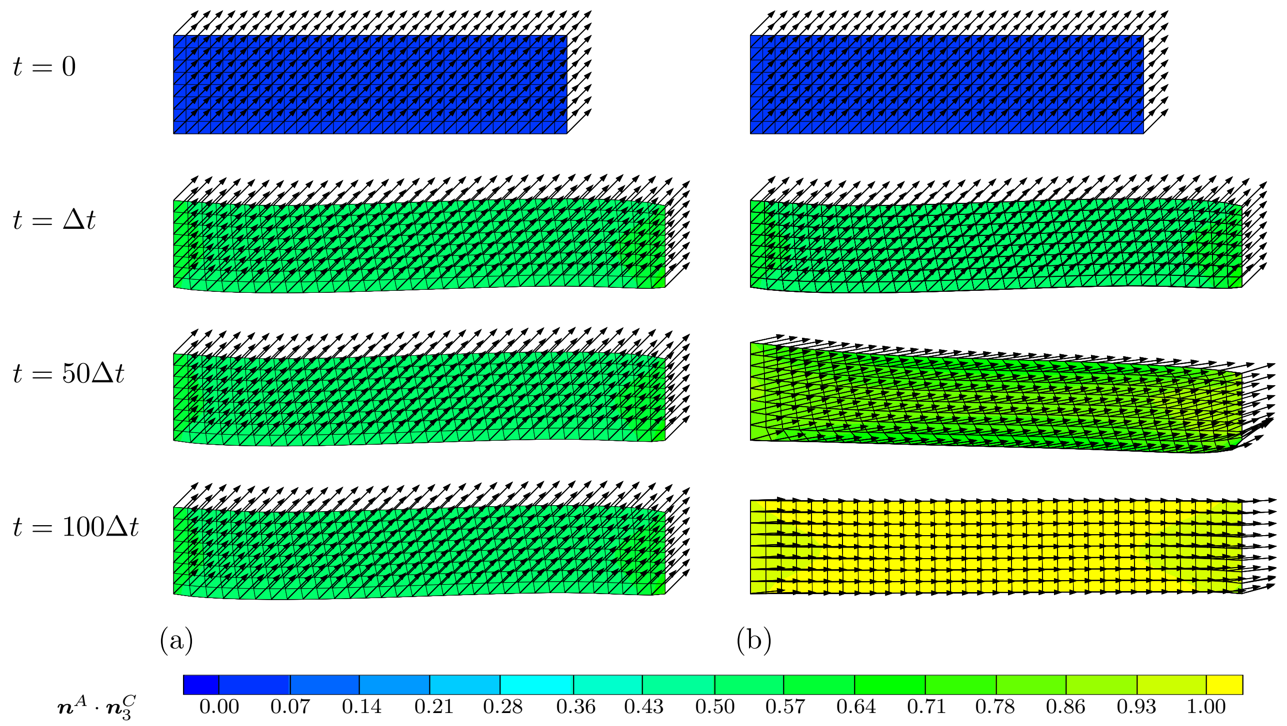


Figure 1: Transverse isotropic strip under tension. (a) Fixed fibre direction. (b) Reorientation.

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[1] E. Kuhl, K. Garikipati, E.M. Arruda, K. Grosh 'Remodeling of biological tissue: Mechanically induced reorientation of a transversely isotropic chain network', *Journal of the Mechanics and Physics of Solids* **53**:1552–1573, 2005.

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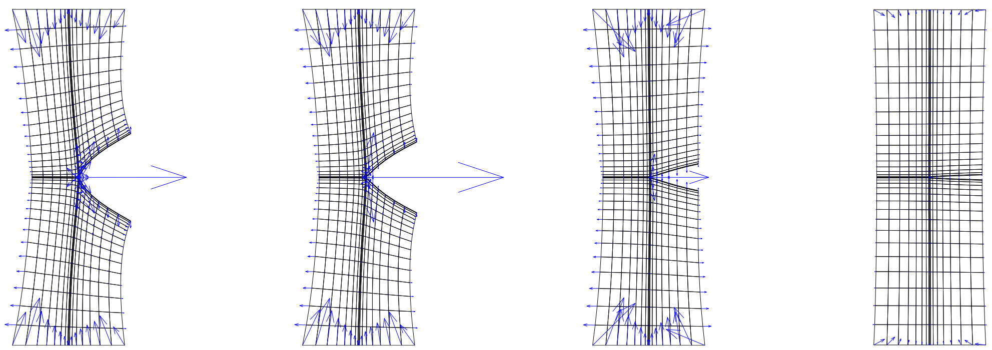
Computational Micromorphic Continua
– A Configurational Mechanics Perspective –

C. Britta Hirschberger, Ellen Kuhl, Paul Steinmann

In contrast to classical – or rather local – continuum mechanics theories, in non-local continua the behaviour of a material point is not only influenced by the point itself but also by its vicinity. Such a non-locality may for instance enter as micro-continua being inherent at each physical point of the macro-continuum and being allowed to undergo independent deformations. In the *micromorphic continuum theory* (see e. g. [1], [2]) the deformations of the micro-continuum are assumed to be affine and the size of the micro-continuum introduces a scale-dependence into the theory. In the kinematical descriptions we distinguish between the macro- and the micro-deformations: Particularly, the macro-continuum kinematics is described by a macro map and a macro tangent map, whereas the affine micro mapping is described by a micro-deformation map and its gradient with respect to macro coordinates which represents a third-order tensor providing a link between the two scales. Energy and balance considerations lead to the definition of stress quantities being conjugate to the aforementioned kinematics. In the present work both stress and deformation quantities as well as the balance relations are viewed from a configurational-mechanics perspective, i. e. different stress formats are obtained, including Eshelby-type stresses which exclusively act on the material manifold. This allows for the application of the material force method [3] which is anticipated to give an insight into the behaviour at inhomogeneities. Upon constitutive assumptions for the macro- and micro-continuum, finite-element approximations are derived. As one example a cracked specimen has been numerically investigated with respect to its behaviour at different characteristic micro-continuum sizes and modifications in the constitutive parameters. Figure 1 displays the discrete material forces evaluated at the finite-element nodes. **References**



$l = L_0/\infty$ $l = L_0/20$ $l = L_0/5$ $l = L_0/1.25$

Figure 1: Cracked specimen under uni-axial tension: Longitudinal Cauchy-type macro-stress at variation of the characteristic size of the micro-continuum

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Modelling and Simulation of Polymer Interphases

Mokarram Hossain, Ralf Denzer, Gunnar Possart, Paul Steinmann

Nowadays, adhesives have many commercial and engineering applications. The adhesive forms a tiny boundary layer near to the adherent [Fig. 1]. Due to this layer the bonding behaviour of the adhesive throughout the whole region between adhesive and adherent is not homogeneous. Therefore, these interphases between adhesive and adherent require special attention. In this investigation, we will model the interphases between adhesive and adherent.
Non-linear models for polymeric material have to be implemented and extended since the distribution of material parameters depends on the distance from the substrate. Simulation results should be compared to experimental data that will be obtained by other research groups.

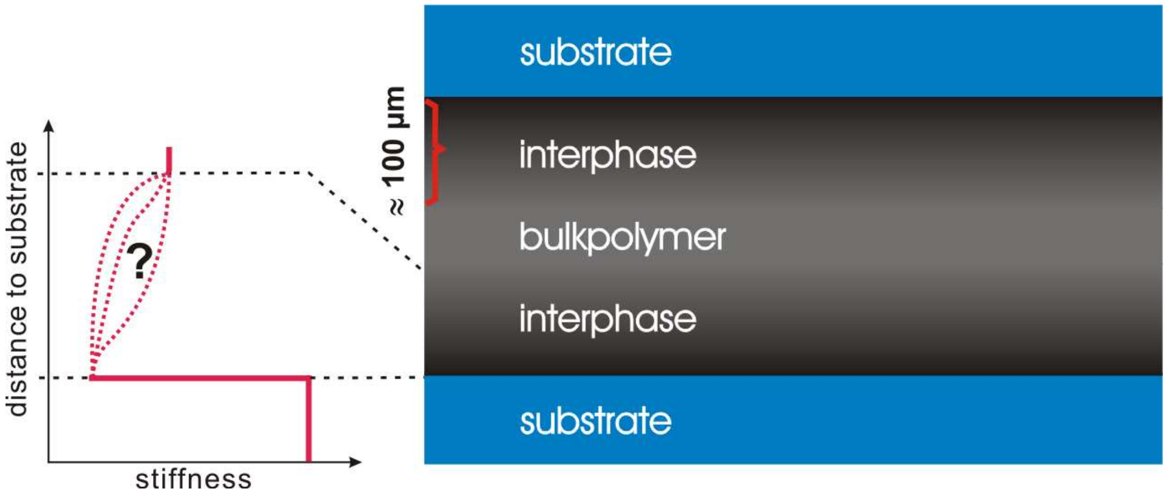

Figure 1: Different layers in adhesive bondings

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New discretization methods for the simulation of cracks in engineering materials

Philippe Jäger, Julia Mergheim, Ellen Kuhl, Paul Steinmann

Strong and weak discontiniuties can appear in different fields of mechanics. Some obvious examples where strong discontinuities arise are stationary and propagating cracks. The objective of this work is to expand the geometrically nonlinear approach for a mesh independent finite framework for the modelling of stationary and propagating cracks [3] on three dimensional continua. By essentially doubling the degrees of freedom in the discontinuous elements, this algorithm allows for arbitrary strong discontinuities which are not restricted to inter-element boundaries. The deformation field is interpolated independently on both sides of the discontinuity according to [1]. Therefore the weak formulation contains an additional term due to the cohesive tractions.

$$\int\limits_{\mathcal{S}^+\cap\mathcal{S}^-} \delta\boldsymbol{\epsilon} : \boldsymbol{\sigma} \, dV + \underbrace{\int\limits_{\overline{\gamma}} [\![\delta\boldsymbol{u}]\!] \cdot \boldsymbol{t}([\![\boldsymbol{u}]\!]) \, dA}_{\text{internal cohesive work}} = \int\limits_{\partial S_t} \delta\boldsymbol{u} \cdot \boldsymbol{t} \, dA$$

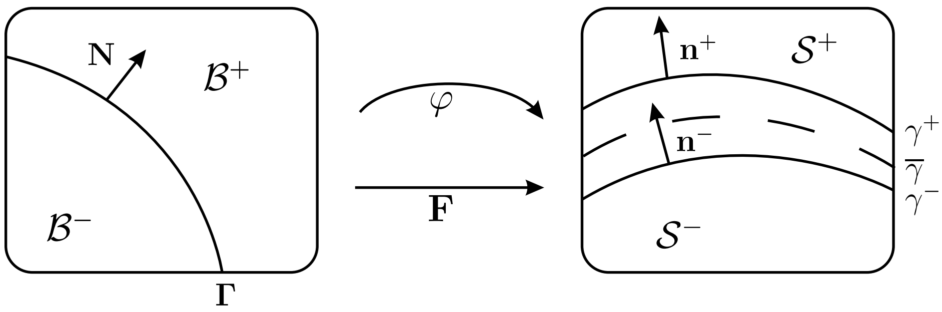

Figure 1: Strong discontinuity kinematics

Rather than following the classical X-FEM approach and introducing jumps in the deformation field as additional unknowns, this formulation is based exclusively on deformation degrees of freedom. While the X-FEM requires additional transition elements, the modifications are strictly local here and only affect the discontinuous elements themselves, see [2].

References

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Macromechanical modeling of microstructured continua: towards computational extended continuum mechanics

Nina Kirchner, Paul Steinmann

The multitude of extended continnum theories describing microstructured media motivates the question whether there exists a generic framework that contains a "hierarchy" of competing model approaches. With such hierarchy at hand, it is easy to detect possible structural similarities of different models/theories, while these might be disguised if such models are treated isolated from each other. The similarities, in turn, can be exploited when deriving algorithms for a broad class of microstructured materials. Thus, considerable attention has within this project been focused on the identification of the relative positions of two representatives of extended continuum theories based on the introduction of structural variables (namely micromorphic continuum formulations and continuum theories for materials of grade N, encompassing in particular so-called gradient continua) in a unified framework given by variational principles, see [1].

The theoretical analysis reveals that threedimensional inelastic behavior of gradient as well as micromorphic materials subject to finite strains can be treated efficiently by the same numerical algorithms.Demonstrating applicability at an early stage, a microstretch continuum theory is used in strain softening plasticity, while fracture mechanics problems are tackled by employing a material force method for gradient continua.

Modeling microstretch materials (which constitute a subclass of micromorphic continua as an isotropically deforming vector triad is attached to each point to describe the microstructure) by means of a variational formulation is expected to initiate an increasing use of microstretch theories and corresponding numerical methods in engineering: the majority of articles dealing with microstretch continua published from the 1990s on is primarily written in a mathematical spirit and utilizes the balance equations of microstretch materials as derived in [2] (by considering invariance properties of a modified energy balance) as a starting point. Moreover, the mathematical analysis of microstretch solids is at present restricted to the static case and linear elastic bodies in an infinitesimal theory.

In the variational setting the constitutive quantities arising for microstretch materials are given in terms of derivatives of the stored energy - prescribing its explicit form thus allows us to specify constitutive material behavior. We have accounted for inelastic material behavior by formulating an associative, deviatoric elastoplastic theory for the geometrically linear case. Integrating the stress–strain relations by means of an unconditionally stable, fully implicit Euler backward scheme, a standard radial return algorithm can be applied for a particular choice of parameters which seems admissible as long as no further benchmarks or material parameter sets for real materials are available. In general, however, an implementation of plastic material behavior of microstretch materials requires a generalization of the classical radial return algorithm due to the occurrence of a parameter set which weights the influence of microstructural quantities on the yield function.

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Parameter identification for the finite element analysis of rubber like polymers

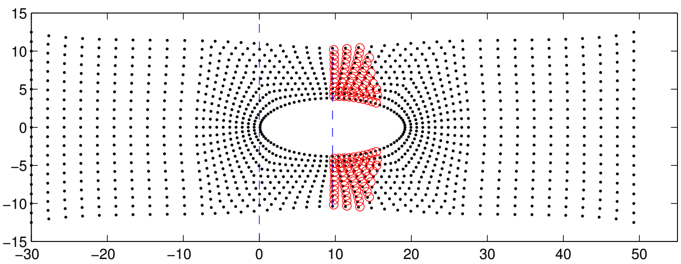
Bernd Kleuter, Paul Steinmann

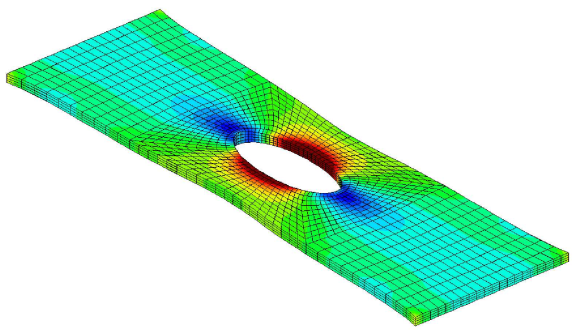
Viscoelastic materials like elastomers are applied in various fields of civil and mechanical engineering. This work is concerned with parameter identification for a finite viscoelastic constitutive law for different materials. The direct problem within the finite element method and its integration method were focused first. It is a finite viscoelastic constitutive law in principal directions which is based on the multiplicative decomposition of the deformation gradient into elastic and viscous parts. For the inverse problem the identification algorithm and the associated sensitivity analysis needed to analyze inhomogenous displacement fields were considered. A gradient based optimization algorithm, the Levenberg Marquardt method, is applied for a least squares type objective function. Then different laboratory tests for a polyurethane adhesive were made together with D. Vogt and P. Geiss [1] and tests for a polyurethane foam and filled rubber like polymers were made together with M. Bosseler and R. Renz [2]. In these different cyclic and quasistatic tensile and pressure tests digital image correlation in 3d was used as field measurement technique. The measured non-uniform displacement fields were interpolated on the coordinates of the so called identification nodes of the associated FE-Models. In the following identification procedure generality for the identified 7 material parameters for different load cases had to be established. So all different tests were considered in one least squares sum for each different material. For the identification the forces in the tests and the force loads in the FE calculation were the same. The least squares sum of the experimental displacements and the FE displacements at the identification nodes were minimized by varying the material parameters. The results for a polyurethane adhesive relaxation test are depicted below.

End of iteration with optimal material parameters:

μ^{eq} [MPa]	α^{eq}	μ^{neq} [MPa]	α^{neq}	k^{eq} [MPa]	k^{neq} [MPa]	τ [s]
0.317966	2.32189	1.14988	1.29458	2.03756	0.888432	2.17529

Interpolated measured displacements (red) over the nodes of the simulation for the load 40 (120s-end of test).





[1]Work Group for Materials and Surface Technology (AWOK), TU Kaiserslautern
[2]Lehrstuhl für Ressourcengerechte Produktentwicklung (RPE), TU Kaiserslautern

Computational modeling of phase separation

Ellen Kuhl, Daniel W. Schmid

Most rocks and minerals found at or near the earth surface have a complex history and were formed at completely different pressure and temperature conditions than those that prevail at the surface of our planet. Minerals that form solid solutions may, under certain conditions, adjust to the lowered temperatures by unmixing or exsolution. The patterns and chemical compositions of mineral exsolution and symplectites potentially contain crucial information for the reconstruction of the geological history of an outcrop or region, see figure 1, left.

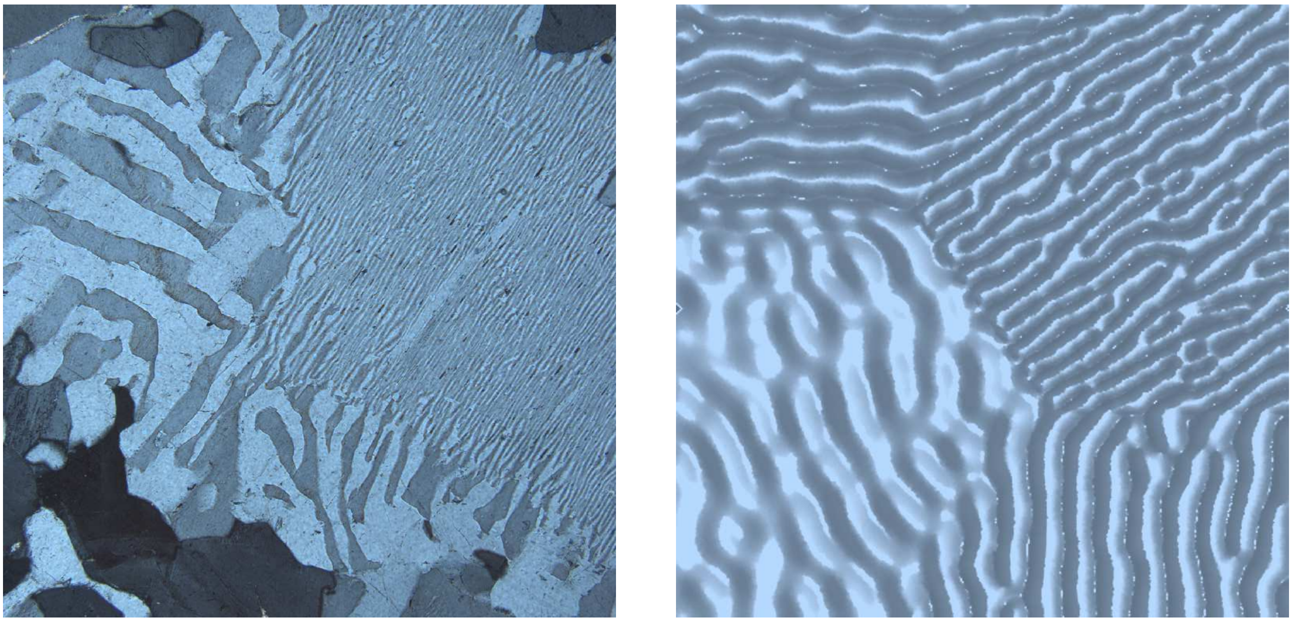


Figure 1: Left: Example of mineral exsolution: Alkali-feldspar unmixing in perthite – Right: Numerical simulation based on anisotropic fourth order diffusion

Within this project, a new finite element based simulation technique for mineral growth governed by the classical Cahn-Hilliard equation has been derived. The particular format of the underlying Flory-Huggins free energy for non-ideal mixtures is characterized through a double-well potential. In contrast to the traditional Fickian diffusion, it allows for uphill diffusion driven by gradients in the chemical potential rather than by gradients of the concentration field itself. The Flory-Huggins free energy alone provides the adequate framework for spinodal decomposition in non-ideal mixtures, however, it is not able to describe the process of phase separation appropriately. To this end, the free energy is supplemented by an additional surface energy term introducing fourth order gradients of the concentration field. For the finite element discretization, the governing fourth order diffusion equation is reformulated in terms of a system of two coupled second order equations. The basic features of the Cahn-Hilliard equation are elaborated by means of selected geologically relevant examples. In particular, isotropic and anisotropic mineral growth, as depicted in figure 1, right, and symplectite formation are studied and the long term response in the sense of Ostwald ripening is elaborated.

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The discrete null space method for flexible multibody dynamics

Sigrid Leyendecker, Peter Betsch, Paul Steinmann

The modeling of flexible multibody systems in nonlinear structural dynamics as finite dimensional Hamiltonian system subject to holonomic constraints constitutes a general framework for a unified treatment of rigid and elastic components. Internal constraints, which are associated with the kinematic assumptions of the underlying continuous theory, as well as external constraints, representing the interconnection of different bodies by joints, can be accounted for in a likewise systematic way.
The discrete null space method developed in [1] provides an energy-momentum conserving integration scheme for the DAEs of the motion of the constrained mechanical system. The resulting reduced time stepping scheme performs advantageously concerning different aspects: the constraints are fulfilled exactly, the condition number of the iteration matrix during the iterative solution procedure is independent of the time step and the dimension of the system of nonlinear equations is reduced to the minimal possible number saving computational costs. The discrete null space method can be applied efficiently to open kinematic chains as well as to closed loop systems [2]. The multibody system under consideration is a three dimensional slider–crank mechanism. Fig. 1 shows a series of the motion and deformation during the first and second revolution coloured by the norm of the resulting bending moments and forces.

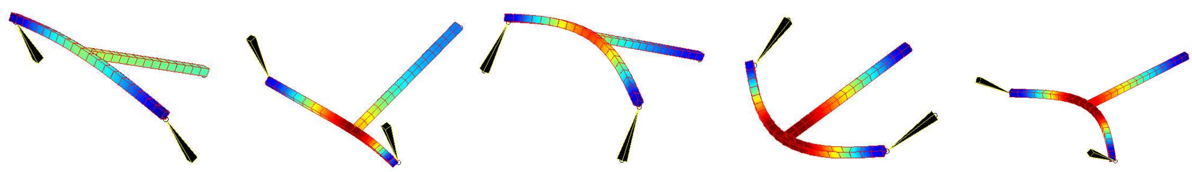

Figure 1: Motion and deformation of the spatial slider–crank mechanism.

Table 1 summarises the simulations using the constrained scheme and the D'Alembert–type scheme with nodal reparametrisation deduced by the discrete null space method. Both schemes fulfil the constraints exactly. Using the time step $\Delta t = 0.01$, the condition numbers differ by six orders of magnitude. A remarkable difference is in the dimensions of the systems of equations of motion, what has a big impact on the numerical costs.

scheme	constraint fulfilment	condition number	$\sharp$ unknowns	CPU–time
constrained	exact	$\mathcal{O}(10^{10})$	722	2.3
D'Alembert–type, rep.	exact	$\mathcal{O}(10^{4})$	214	1

Table 1: Comparison of the simulations using different schemes.

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Failure of granular materials at different scales

Holger Meier, Ellen Kuhl, Paul Steinmann

In recent years there has been an increase in interest in granular and discontinuous media. We apply a computational homogenization method in order to complete the task of modelling this kind of media in three dimensions.
Two scales are to be considered (see Figure 1): First, the macro scale assuming continuous media. Second, the micro scale which represents granular and discontinuous media, see e.g. Miehe and Dettmar [3]. The finite element method is applied on the macro scale. Three dimensional discrete elements are employed on the micro scale. On the micro level a boundary value problem is considered which is driven by the macro scale deformation gradient. Static condensation of the micro scale stiffness matrix and the use of the averaging theorems [1] are utilized to obtain the macro scale constitutive operator [2].

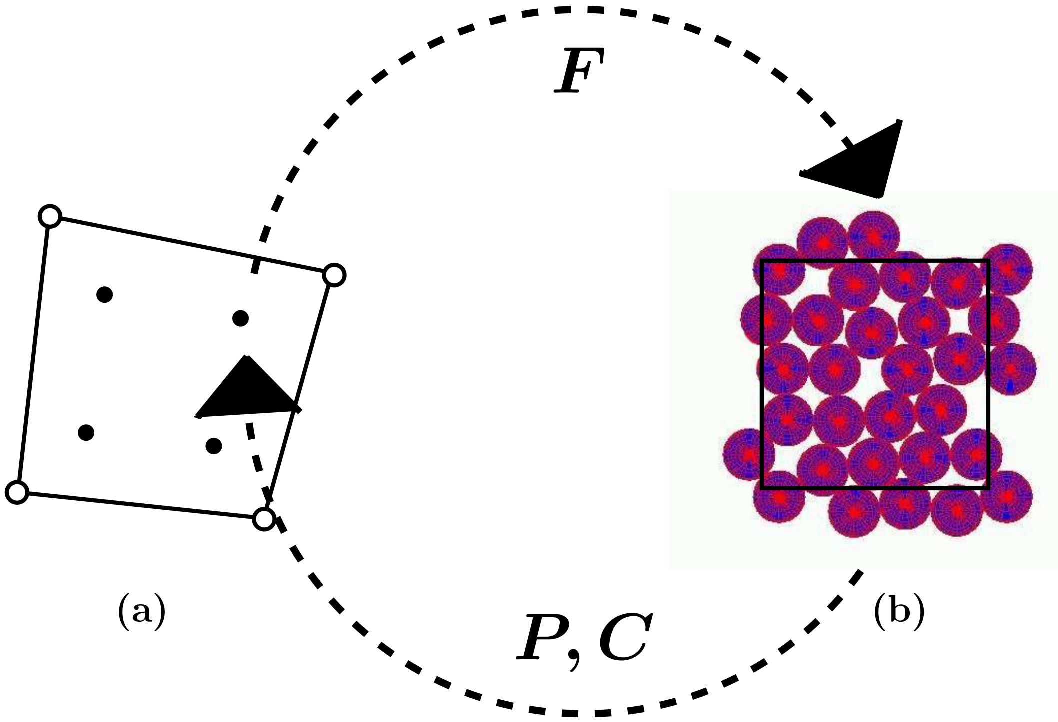

Figure 1: 2D micro-macro transition: (a) standard finite element on the macro level. (b) discontinuous granular representative volume element on the micro level. The mircostructure (b) is driven by the macroscopic deformation gradient tensor $\boldsymbol{F}$ and returns the macroscopic first Piola Kirchhoff stress $\boldsymbol{P}$ as well as the macroscopic constitutive operator $\boldsymbol{C}$. The Hill-Mandel condition [1] is used.

References

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Generalised strain measures for finite inelasticity

Andreas Menzel

The application of different stretch representations and strain measures within nonlinear continuum mechanics has been under discussion for several decades. General pushforward and pullback transformations of such strain measures to different configurations in the context of for example multiplicative elastoplasticity are of particular interest for efficient numerical algorithms and computational applications.

As a key kinematic feature for the subsequent elaborations, we accept the nowadays well–established multiplicative decomposition of the deformation gradient, $\boldsymbol{F} \doteq \boldsymbol{F}_{\rm e} \cdot \boldsymbol{F}_{\rm p}$ with $\boldsymbol{F}_{\rm e} = \boldsymbol{R}_{\rm e} \cdot \boldsymbol{U}_{\rm e} = \boldsymbol{v}_{\rm e} \cdot \boldsymbol{R}_{\rm e}$, and introduce two Seth–Hill–type (intermediate elastic) strain families

$$\begin{aligned} \boldsymbol{E}_{{\rm e}\,(m)} &= \tfrac{1}{m}\,[\,\boldsymbol{U}_{\rm e}^{m} - \boldsymbol{I}\,] \quad \text{for } m>0\,, & \boldsymbol{E}_{{\rm e}\,(0)} &= \tfrac{1}{2}\ln(\boldsymbol{U}_{\rm e}^{2}) \quad \text{for } m=0\,,\\ \boldsymbol{K}_{{\rm e}\,(m)} &= \tfrac{1}{m}\,[\,\boldsymbol{I} - \boldsymbol{U}_{\rm e}^{-m}\,] \quad \text{for } m>0\,, & \boldsymbol{K}_{{\rm e}\,(0)} &= -\,\tfrac{1}{2}\ln(\boldsymbol{U}_{\rm e}^{-2}) \quad \text{for } m=0\,. \end{aligned}$$

Apart from further material representations, we additionally establish the following (spatial elastic) generalised strain measures

$$\begin{aligned} \boldsymbol{e}_{{\rm e}\,(m)} &= \tfrac{1}{m}\,[\,\boldsymbol{I} - \boldsymbol{v}_{\rm e}^{-m}\,] \quad \text{for } m>0\,, & \boldsymbol{e}_{{\rm e}\,(0)} &= -\,\tfrac{1}{2}\ln(\boldsymbol{v}_{\rm e}^{-2}) \quad \text{for } m=0\,,\\ \boldsymbol{k}_{{\rm e}\,(m)} &= \tfrac{1}{m}\,[\,\boldsymbol{v}_{\rm e}^{m} - \boldsymbol{I}\,] \quad \text{for } m>0\,, & \boldsymbol{k}_{{\rm e}\,(0)} &= \tfrac{1}{2}\ln(\boldsymbol{v}_{\rm e}^{2}) \quad \text{for } m=0\,. \end{aligned}$$

With these definitions at hand, one easily verifies that for instance $\boldsymbol{E}_{{\rm e}\,(m)}$ and $\boldsymbol{k}_{{\rm e}\,(m)}$ share identical eigenvalues, namely $\boldsymbol{R}_{\rm e} \cdot \boldsymbol{E}_{{\rm e}\,(m)} \cdot \boldsymbol{R}_{\rm e}^{\rm t} = \boldsymbol{k}_{{\rm e}\,(m)}$ as well as $\boldsymbol{R}_{\rm e} \cdot \boldsymbol{K}_{{\rm e}\,(m)} \cdot \boldsymbol{R}_{\rm e}^{\rm t} = \boldsymbol{e}_{{\rm e}\,(m)}$, respectively. The by far more interesting relation, however, consists of the transformation

$$\boldsymbol{F}_{\rm e}^{-\rm t} \cdot \boldsymbol{E}_{{\rm e}\,(m)} \cdot \boldsymbol{F}_{\rm e}^{-1} = \boldsymbol{v}_{\rm e}^{-2} \cdot \boldsymbol{k}_{{\rm e}\,(m)}\,, \qquad \boldsymbol{F}_{\rm e} \cdot \boldsymbol{K}_{{\rm e}\,(m)} \cdot \boldsymbol{F}_{\rm e}^{\rm t} = \boldsymbol{v}_{\rm e}^{2} \cdot \boldsymbol{e}_{{\rm e}\,(m)}\,,$$

which enables us to express the strain energy ψ by means of different sets of arguments. In this regard, let ψ be an isotropic tensor function determined in terms of a representative strain measure and – to capture elastic anisotropy – an additional structural tensor $\boldsymbol{A}_{\rm e}$ or $\boldsymbol{a} = \boldsymbol{F}_{\rm e} \cdot \boldsymbol{A}_{\rm e} \cdot \boldsymbol{F}_{\rm e}^{\rm t}$, respectively. In view of elastoplastic behaviour, ψ allows representation as

$$\psi \doteq \psi(\boldsymbol{E}_{{\rm e}\,(m)}, \boldsymbol{I}, \boldsymbol{A}_{\rm e}) = \psi(\boldsymbol{v}_{\rm e}^{-2} \cdot \boldsymbol{k}_{{\rm e}\,(m)}, \boldsymbol{v}_{\rm e}^{2}, \boldsymbol{a})\,.$$

By assuming $\boldsymbol{A}_{\rm e} \doteq$ const, one obtains a set of five invariants ($j = 1, 2, 3$; $\alpha = 1, 2$), to be specific

$$I_j = \boldsymbol{I} : \boldsymbol{E}^{j}_{{\rm e}\,(m)} = \boldsymbol{I} : \boldsymbol{k}^{j}_{{\rm e}\,(m)}\,, \qquad I_{\alpha+3} = \boldsymbol{I} : [\,\boldsymbol{E}^{\alpha}_{{\rm e}\,(m)} \cdot \boldsymbol{A}_{\rm e}\,] = \boldsymbol{I} : [\,\boldsymbol{v}_{\rm e}^{-2} \cdot \boldsymbol{k}^{\alpha}_{{\rm e}\,(m)} \cdot \boldsymbol{a}\,]\,.$$

Similar investigations can also be applied to related yield functions and directly carry over to the modelling of for example viscoelastic response.

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Towards the algorithmic treatment of 3D strong discontinuities

Julia Mergheim, Ellen Kuhl, Paul Steinmann

Within this project, a geometrically nonlinear finite element framework for the modeling of propagating discontinuities in three dimensional continua is developed. By doubling the degrees of freedom in the discontinuous elements, the algorithm allows for arbitrary discontinuities which are not restricted to inter-element boundaries. The deformation field is interpolated independently on both sides of the discontinuity. On the discontinuity surface, the jump in the deformation is related to the cohesive tractions to account for smooth crack opening. Computational difficulties characteristic of three dimensional crack propagation are addressed. The performance of the method is elaborated by means of the classical peel test in the three-dimensional setting.

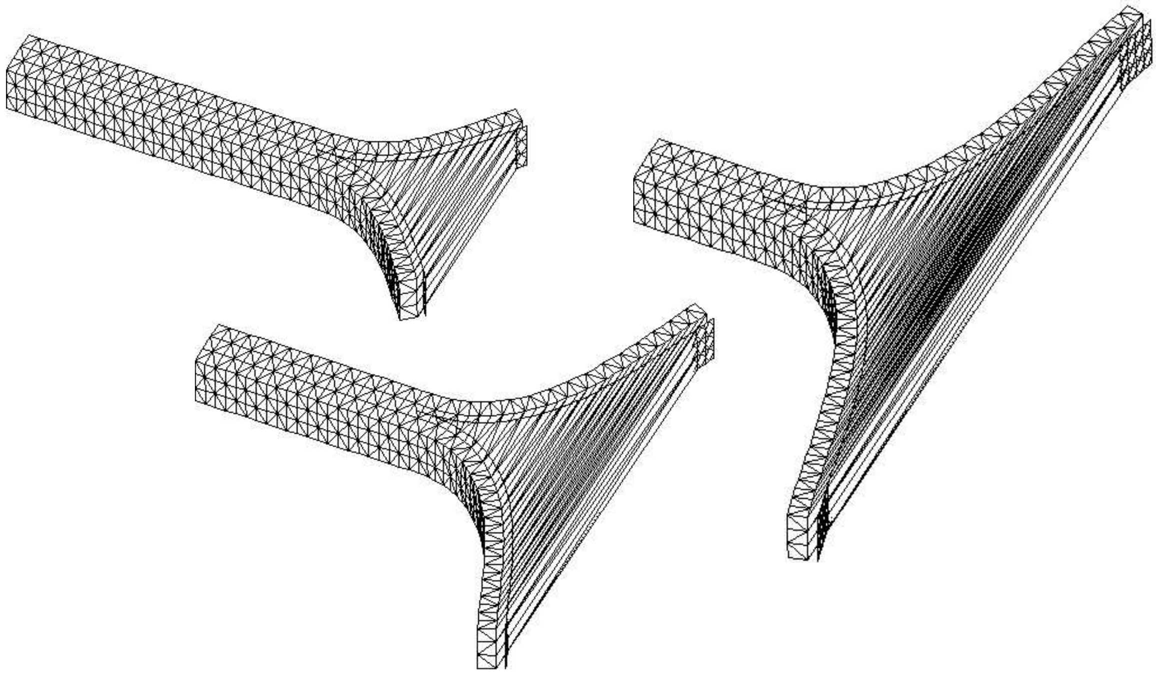

Figure 1: Peel test – Deformation of the structure at different stages of loading

The deformation of the structure at different loading stages is pictured in figure 1. The response is symmetric and the discontinuity propagates along the center line but is obviously not aligned with the element boundaries. While the classical X-FEM requires additional transition elements, our modifications are strictly local and only affect the discontinuous elements themselves. The suggested method is thus believed to be extremely powerful in simulating propagating discontinuities not only in two but also in three dimensional continua. Its extension to non-planar crack propagation is part of current research.

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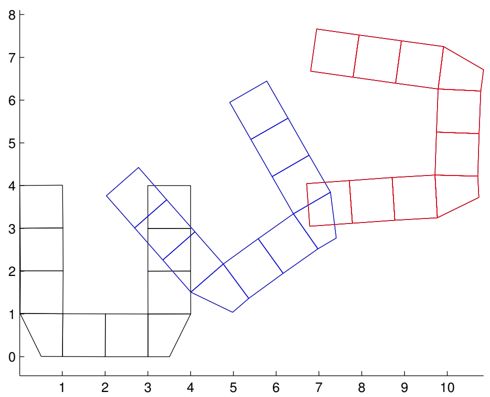
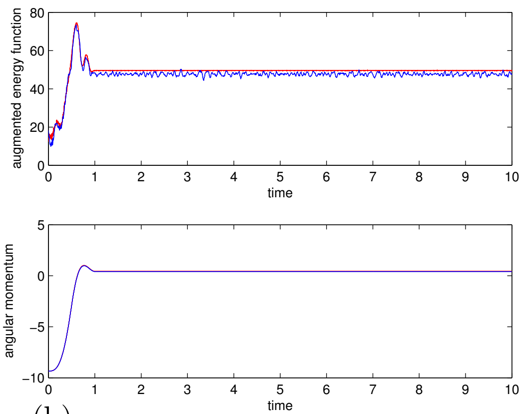
Galerkin-based Time-Stepping Schemes for Geometrically Nonlinear Plastodynamics

Rouven Mohr, Andreas Menzel, Paul Steinmann

Computational modelling often demands the incorporation of dynamic effects. The consideration of computational continuum dynamics requires in particular advanced numerical techniques to satisfy the classical balance laws like balance of linear and angular momentum or the laws of thermodynamics. Energy- and momentum-conserving time integrators are well-established in computational dynamics for the elastic case [1, 2]. Algorithmic conservation of energy and angular momentum have been shown to be closely related to quadrature formulas that were required for the calculation of time integrals. In this contribution we deal with the enhancement of these concepts for geometrically nonlinear plasticity. First, we apply concepts of geometrically nonlinear continuum mechanics and finite elements in space to receive a semidiscrete system of equations of motion based on a Hamiltonian-type formalism. The formulation of finite plasticity adopts a multiplicative decomposition of the deformation gradient in an elastic and a plastic part, see [3]. For the temporal approximation of the semidiscrete system finite elements are used as well.
For the computation of the example we have applied a cG(1)-method in combination with a standard Gauss quadrature rule for the time integrals (mid-point scheme). This example deals with the motion of a Flying-U under plastic deformation, see (a). The resulting conservation properties – the augmented energy function $\widetilde{H} := H + D^{int}$ and the angular momentum $\boldsymbol{L}$ – can be observed in (b).



(a)



(b)

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Constitutive modelling and finite element simulation of cathodic electrodeposition processes

Gunnar Possart, Paul Steinmann, Oliver Kurz, Matthias Schmidt

Cathodic electrodeposition has been used for priming and coating of metallic components for decades and in a large number of industrial applications. Such processes base upon the application of organic coatings from aqueous solutions to conductive substrates. The component to be coated is immersed into the lacquer and a direct current is applied upon which positively charged polymers migrate electrophoretically to the cathode, become insoluble and build an insulating layer of paint. Critical process parameters are not only the duration, progression and amplitude of applied voltage or current but also the conductivity of substrate and dilution, the geometry of the assembly to be coated and possible surface pretreatments.
A constitutive model has been developed and implemented which is able to map the most important effects and dependencies. The coating thickness, for example, depends nonlinearly on the local current density at the surface and is realized by an exponential relation between growth velocity and current density. The coating resistivity is defined also nonlinearly by the growth velocity, i.e. fast growing layers exhibit lower resistivities. This effect is directly related to the porosity of the deposited layer and significantly affects mechanical behavior and long term durability of the coating.

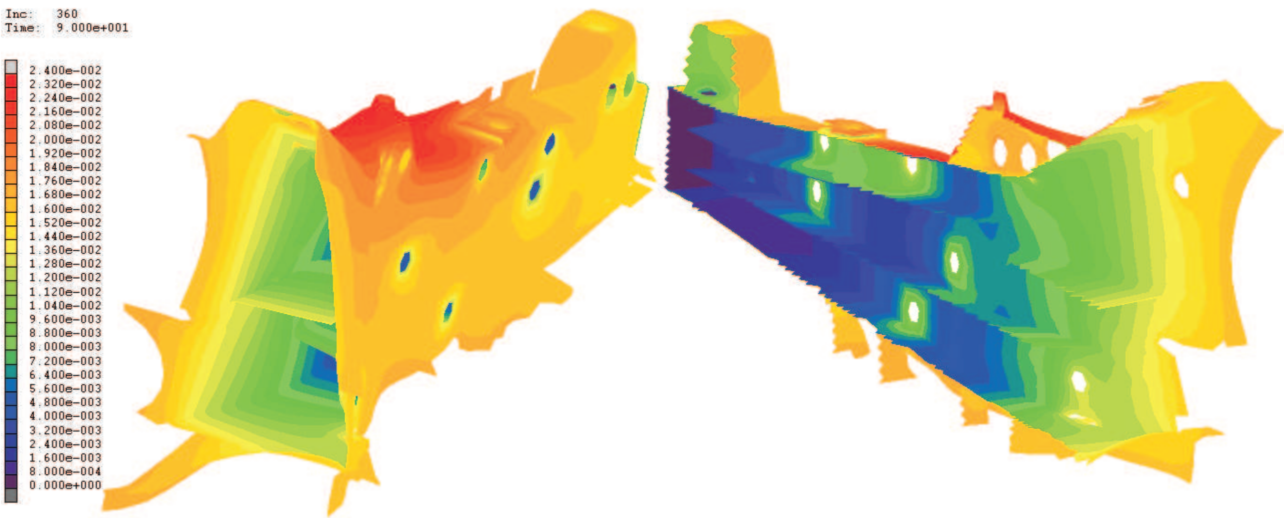

Fig. 1: Coating thickness of a longitudinal chassis beam after $90s$ of electrodeposition at $280V$

The method has proven to account for all the relevant properties of electrodeposition and permits comprehensive parameter studies that lead to a significant reduction of expenditures in automotive industry.

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On the Modelling and Computation of Spinning Wheels

Sarah Ricker, Andreas Menzel, Paul Steinmann

Spinning Wheels, or rather steady cylinder-like deformable bodies occur in many mechanical (contact) problems, e.g. car or aircraft tires, gears or grinding processes. In order to avoid a full dynamical calculation and to obtain a steady-state formulation the present elaboration makes use of a model which has been advocated in the work of Oden, see [1], and has also been applied in the paper of Govindjee, see [2]. In this model, a configuration between the material and spatial configuration is introduced, in which the coordinate system spins around the middle of the cylinder - according to the movement of the cylinder itself - instead of the cylinder spinning around the coordinate system.
After developing the discretized and linearized weak form for the free spinnning problem, a normal contact force and a special tangential contact force are included via a penalty formulation, whereby the latter force represents an adhesion of the cylinder on the basement as soon as both bodies get in contact.

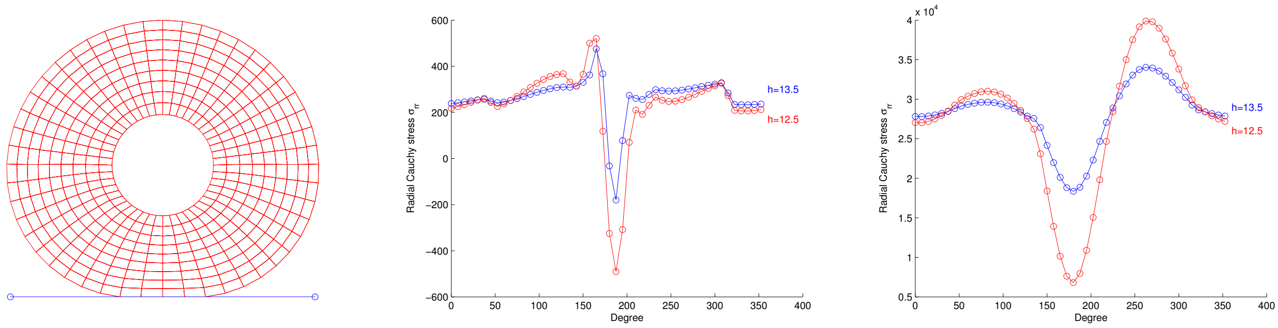


Figure 1: (a) Deformed mesh for spinning wheel with normal contact (b) Outer radial Cauchy stresses for different magnitudes of contact (c) Corresponding inner radial Cauchy stresses

References

[1] J.T. Oden and T.L. Lin. On the general rolling contact problem for finite deformations of a viscoelastic cylinder. *Computer Methods in Applied Mechanics and Engineering*, **57**, 297–367, 1986.

[2] S. Govindjee and P.A. Mihalic. Viscoelastic constitutive relations for the steady spinning of a cylinder. *Technical Report.* University of California at Berkeley, 1998

Visualization of Multidimensional Phase Space Portraits in Structural Dynamics

Patrick R. Schmitt, Paul Steinmann

Within the Hamiltonian setting of classical mechanics the behavior of a dynamical system is typically visualized in terms of the canonical phase space coordinates, i.e. the position and the canonical momentum in a so called phase space portrait (Fig. 1). The investigation of elastodynamic systems modelled by finite element simulations leads to a high dimensionality of phase space, i.e. twice the number of nodal degrees of freedom (DOF). Therefore visualization only seems possible via projection techniques, see Fig. 2 for an example calculated by the implementation in [1] and visualized by a C++/OpenGL-based post-processor. In order to study the overall phase space structure a reduction of the problem's dimensionality seems absolutely necessary which leads us to the theory of pseudo-rigid bodies. A pseudo-rigid or affinely-rigid body is a continuum capable of undergoing only spatially homogeneous deformation. At first glance this seems to be an extreme simplification but the pseudo-rigid body model still captures many interesting features of the full infinite-dimensional elastodynamical model. For example the usual constitutive equations of linear elasticity can be prescribed. The big advantage lies in the applicability of Lie group theoretical methods in order to exploit the geometrical structure underlying the problem. The configuration space Q can be identified with the Lie group $GL^+(3,\mathbb{R}) \ltimes \mathbb{R}^3$ where $GL^+(3,\mathbb{R}) = \{g \in GL(3,\mathbb{R}) | \det g > 0\}$ is the identity component of the general linear group. In a Hamiltonian setting the phase space is just the cotangent bundle of the configuration manifold, i.e. T^*Q, which has a natural symplectic structure. Thus geometric numerical integration schemes [2] are well suited to conserve the problem's inherent structure.

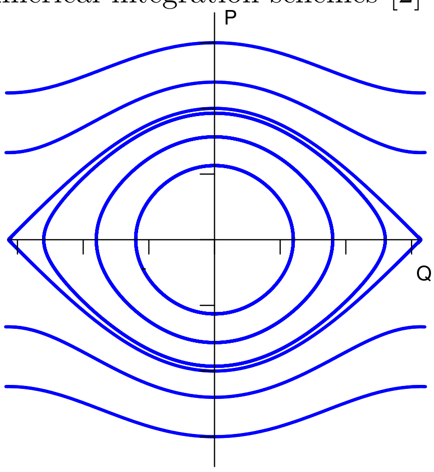


Figure 1: phase space plot of the 2D mathematical pendulum (1 DOF)

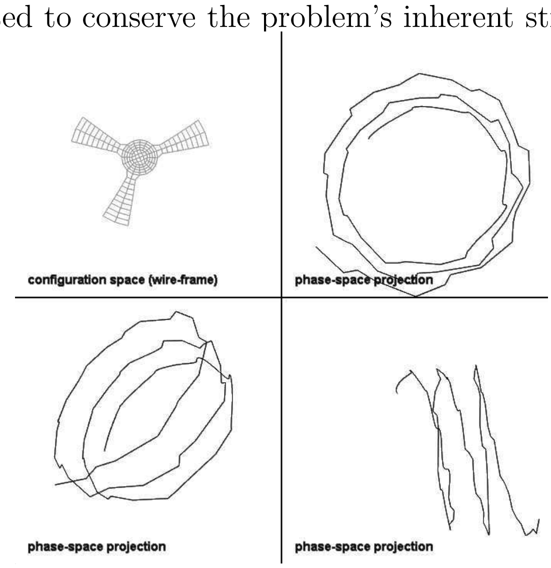


Figure 2: different views of the $\{q_1, p_1, p_2\}$-projection for a single node of a 2D hyperelastic rotor

References

[1] M. Gross: Conserving Time Integrators for Nonlinear Elastodynamics, PhD thesis, University of Kaiserslautern, 2004

[2] E. Hairer, Ch. Lubich and G. Wanner: Geometric Numerical Integration, Springer Series in Computational Mathematics **31**, Springer-Verlag, 2002

Theoretical and Numerical Investigations on Laminar Welded Metal/Fiber-Plastic Composites

Johannes Utzinger, Andreas Menzel, Ellen Kuhl, Paul Steinmann

In the scope of the DFG research group 524 "Manufacturing, analysis and simulation of laminar welded metal/fiber-plastic composites" consisting of 7 subprojects, the modeling and numerical treatment of such materials is the aim of subproject 7.

The main problem is given by the modeling of interfaces between the bulk materials on a meso scale and the introduction of constitutive laws for an interface element formulation. These include elasticity, plasticity, viscosity, damage and combinations of these.

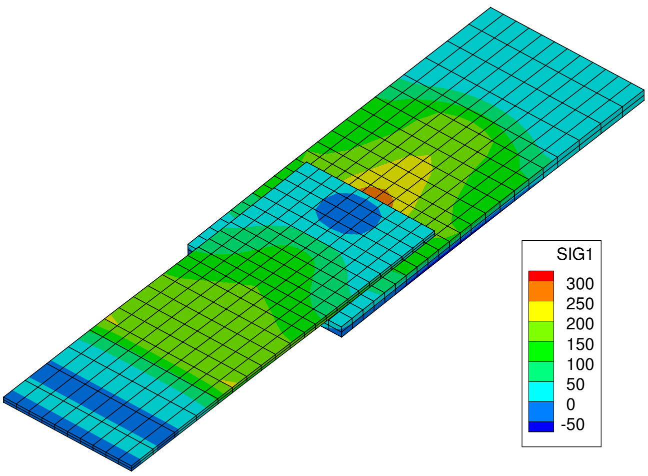
Typically, interface elements are given in a downgraded dimension compared to the surrounding normal finite elements. The traction vector in the interface and the relative displacement of the interface sides are the energetically conjugated vectorial variables.

By comparison to experimental and analytical results of normed tests, it is possible to achieve exact replicas of global load-displacement-curves. Under usage of locally resolved optical and thermical deformation measurements accomplished by subproject 5, it is conceivable to adjust the simulations locally.

Towards a better understanding of imperfections in the welded areas, investigations concerning conciously created imperfections have begun in close cooperation with subprojects 3 and 5.

Additionally, a more theoretical approach towards continuum interface problems is proceeded, whereas the possibilities of bifurcation and well posedness in general are discussed in dependency to the material laws of the continuum and the interface. In this regard, a collaboration exists with the LMT at Cachan/Paris.

In the figure, stresses in the loading direction are shown in the simulation of a shear tension test applied to a specimen welded by ultrasonic vibrations, manufactured by subproject 1.



Numerical Modelling of Nonlinear Electroelasticity

Duc-Khoi Vu, Paul Steinmann

In the last few years there is a growing interest for smart materials that exhibit large displacement and change their mechanical behavior in response to the application of electric fields[1,2]. This class of materials attracts special attention due to their potential for providing relatively simple and quiet variable-stiffness devices for use as rapid-response interfaces between electronic controls and mechanical systems. However the nonlinear electro-mechanic coupling effect exhibited by these materials also poses a new challenge in applied mechanics. In this work we focus on the numerical modelling of the nonlinear electroelastic behavior of systems made of the above mentioned smart materials.

Although basic equations and some analytical analyses for nonlinear electroelasticity were published, very few numerical studies are known in this field. By restricting our attention to the quasi-static theory of nonlinear electroelasticity, a variational formulation for the problem can be established as:

$$\int_{B_0} (\partial_{\mathbf{F}} W : \delta\mathbf{F}) \, \mathrm{d}V + \int_{B_0} (\partial_{\mathbf{E}} W \cdot \delta\mathbf{E}) \, \mathrm{d}V - \int_{\partial B_0} (\delta\Phi \cdot \mathbf{t}) \, \mathrm{d}A + \int_{\partial B_0} (\delta\phi q) \, \mathrm{d}A = 0 \tag{3}$$

where W is the free energy, $\mathbf{F}$ denotes the deformation gradient tensor, $\mathbf{E}$ denotes the electric field vector, Φ is the displacement vector, ϕ is the electric potential, $\mathbf{t}$ is the external pressure and q denotes the electric charge applied on the boundary of the system under consideration with the reference configuration B_0. Note that for simplicity mechanical body forces are not considered. By using Finite Element Method, the linearization of (1) can be discretized, which in turn gives a system of nonlinear equations. A numerical example is shown in Fig. 1. where a rectangular plate with a central hole is subjected to electric potential loading at the two ends.

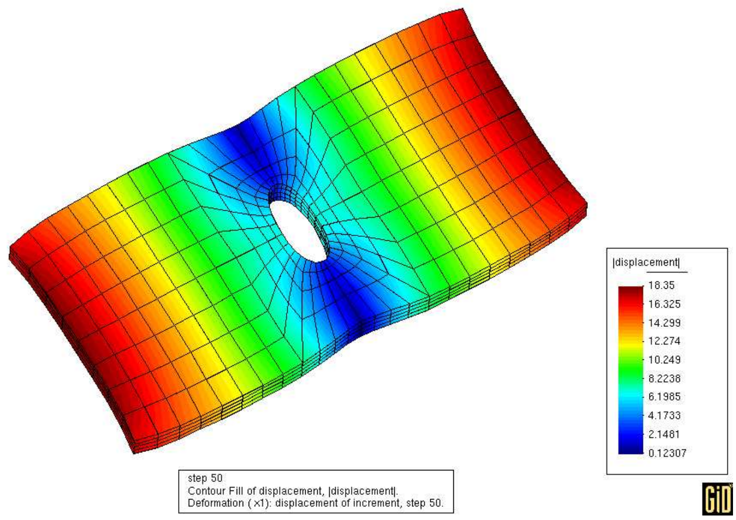


Fig.1 Displacement at $\Delta\phi$=100V

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[1] Dorfmann A., Ogden R. W.: Nonlinear electroelasticity, Acta Mechanica 174, 167-183 (2005).

[2] Bar-Cohen Y.: Electro-active polymers: current capabilities and challenges, Paper 4695-02, EA-PAD Conference, San Diego, CA, March 18-21 (2002).

4 Activities in 2005

4.1 Lectures

- Technische Mechanik I
- Technische Mechanik II
- Technische Mechanik III
- Technische Mechanik IV
- Elemente der technischen Mechanik I
- Elemente der technischen Mechanik II
- Finite Elemente
- Nichtlineare Finite Elemente
- Strukturmechanik
- Kontinuumsmechanik
- Nichtlineare Kontinuumsmechanik
- Plastomechanik
- Materialmechanik
- Bruchmechanik
- Biomechanik
- Maschinendynamik
- Höhere Dynamik
- Analytische Finite Elemente
- Randelemente
- Fernstudiengang Früheinstieg in den Maschinenbau, Technische Mechanik I
- Fernstudiengang Früheinstieg in den Maschinenbau, Technische Mechanik II

4.2 Student research projects theses

- Henrik Schmidt, *Implementierung von Finiten Elementen und Finiten Differenzen Methoden zur Lösung eines nicht-klassischen Wämeleitproblems,*
  Juni 2005
  Betreuer: Dipl.-Math. S. Bargmann
- Stephan Schnorpfeil, *Numerische Lösung der nichtklassischen Wärmeleitung in MATLAB mit Hilfe der Finiten Element Methode,*
  Juni 2005
  Betreuer: Dipl.-Math. S. Bargmann

- Huimin Pi and Friedrich Schäfer, *Analytische Betrachtung zweier Peeling Probleme (Projektarbeit),*
  Juni 2005
  Betreuer: JP Dr.-Ing. habil. E. Kuhl, Dr.-Ing. A. Menzel

- Stefan Uljantschik, *Implementierung der elektromechanischen Kopplung zur FE-Berechnung von piezoelektrischen Materialien,*
  Juli 2005
  Betreuer: Dipl.-Ing. J. Mergheim

4.3 Diploma Theses

- Rouven Mohr, *Theorie und Numerik geometrisch linearer Thermo-Viskoplastizität unter Berücksichtigung von Schädigungseinflüssen,*
  Januar 2005
  Betreuer: Dipl.-Ing. O. Häsner

- Ramona Maas, *Biomechanics of Soft Tissues: On the Implementation of Material Growth into the Commercial Finite Element System ABAQUS,*
  Juli 2005
  Betreuer: Dipl.-Ing. Grieta Himpel, JP Dr.-Ing. habil. E. Kuhl

- Sarah Ricker, *On the Modeling and Computation of Spinning Wheels,*
  Juli 2005
  Betreuer: Dr.-Ing. A. Menzel, Prof. Dr.-Ing. P. Steinmann in Zusammenarbeit mit dem Fachbereich Mathematik

- Alex Barbera, *Computer Simulation of a Grinding Machine,*
  August 2005
  Betreuer: Prof. Dr.-Ing. P. Steinmann

- Kathrin Wippel, *Erstellung eines Finite Elemente Modells einer Hüftinterimsprothese aus PMMA und Vergleich der rechnerischen Bruchlasten mit den experimentell ermittelten Befunden,*
  Dezember 2005
  Betreuer: JP Dr.-Ing. habil. E. Kuhl in Zusammenarbeit mit der Universite du Luxembourg

- Paul Fischer, *Analytical and numerical approximation of the Cahn-Hilliard equation,*
  Dezember 2005
  Betreuer: JP Dr. Martin Grothaus und JP Dr.-Ing. habil. E. Kuhl

4.4 Theses

- R. Denzer, *Computational Configurational Forces*, PhD Thesis

- A. Arockiarajan, *Computational Modeling of Domain Switching Effects in Piezoceramic Materials – A Micro-Macro Mechanical Approach*, PhD Thesis

- B. Delibas, *Rate Dependent Nonlinear Properties of Perovskite tetragonal Piezoelectric Materials Using a Micromechanical Model*, PhD Thesis

- J. Mergheim, *Computational Modeling of Strong and Weak Discontinuities*, PhD Thesis

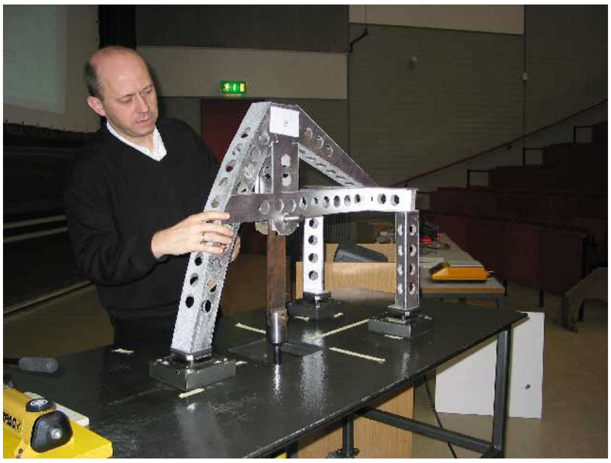
4.5 Colloquium for Mechanics

13.01.05	Baris Irhan, *Enhanced Finite Element Formulations for the Modeling of Strong Discontinuities*
20.01.05	Dr.-Ing. Claus Oberste-Brandenburg Ruhr-Universität-Bochum *Ein numerisches Verfahren zur Beschreibung der Bewegung von Unstetigkeitsflächen in Kontinua*
27.01.05	Dipl.-Ing. Bernd Kleuter Lehrstuhl für Technische Mechanik, TU Kaiserslautern *Parameter identification for finite deformation viscoelasticity analyzing inhomogenous displacement fields*
10.02.05	Cand.-Ing. Bernd Lenhof Lehrstuhl für Technische Mechanik, TU Kaiserslautern *Mechanical Integration of the Dynamics of Rigid Bodies Connected by Joints*
04.04.05	Dipl.- Ing. Rouven Mohr Lehrstuhl für Technische Mechanik, TU Kaiserslautern *Theory and numerics of geometrically linear thermo-viscoplasticity including damage effects*
02.05.2005	Dipl.- Ing. Britta Hirschberger Lehrstuhl für technische Mechanik, TU Kaiserslautern *Numerische Simulation der Dehnungslokalisierung unter Zuhilfenahme der Cosserat-Theorie*
12.05.2005	cand.-Ing. Stefan Uhlar Lehrstuhl für Technische Mechanik, TU Kaiserslautern *Nonlinear stability-analysis of high speed rotors*
09.06.2005	Dipl.- Ing. Frank Längler KK3 - Material Characterization; Fraunhofer-Institute for Non-Destructive Testing, Saarbrücken *Kontinuumsmechanische Erweiterung der Ultraschallspannungsanalyse zur Beschreibung des Spannungszustands im gesamten Bauteil*
16.06.2005	Prof. Michael Ortiz Computational Solid Mechanics Group; California Institute of Technology *Multiscale Modeling of Materials: Linking Microstructure and Macroscopic Behaviour*
28.06.2005	cand.-Ing. Stephan Schnorpfeil and cand.-Ing. Henrik Schmidt Lehrstuhl für Technische Mechanik, TU Kaiserslautern *Anmerkungen zur Theorie und Numerik nicht-klassischer Wärmeleitung*
30.06.2005	Prof. Dr. Christian Wieners Institut für Praktische Mathematik, Universität Karlsruhe (TH) *Effiziente numerische Methoden in der Elasto-Plastizität*
04.07.2005	M. Sc. Robin Ching Lehrstuhl für technische Mechanik, TU Kaiserslautern *Finite Element Rail Vibration Dynamics: Multi-body Dynamics of Modern High-speed Train*
07.07.2005	Dipl.- Ing. Iuliana Matei Fraunhofer ITWM, Kaiserslautern *Topologieoptimierung für Gußteile*

11.07.2005	Dipl.-Math. techn. Sigrid Leyendecker Lehrstuhl für technische Mechanik, TU Kaiserslautern *Mechanical integration of multibody dynamics by the discrete null space method*
14.07.2005	Prof. Krishna Garikipati Department of Mechanical Engineering, University of Michigan *Discontinuous Galerkin methods for gradient theories in continuum mechanics*
18.07.2005	cand.-Ing. Ramona Maas Lehrstuhl für Technische Mechanik, TU Kaiserslautern *Implementierung von Materialwachstum in das kommerzielle Finite Elemente System ABAQUS*
22.09.2005	Prof. N. Sukumar Department of Civil and Environmental Engineering, University of California *Adaptive Computations on Conforming Quadtree Meshes*
27.09.2005	Prof. Anna Pandolfi Dipartimento di Ingegneria Strutturale, Politecnico di Milano, Italy *Cohesive models of fracture and 3d fragmentation procedure*
20.10.2005	Duc-Khoi Vu Lehrstuhl für Technische Mechanik, TU Kaiserslautern *Application of dual programming in limit and shakedown analysis*
27.10.2005	Natalia A. Konchakova Lehrstuhl für Technische Mechanik, TU Kaiserslautern *Plastic deformation of brittle fracture material*
08.12.2005	Peter Pospiech Klinik für zahnärztliche Prothetik und Werkstoffkunde, Universität des Saarlandes *Jede Lücke eine Brücke? Zur Problematik des vollkeramischen Brückenbaues im Mund*
15.12.2005	cand.-ing. Kathrin Wippel Lehrstuhl für Technische Mechanik, TU Kaiserslautern *Erstellung eines FE Modells einer Hüftinterimsprothese aus Plexiglas*

4.6 Ultimate Load Contest

Taking place at february 17th for the sixth time since 2000, the Ultimate Load Contest attracted 10 participating groups this year, consisting of students of all engineering disciplines. The object of this contest is an optimization problem in applied mechanics: built out of hard masonite, an engineering structure is loaded until it collapses. The structure is supported at three points and should have a weight of 2 kg. Nearly 200 spectators were thrilled by the event and the diversity of its ideas. As a reward for the efforts, presents were handed over to all participants. Being an exciting supplement to an engineering students curriculum, the Ultimate Load Contest deepens and enhances the theoretical part of education in Applied Mechanics by giving it a demonstrative dimension. Increasing numbers of spectators and participants are encouraging the Chair for Applied Mechanics to intensify the work on this highlight.



4.7 Joint Research Training Activities

- DFG Graduiertenkolleg 814

  "Ingenieurmaterialien auf verschiedenen Skalen:
  Experiment, Modellierung und Simulation"

- DFG Forschergruppe

  "Herstellung, Eigenschaftsanalyse und Simulation geschweißter
  Leichtbaustrukturen aus Metall/Faser-Kunststoff-Verbunden"

- RLP Graduate School

  "Engineering Materials and Processes"

5 Talks

1. A. Arockiarajan, B. Delibas, A. Menzel, and W. Seemann. Computational modeling of nonlinear bahavior piezoelectric materials. Seminar Mechanik und Numerische Mathematik, Modellierung ferroelektrischer Piezokeramiken, Essen, 22.07.2005.

2. A. Arockiarajan, B. Delibas, A. Menzel, and W. Seemann. Finite element modeling of piezoelectric materials under electromechanical loading. 46th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials, Austin, USA, 17.04. – 25.04.2005.

3. A. Arockiarajan, B. Delibas, A. Menzel, and W. Seemann. Studies on nonlinear electromechanical behavior of piezoelectric materials using finite element modeling. 76th GAMM Annual Conference, Luxemburg, Luxemburg, 28.03–01.04.2005.

4. A. Arockiarajan, B. Delibas, A. Menzel, and W. Seemann. Studies on nonlinear electromechanical behavior of piezoelectric materials using finite element modeling. International Workshop on Piezoceramic Materials and Applications, Paderborn, 22.05 – 26.05.2005.

5. S. Bargmann and P. Steinmann. Computational modeling of thermal waves. GACM 2005, Bochum, Germany, 05.–07.10.2005.

6. S. Bargmann and P. Steinmann. On the theory and numerics of non-classical heat conduction. 76th GAMM Annual Conference, Luxemburg, Luxemburg, 28.03–01.04.2005.

7. R. Ching. Experimental Methods and Computer Model of High Speed Grinding. SPP1180 Group Meeting, TU-Hannover, 11.10.2005.

8. R. Ching and S. Ricker. Computation Models and Algorithms. SPP1180 Group Meeting, TU-Hannover, 30.11.2005.

9. A. Constantiniu and P. Steinmann. Attempts Towards a Novel Meshless Finite Element Method. Third International Workshop: Meshfree Methods for Partial Differential Equations, Bonn, Germany, 12.–15.09.2005.

10. A. Constantiniu and P. Steinmann. Towards a Novel Meshless Finite Element Method. 76th GAMM Annual Conference, Luxemburg, Luxemburg, 28.03–01.04.2005.

11. A. Constantiniu and P. Steinmann. Towards a Novel Meshless Finite Element Method. GK Workshop: Micro-Macro-Interactions in Structured Media and Particle Systems, Kassel, Germany, 10. – 11.06.2005.

12. R. Denzer, A. Menzel, F.J. Barth, and P. Steinmann. Material force method: dissipative materials & fracture. 76th GAMM Annual Conference, Luxemburg, Luxemburg, 28.03–01.04.2005.

13. R. Denzer and P. Steinmann. Advances in the numerics of material forces: Damage & crack kinking. International Symposium on the Mechanics of Material Forces, Symi, Greece, 03.–08.07.2005.

14. R. Denzer and P. Steinmann. Material forces in fracture mechanics of functionally graded materials. 8th U.S. National Congress on Computational Mechanics, Austin, TX, USA, 24.–27.07.2005.

15. R. Denzer and P. Steinmann. On recent progress in the theory and numerics of material forces. 11th International Conference on Fracture, Turin, Italy, 22.–25.03.2005.

16. J. Glaser and P. Steinmann. X-FEM Crack Simulation Based on the Material Force Method. 76th GAMM Annual Conference, Luxemburg, Luxemburg, 28.03–01.04.2005.

17. G. Himpel, E. Kuhl, A. Menzel, and P. Steinmann. Modelling of Mass Changes in Anisotropic Materials. 76th GAMM Annual Conference, Luxemburg, Luxemburg, 28.03–01.04.2005.

18. G. Himpel, E. Kuhl, A. Menzel, and P. Steinmann. Theory and implementation of Mass Changes in Transversely Isotropic Materials. 8th International and Interdisciplinary Essen Symposium on Biomaterials and Biomechanics: Fundamentals and Clinical Applications, 21.-23.09.2005, Essen, Germany.

19. C. B. Hirschberger. An introduction to non-local continuum theories. Seminar of the Department of Civil and Environmental Engineering, University of California Davis, USA, 08.11.2005.

20. N. Kirchner. Modeling microstretch continua. Seminar 'AG Partielle Differentialgleichungen', TU Darmstadt, July 2005.

21. N. Kirchner and P. Steinmann. Towards computational mechanics of microstretch continua. International Workshop on Advanced Models of Foam, Saarbrücken, November 2005.

22. B. Kleuter and P. Steinmann. Parameter identification for finite deformation viscoelasticity analyzing inhomogeneous displacement fields. 76th GAMM Annual Conference, Luxemburg, Luxemburg, 28.03–01.04.2005.

23. B. Kleuter and P. Steinmann. Parameter identification for finite deformation viscoelasticity analyzing inhomogeneous displacement fields. GACM Conference, Bochum, 05.10–07.10.2005.

24. B. Kleuter and P. Steinmann. Parameter identification for the FE analysis of viscoelastic adhesives at large strains. Poster Presentation, IWCMM 15, Düsseldorf, Germany, 19.09.–20.09.2005.

25. B. Kleuter and P. Steinmann. Parameter identification for the finite element analysis of rubber like polymers. Chair of Applied Mechanics, University of Paderborn, 01.12.2005.

26. B. Kleuter, P. Steinmann, D. Vogt, and P. Geiss. Parameter identification for the FE analysis of viscoelastic adhesives at large strains. Poster Presentation, SwissBonding, Rapperswil, Switzerland, 23.05.–25.05.2005.

27. E. Kuhl. Continuum biomechanics - Everything grows. Computational Solid Mechanics Group Seminar, California Institute of Technology , USA, 11.03.2005.

28. E. Kuhl. Continuum biomechanics - Pantha psiloni. Invited Lecture, ETH Zürich, Switzerland, 07.04.2005.

29. E. Kuhl. Continuum biomechanics - Pantha psiloni. Mechanical Engineering Seminar, California Institute of Technology, USA, 29.03.2005.

30. E. Kuhl. Form follows function - Natürlich optimierte Strukturen in der Biomechanik. Invited Lecture, University of Stuttgart, 29.04.2005.

31. E. Kuhl. Kontinuumsmechanik offener Systeme. Invited lecture, University of Kassel, 21.12.2005.

32. E. Kuhl. Kontinuumsmechanik offener Systeme – Smart Structures in der Natur. Invited Lecture, University of Karlsruhe, 18.11.2005.

33. E. Kuhl. On the fundamental difference between engineering materials and living tissues. Department of Civil and Environmental Engineering, UC Davis, USA, 28.10.2005.

34. E. Kuhl. Pantha psiloni - Everything grows. Invited lecture, Max-Planck-Institute for Mathematics in the Sciences, Leipzig, 23.11.2005.

35. E. Kuhl, G. Himpel, R. Maas, and A. Menzel. A kinematic approach towards biological growth within the framework of open system thermodynamics. Computational Plasticity VIII, Barcelona, Spain, 05.09.2005.

36. E. Kuhl, G. Himpel, A. Menzel, K. Garikipati, E. Arruda, and K. Grosh. Remodeling in biological tissues based on a micromechanically motivated chain network model. US National Conference of Computational Mechanics 8, Texas, USA, 25.07.2005.

37. E. Kuhl, G. Himpel, A. Menzel, and P. Steinmann. Modelling and simulation of biological growth phenomen. Mathematical Methods and Models of Continuum Biomechanics, MFO, Oberwolfach, 24.02.2005.

38. E. Kuhl, G. Himpel, A. Menzel, and P. Steinmann. Modelling and simulation of isotropic and anisotropic biological growth. Plasticity'05, Keynote Lecture, 08.01.2005.

39. S. Leyendecker, P. Betsch, and P. Steinmann. Conserving integration of constrained geometrically nonlinear beam dynamics. Sixth Conference on Structural Dynamics, EURODYN05, Paris, France, 04–07.09.2005.

40. S. Leyendecker, P. Betsch, and P. Steinmann. The discrete null space method for constrained mechanical systems in nonlinear structural and multibody dynamics. 76th GAMM Annual Conference, Luxemburg, Luxemburg, 28.03–01.04.2005.

41. S. Leyendecker, P. Betsch, and P. Steinmann. The discrete null space method for multibody dynamics - an application to closed loop systems. International Conference on Computational & Experimental Engineering and Sciences , ICCES'05, Chennai, India, 01.–06.12.2005.

42. S. Leyendecker, P. Betsch, and P. Steinmann. The discrete null space method for multibody dynamics with application to closed loop systems. 2nd Workshop on Numerical Methods in Multibody Dynamics, Bad Herrenalb, Germany, 26–28.10.2005.

43. S. Leyendecker, P. Betsch, and P. Steinmann. Mechanical integration of multibody dynamics by the discrete null space method. Multibody Dynamics 2005, International Conference on Advances in Computational Multibody Dynamics, Madrid, Spain, 21.–24.06.2005.

44. S. Leyendecker, P. Betsch, and P. Steinmann. Mechanical integration of multibody dynamics by the discrete null space method. DFG's International Research Training Group (IRTG): Visualization of Large and Unstructured Data Sets, Kaiserslautern, Germany 11.07.2005.

45. A. Menzel. Adaptation of anisotropic biological tissues. Fourth Gamm–Seminar on Microstructures, Będlewo, Poland, 14.01.–16.01.2005.

46. A. Menzel. Adaptation of anisotropic biological tissues – a computational approach for growth and fibre reorientation. France–Berekeley Workshop on Biomechanics, LMM, Paris, 22.03.2005.

47. A. Menzel. Kontinuumsmechanische Modellierung adaptiver Materialien. Seminar für Mechanik, Universität Karlsruhe (TH), 18.11.2005.

48. A. Menzel, A. Arockiarajan, B. Delibas, and W. Seemann. Micromechanical modeling of rate dependent domain switching effects in piezoelectric materials. International Conference on Computational and Experimental Engineering and Sciences, ICCES'05, Chennai, India, 01.–06.12.2005.

49. A. Menzel and E. Kuhl. Fibre reorientation for transversely isotropic and orthotropic tissue adaptation. Mathematical Methods and Models of Continuum Biomechanics, MFO, Oberwolfach, 21.–25.02.2005.

50. A. Menzel and P. Steinmann. Configurational forces in multiplicative elasto–plasticity. Computational Plasticity VIII, Barcelona, Spain, 07.–09.09.2005.

51. J. Mergheim, E. Kuhl, and P. Steinmann. Computational modelling of cohesive cracks at finite strains. 76th GAMM Annual Conference, Luxemburg, Luxemburg, 28.03–01.04.2005.

52. J. Mergheim and P. Steinmann. A computational method for the fe simulation of strong and weak discontinuities. 76th GAMM Annual Conference, Luxemburg, Luxemburg, 28.03–01.04.2005.

53. R. Mohr, A. Menzel, and P. Steinmann. Aspects on Energy Consistency of Geometrically Nonlinear Plastodynamics. International Conference on Computational and Experimental Engineering and Sciences, ICCES'05, Chennai, India, 01.–06.12.2005.

54. P. Steinmann. Coupled Modelling and Simulation of Electro-Elastic Materials at Large Strains. Coupled Problems'05, ECCOMAS, Santorini, Greece, 25–27.05.2005.

55. P. Steinmann. A FE Approach for the Computation of Strong and Weak Discontinuities at Finite Strains. COMPLAS'05, Computational Plasticity VIII, Barcelona, Spain, 07.–09.09.2005.

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