Annual Report 2009

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1 Preface

The present booklet reports on the activities ongoing at the Chair of Applied Mechanics, University of Erlangen-Nuremberg demonstrating that it is constantly developing in a very satisfactory manner during the year 2009.

This success is exclusively due to the hard work and never ending enthusiasm for scientific research and teaching in the area of applied mechanics, demonstrated by 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 Erlangen-Nuremberg and should convince the reader about the high degree of dedication and ambition of all the members of this group.

Paul Steinmann, Kai Willner

2 Members of the Chair of Applied Mechanics

Professorship for Continuum Mechanics: Prof. Dr.-Ing. habil. Paul Steinmann (Head of the Chair)

Professorship for Structural Mechanics: Prof. Dr.-Ing. habil. Kai Willner

Professorship for Computational Mechanics: JP Dr.-Ing. Julia Mergheim (since 01.07.)

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Student Assistants

Student assistants are mainly active as tutors for young students in basic and advanced lectures at the BA- and MA-level. Their indispensable contribution to high quality teaching at LTM is invaluable, thus financial support from the students enrollment fees as requested at Bavarian universities is gratefully acknowledged.

New Borns (possible candidates for future students in mechanics)

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Wilhelm Weber, Paul Steinmann, Günther Kuhn

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Werner Winter, Thomas Krafft, Matthias Karl, Paul Steinmann

Experimental and numerical analysis of crack growth and affiliated parameter optimization

Volker Barth, Paul Steinmann

This work is split into three parts. Part one, the experimental crack growth analysis, dealt with the creation of a software tool, which is capable of analyzing experimental crack growth data. This software tool processes digital black and white pictures of a crack specimen taken during the crack growth. The output of the software is the current position of the crack tip, respectively the rate of the crack growth, with respect to the stress cycles and the crack start point.

Figure 1: sketch of a partially cracked specimen using extended finite elements

The second part of this work, the numerical simulation of the crack growth, is carried out by extending the chair's own finite element program PhoeniXwith an additional element type, an extended finite element. This element is characterized by the extension of the standard FE formulation with a problem specific term (enrichment). This problem specific term consists of a shape function N (which may be identical to the shape function N of the standard FE part), a problem specific function ψ and additional degrees of freedom \tilde{u} :

$$
u^{h}(\mathbf{x}) = \sum_{i \in I} N_{i}(\mathbf{x}) u_{i} + \sum_{i \in I^{*}} \tilde{N}_{i}(\mathbf{x}) \psi(\mathbf{x}) \tilde{u}_{i}
$$

In the last part of the work, the results of the numerical and the experimental analysis will be compared. A parameter optimization will be carried out with the aim of improving the numerical analysis of the crack growth.

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Interaction of Process and Machine for High-Performance Surface Grinding

Aous Bouabid and Paul Steinmann

Grinding processes have been extensively studied in the last decades within a modelling and an experimental framework [1]. While the focus of these studies lies in basic aspects of grinding, e.g., the relationship between process parameters and resulting cutting forces, the treatment of grinding processes within a more complex framework, that takes into account the interaction between process and structure, became more and more important in the last years. Recent simulation and experimental approaches to model complex coupled grinding processes have been reported in [2] and [3]. One of the major difficulties encountered when coupling different simulation models is the complexity of the interacting models, on the one side, and of the coupling schemes, on the other side. These schemes often require some more modelling details than each of the models can, however, provide. Indeed, available models do, in many cases, not need to incorporate such details in order to appropriately function - each for its own.

The experienced engineer will extract the essence of each of the models to be coupled, and derive, thus, from a complex model simpler models, that can be analyzed in a much shorter time, while providing quite primordial process characteristics at an early simulation stage. Fig. 1 shows a stability card, simulated using a simplified model of a grinding wheel. The stability card gives the critical frequencies of the grinding force excitation, that render excessive high deformations of the grinding wheel, i.e., that cause the grinding process to become non-stable. The model does, on the one side, not cover all physical aspects related to the grinding process. It gives, however, an idea about position and order of magnitude of critical frequencies.

Figure 1: Simulated stability card for a high-performance grinding process.

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Electronic electro-active polymers under electric loading: Experiment, modelling and simulation

Hernán De Santis, Duc Khoi Vu, Paul Steinmann

Electroactive polymers are elastomeric materials that change their shape significantly when subjected to electrical stimulation. In the particular case of electronic electroactive polymers (EEAP) this deformation arises as a consequence of electrostatic forces between two electrodes that compress the polymer, and the mechanical response is influenced both by the mechanical and the electrical properties of the material. Understanding the behaviour of EEAP plays a key role in the development of artificial muscles, where electroactive polymers are used as actuators. Experimental tests, mathematical modelling and numerical simulations of EEAP were already developed to a certain extent in the past, but only one-sided coupling models have been used to model the interaction between the electric field and the elastic body, therefore assuming that the electric field is linear. For this reason, there still exist discrepancies between experimental data and numerical simulations. In this project, an appropiate experimental testing procedure is being set up in order to capture all the important electro-mechanical properties of EEAP under both electric and mechanical loading. Then the electro-mechanical coupling phenomenon will be modeled by using the principles of hyperelasticity and viscoelasticity. Finally, by using a variational approach, a formulation representing the fully-coupled problem will be derived, discretized, linearized and solved with the Finite Element Method.

Figure 1: Experimental setup used in the electro-mechanical testing of EEAP

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$C¹$ continuous discretization of nonlinear gradient elasticity

Paul Fischer, Julia Mergheim, Paul Steinmann

The modeling of materials that exhibit size effects is of high interest. However this effect can not be modeled within the framework of the classical Boltzmann theory. To overcome this problem, extended models like gradient elasticity are used. The main issue in the numerical modeling of gradient elasticity is that a \mathcal{C}^1 continuous approximation for the deformation is required.

Several methods to construct \mathcal{C}^1 continuous shape functions are compared to each other [1,2]. The classical \mathcal{C}^1 continuous 2D elements are reparametrized in terms of Bernstein-Bézier patches, to facilitate the computation of the element shape functions. An alternative approach where only the displacement and its gradient are interpolated at the nodes is the use of the \mathcal{C}^1 natural element method. Unfortunately, all these methods suffer from the linear approximation of the geometry, see Figure 1.

Unlike the earlier formulations, the quadrilateral Bogner-Fox-Schmidt element is used in an isoparametric setting. Therefore, the main difficulty lies in the construction of suitable meshes. A simple a priori mesh optimization algorithm has been developed, which results in a significant improvement of the performance of these elements, see Figure 2.

Figure 1: Comparison of the convergence behavior of several \mathcal{C}^1 continuous methods for a nonlinear thick hollow cylinder with external pressure.

Figure 2: Contour plots for the local error $||\mathbf{u}^h - \mathbf{u}^a||_2/||\mathbf{u}^a||_2$. Left: Argyris element. Center: Bogner-Fox-Schmidt with linear mesh optimization. Right: Bogner-Fox-Schmidt without mesh optimization.

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Isogeometric Approaches in Computational Shape Optimization

Jan Friederich, Paul Steinmann

Shape optimization of elastic mechanical structures is an important issue in computational mechanics and engineering. Classical hybrid approaches combine a geometric parametrization of the boundary (given by B´ezier curves and surfaces, B-splines or NURBS) with an analysis model of the structure (given by a FEM-discretization). The geometric parametrization on the one hand provides the design variables, the FEM-model on the other hand is used for the Galerkin-based computation of the state variables and sensitivities.

In contrast to the isoparametric approach of Scherer [1], the goal of this project is to develop exclusively isogeometric strategies by employing a new method, called "Isogeometric Analysis", that has been recently introduced by Hughes et al. [2]. Basically relying on the isoparametric concept for the FEM, this approach uses basis functions generated from NURBS to describe the geometry of the model as well as to solve the PDE of the mechanical problem. This method exhibits several advantages: It enables a precise geometric definition of complex designs independently of the resolution of the discretization; it provides simpler and further strategies of mesh refinement; finally, $C¹$ and higher-order continuity can be achieved easily without introducing extra degrees of freedom.

In the context of a shape optimization problem, isogeometric strategies allow for an integration of the geometry model and the analysis model, since a precise geometric parametrization of the boundary is naturally given and the design variables are directly at hand.

Figure 1: Example of an isogeometric discretization: Infinite plate with circular hole. a) Net of control points. b) Refined element mesh. (Cf. [3])

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Modelling of jointed structures in the frequency domain

Johannes Geisler, Kai Willner

This contribution deals with numerical and experimental investigations of jointed structures. Here, nonlinear friction forces in contact interfaces are important especially with respect to stiffness and damping properties.

In numerical studies Zero Thickness Elements are applied for the discretization of contact interfaces in the framework of the Finite Element Method. In time domain, structural answers can be calculated for arbitrary excitations, including transient effects. Especially for harmonic excitations, often only the steady state is of interest. In the linear case a direct computation of the steady state in the frequency domain is possible, whereas for nonlinear problems like the considered ones with contact interfaces, a special treatment of nonlinear contact stresses has to be applied. Therefor the harmonic balance method is utilized, which leads to a complex nonlinear system of equations in the frequency domain. This is solved for the stationary answer of the structure, [1], [2].

As an example, a system consisting of two bolted beams is considered. In the following figure magnitudes of calculated and measured frequency response functions $|H|$ are shown for harmonic excitation of the structure around its first resonance frequency. Good agreement between measurement and computation using the harmonic balance method is observed.

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On Inverse Form Finding for Hyperelasticity in Logarithmic Strain Space

Sandrine Germain, Michael Scherer, Paul Steinmann

We extended the method proposed in [1] to anisotropic hyperelasticity that is based on logarithmic strains. We formulate the problem using the inverse kinematics. The deformed configuration is given and the inverse deformation mapping that determines the undeformed shape is the primal unknown. The governing equation for the numerical analysis based on finite elements is a weak form of the balance of momentum, that is formulated in terms of the deformed configuration using the Cauchy stress tensor. The free energy density is expressed as a function of the logarithmic strain and the anisotropic stiffness tensor.

The motivation for the use of the logarithmic strain space formulation lies in the fact that the fourth order stiffness tensor is known for many symmetry classes of anisotropic materials and it mimics the small strain format. The use of a spectral decomposition on the right Cauchy-Green tensor to compute the Hencky strain tensor has a considerable advantage. The logarithm is applied on the eigenvalues and not on the complete tensor.

Figure 1: Tension test of a rectangular bar in the final configuration.

Figure 2: Undeformed bar in the initial configuration.

As an example, we consider a tension test of a rectangular bar in 3D. The shape is divided in two equal parts with different anisotropic principal direction orientations. The two lower corner points of the cross section of the rear face are fixed. The domain was discretized using trilinear hexahedral finite elements. An orthotropic material is considered. Figure 2 shows the computed undeformed shape in the initial configuration. We obtained a quadratic evolution of the residual norm as a function of iterations using the Newton-Raphson method.

This work was supported by the German Research Foundation (DFG) under the Transregional Collaborative Research Center SFB/TR73 project.

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Experimental and numerical investigations of the normal and tangential contact behavior of rough metallic surfaces

Daniel Goerke and Kai Willner

To determine geometrical parameters of rough surfaces uniquely a fractal regular description is used. Therefore measured structure functions are approximated by a three-parameter function, employing the RMS-value of the roughness, a transition length x_T between fractal behavior at high wavenumbers and stationary behaviour at low wavenumbers, and the fractal dimension D in the fractal region, respectively, as intrinsic parameters to describe an isotropic rough surface. In order to study the influence of the different parameters and to develop constitutive contact laws, it is necessary to generate surfaces numerically. They are used in normal and tangential contact simulations based on elastic halfspace theory [1]. In addition finite element models with geometrical irregularities are applied to examine the influence of waved and skewed surfaces on the contact behavior [2].

All simulations are tested against experimental data. In a normal contact test setup the pressure gap relationship is measured [2,3] and in a tangential contact test setup (Figure 1) the contact behavior is determined by load-displacement curves (Figure 2) to analyze the influence of the material and the surface production process on the tangential contact stiffness k_T , the microslip and the friction coefficient. With a second tangential contact setup tests with different velocities and small loads are performed.

Figure 1: Tangential contact setup with piezo actuator and two extensometers

Figure 2: Load-displacement curves of ground, hardened steel against stainless steel under cyclic tangential loading, normal force $F_N = 2$ kN

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Constitutive friction law for the description and optimisation of Tailored Surfaces

Franz Hauer, Kai Willner

Friction between tools and workpieces is an important parameter in forming processes. It strongly influences the quality of products and machine forces. Tailored surfaces are employed to influence friction systematically. The aim of the project is to simulate the contact between tools and workpieces numerically and to form a constitutive friction law for tailored surfaces. Particular attention is drawn on surface roughness and lubricants. A special feature of forming processes is large contact pressure leading to plastic deformation of surface asperities, which has to be considered in the numerical model. Simulations are performed by a halfspace model whose advantage is the lower numerical effort compared to finite element or boundary element method. The halfspace model is based on potential functions by Boussinesq and Cerruti.

$$
F_1 = \int_{\Gamma} \int q_x(\xi, \eta) \Omega \, d\xi \, d\eta \qquad F = \frac{\partial F_1}{\partial z} = \int_{\Gamma} \int q_x(\xi, \eta) \log (\rho + z) \, d\xi \, d\eta
$$

\n
$$
G_1 = \int_{\Gamma} \int q_y(\xi, \eta) \Omega \, d\xi \, d\eta \qquad G = \frac{\partial G_1}{\partial z} = \int_{\Gamma} \int q_y(\xi, \eta) \log (\rho + z) \, d\xi \, d\eta
$$

\n
$$
H_1 = \int_{\Gamma} \int p(\xi, \eta) \Omega \, d\xi \, d\eta \qquad H = \frac{\partial H_1}{\partial z} = \int_{\Gamma} \int p(\xi, \eta) \log (\rho + z) \, d\xi \, d\eta
$$

\n
$$
\rho = \sqrt{x^2 + y^2 + z^2} \qquad \Omega = z \log (\rho + z) - \rho
$$

Displacements on the surface and within the solid can be calculated by means of the potential functions which are integrated over evenly spaced surface patches.

$$
\Psi_1 = \frac{\partial F_1}{\partial x} + \frac{\partial G_1}{\partial y} + \frac{\partial H_1}{\partial z} \qquad \Psi = \frac{\partial \Psi_1}{\partial z} = \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z}
$$

$$
u_x = \frac{1}{4\pi G} \left\{ 2\frac{\partial F}{\partial z} - \frac{\partial H}{\partial x} + 2\nu \frac{\partial \Psi_1}{\partial x} - z\frac{\partial \Psi}{\partial x} \right\}
$$

$$
u_y = \frac{1}{4\pi G} \left\{ 2\frac{\partial G}{\partial z} - \frac{\partial H}{\partial y} + 2\nu \frac{\partial \Psi_1}{\partial y} - z\frac{\partial \Psi}{\partial y} \right\}
$$

$$
u_z = \frac{1}{4\pi G} \left\{ \frac{\partial H}{\partial z} + (1 - 2\nu)\Psi - z\frac{\partial \Psi}{\partial z} \right\}
$$

The pressure distribution on the surface is determined by minimising the complementary internal potential energy of the halfspace. The stress field within the solid is very important for the calculation of plastic deformations. It can be found by inserting derivatives of the displacements into Hooke's law.

This research project is funded by the DFG (Deutsche Forschungsgemeinschaft) within SFB Transregio 73.

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Towards developing finite strain constitutive models for nano-filled glassy polymers

Mokarram Hossain, Paul Steinmann

Nano-filled amorphous glassy polymers have been widely employed in various practical application areas that cover automotive and construction industry, electronics, optical devices and medical technology, to mention a few. The broad spectrum of application is due to their good processing features, high energy absorption capacity under impact loadings, lower weight relative to glass and excellent optical properties [1,4]. Bulk amorphous glassy polymers exhibit rate-dependent finite elastic-plastic material behaviour. The elastic-plastic response stems from the inherent disordered micro-structure of the material that is formed by linear polymer chains existing in the 'frozen-in' state. In contrast to elastomers or thermosets, they are generally not cross-linked by chemical bonds but their network structure is rather formed by physical junctions, the so-called entanglements. This intrinsic micro-structure brings along the rate and temperature effects prevailing in the material behaviour. The finite elasto-viscoplastic behaviour is not specific only to tough polymers but is also observed in brittle polymers on a much smaller scale, especially in course of crazing. For this reason, both a sound three-dimensional constitutive model accounting for the complicated material behaviour and the associated effective numerical algorithm for the finite element simulations are of great importance.

The typical load-displacement curve of glassy polymer consists of three major parts, i.e., a) the initial linear elastic part which falls in the small strain deformation domain limited by a yield stress that depends on rate, pressure and temperature; b) ideally plastic response e.g. strain softening and c) entropic hardening response due to the chain alignment that also depends on rate and temperature.

In this project, several large strain continuum-based constitutive models for glassy polymers, which have been proposed in the literature [1,2,3], are implemented systematically in an in-house finite element code. The most suitable one is extended to incorporate the influence of the nano particles. The extension toward modelling the nano-particle influence in the amorphous glassy polymer can be conceptualized either by changing the linear elastic energy function, or the visco-plastic evolution (flow) rule or the entropic hardening energy function or changing all two/three parts in a systematic manner. The proposed models will be validated with the experimental data provided by the other partners of the project.

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A finite element framework for continua with boundary energies

Ali Javili, Paul Steinmann

Common modeling in continuum mechanics takes exclusively the bulk into account, nevertheless, neglecting possible contributions from the boundary. However, boundary effects sometimes play a dominant role in the material behavior, the most prominent example being surface tension. Within this project boundary potentials are allowed, in general, to depend not only on the boundary deformation but also on the boundary deformation gradient and the spatial boundary normal. Motivated by this idea, a suitable finite element framework based on rank deficient deformation gradients is established. In essence, the total potential energy functional $I = I(\varphi)$ that we seek to minimize with respect to all admissible variations $\delta\varphi$ (spatial variations at fixed material placement) reads

$$
I(\boldsymbol{\varphi}) := \int_{\mathcal{B}_0} U_0(\boldsymbol{\varphi}, \boldsymbol{F}; \boldsymbol{X}) \, \mathrm{d}V + \int_{\mathcal{S}_0} \mathsf{u}_0(\boldsymbol{\varphi}, \boldsymbol{n}, \widehat{\boldsymbol{F}}; \boldsymbol{X}, \boldsymbol{N}) \, \mathrm{d}A. \tag{1}
$$

Then the minimization of the total potential energy functional, $\delta I(\varphi) = 0$, renders the principle of virtual work including contributions from boundary terms

$$
\int_{\mathcal{B}_0} \mathbf{P} : \text{Grad}\delta\varphi \, \mathrm{d}V + \int_{\mathcal{S}_0} \widehat{\mathbf{P}}^* : \widehat{\text{Grad}}\delta\varphi \, \mathrm{d}A = \int_{\mathcal{B}_0} b_0 \cdot \delta\varphi \, \mathrm{d}V + \int_{\mathcal{S}_0} \widehat{b}_0 \cdot \delta\varphi \, \mathrm{d}A \qquad \forall \delta\varphi. \tag{2}
$$

As an example, due to the surface tension effect, the surface of a body tends to obtain constant curvature, i.e. a cube tends to transform to a sphere. This fact is shown in Figure 1.

Figure 1: Transformation of a cube to sphere due to surface effects.

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Polyhedral finite elements

Markus Kraus, Paul Steinmann

The finite element method is a generally acknowledged and very efficient technique for the numerical solution of partial differential equations. Traditional element formulations are often limited to simple geometries, like hexahedra in 3d. Otherwise, polyhedral finite elements as proposed in [1] with almost arbitrary number of flat faces provide great flexibility meshing complex structures or modelling materials with grained or crystalline polyhedral structure, whereas loss of computational accuracy or higher computational costs are undesired.

A basic algorithm for polyhedral finite element formulations can easily be adopted from the 2d case by splitting the integration domain into many tetrahedral subdomains on which quadrature rules are known [1]. Furthermore, the suggested subdivision of polygons with linear-displacement- or uniformstrain-elements [2] are negotiable as well. More critical is the interpolation in arbitrary element geometries: although many interpolation techniques are available even for concave domains in 2d [3], adequate and general approaches in 3d are missing and need further investigation. Additionally to the deployment and analyses of finite element formulations, some technical aspects occurred: in contrast to standard element geometries, the generalization to polyhedra needs a more general representation of element entities and connectivities. Thus, a polyhedral representation was realized that contains all required datasets and measures like element nodes, node-to-face-connectivities or face normals. Providing arbitrary meshes for polyhedral finite elements, the Adaptive Delaunay Tessellation as proposed in [4] has been extended to technical relevant tessellations in 3d (figure a). By the limitation of common postprocessors to standard elements an interface to Kitware's ParaView has been established that enables the illustration of any (convex) polyhedral mesh (figure b).

(a) polyhedral ADT mesh: color indicating number of element nodes (blue: 4 nodes, red: 8 nodes)

(b) ParaView postprocessor with assembled galenite crystals

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A Variational Multiscale Method for Fracture

Julia Mergheim

Multiscale approaches for the modeling of heterogeneous materials are often based on the concept of homogenization, which requires that the fine scale is much smaller than the coarse scale of the problem, i.e. the scales have to be separated. This condition of scale separation is violated when failure processes are analyzed, which come along with narrow zones of localized deformation or discrete cracks. These zones of localized deformation have to be modelled explicitly within a multiscale framework.

The present multiscale approach adapts the variational multiscale method (VMM), initially introduced by Hughes [1]. The basis of this method is a decomposition of the solution into a coarse scale and a fine scale contribution, the latter incorporating the local behaviour. The VMM is here extended to include propagating cracks [2]. A twoscale approach, macro-meso, is adopted and both scales are discretized with finite elements whereby certain locality assumptions are prescribed to the mesoscopic solution. At the fine scale an evolving mesostructure induced by crack propagation is taken into account. To enhance the efficiency of the approach the fine scale region is adaptively resized, depending on the stress state in the particular elements.

The multiscale framework implies naturally a refined discretization in the area of the crack tip. Nevertheless, when crack propagation is modelled, the crack direction should not depend on the discretization. To prevent constant remeshing a discretization with discontinuous elements, following an approach of Hansbo and Hansbo [3], at the fine scale is applied.

In the figure below the proposed twoscale approach is compared with a full fine scale simulation and the results are in very good agreement.

Three-point bending beam - comparison of twoscale and reference solution, σ_{xx}

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Coupling of particle- and finite-element-based simulations by using a bridging domain

Sebastian Pfaller and Paul Steinmann

The aim of our current research is the coupling of particle based simulations with the Finite Element method. For this end, multi dimensional systems are going to be simulated by utilizing a bridging domain method which is based on the Arlequin method.

The Arlequin framework was originated by Ben Dhia and Rateau [1] to couple different Finite Element domains. It has later been extended to the coupling of particle based systems with continua by several authors, eg. by Guidault and Belytschko [2] or by Bauman, Oden, and Prudhomme [3]. For crucial sections, like the surroundings of cracks or crazes, particle based simulations like Molecular Dynamics are utilized in order to describe the behavior of materials very accurately. Other parts of the system under consideration are modelled at much higher length scales with the Finite Element method.

Figure 1. Uniaxial tension test: Particle domain Ω_d included in a Finite Element domain Ω_c , coupled by a bridging domain Ω_0 ; external forces (red arrows), coupling forces acting on FE nodes (green), and coupling forces acting on particles (blue)

Depending on the characteristics of the problem, a geometrically linear or nonlinear formulation is used. A two-dimensional coupling like it is shown in Figure 1 is running, a extension to three dimensions is being implemented.

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Mechanical interphases in adhesive epoxy-aluminium joints

G. Possart, P. Steinmann

A recently finished collaborative project provided a new experimental method to measure inhomogeneous deformation fields occuring in shear tests of adhesive joints, cf. Fig. 1. These inhomogeneities are assumed to result from gradients in the mechanical properties of the epoxy close to the substrate. The gradients, hitherto only measurable by Brillouin microscopy [1], may be caused by demixing, curing shrinkage or preferred adsorption effects of particular epoxy components during the network formation.

Fig. 1: adhesive joints (FIB-marked) under shear (SEM): inhomogeneous deformations (magnitude dependent on component mixing ratio) [2]

Finite element simulations using different classes of constitutive assumptions have been applied to identify reasons for the inhomogeneous shear behaviour. Thereby it turned out that purely elastic gradients (about ten percent deviation in stiffness) as reported by other authors, would not be sufficient to explain the observed deformations. Also curing shrinkage induced pre-stress is only of minor importance while already small gradients in the plastic material parameters have a significant impact:

Fig. 2: pre-stress due to curing shrinkage vs. plastic gradients

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On Cahn-Hilliard phase field modeling using NEM

Amirtham Rajagopal, Paul Fischer, Paul Steinmann, Ellen Kuhl

We present a natural element method to treat higher-order spatial derivatives in the Cahn-Hilliard equation. The Cahn-Hilliard equation is a fourth-order nonlinear partial differential equation that allows to model phase separation in binary mixtures. Finite element solutions are not suitable because primal variational formulations of fourth order operators are well-defined and integrable only if the finite element basis functions are piecewise smooth and globally \mathcal{C}^1 continuous. To ensure \mathcal{C}^1 -continuity, we develop a natural-element-based spatial discretization scheme. The \mathcal{C}^1 -continuous natural element shape functions are achieved by a transformation of the classical Farin interpolant, which is basically obtained by embedding Sibsons natural element coordinates in a Bernstein-Bézier surface representation of a cubic simplex. For the temporal discretization, we apply an unconditionally stable Euler backward time integration scheme supplemented with an adaptively adjustable time step size. Figure 1 shows the influence of initial conditions on the phase seperated concentration profiles.

Figure 1: Isotropic diffusion: Influence of initial concentration (a) $c^{ini} = 0.28$ (b) $c^{ini} = 0.72$ (c) $c^{ini} = 0.63$ (d) $c^{ini} = 0.5$

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A fictitious energy approach for shape optimization

Michael Scherer and Paul Steinmann

Our work deals with shape optimization of continuous structures. As in early works on shape optimization, coordinates of boundary nodes of the FE mesh are directly chosen as design variables. Convergence problems and problems with jagged shapes are eliminated by a new regularization technique. We introduce a *fictitious total strain energy* that measures the shape change of the optimized design with respect to the initial design. An inequality constraint added to the shape optimization problem limits the fictitious energy. This *energy constraint* is the key feature of our approach. It defines a feasible design set whose size can be varied by one parameter, the upper energy limit. The energy constraint improves the solvability of nodebased shape optimization problems significantly such that standard gradient-based nonlinear programming methods can be applied. Since the regularization is based on a fictitious energy functional, it does not cause mesh dependency. If the mesh is successively refined, the shape optimization converges to a final design. A numerical example for a shape optimization subject to an energy constraint is given in Figure 1. For further details on the proposed regularization technique and further numerical examples we refer to Scherer et al. [1].

Figure 1. Numerical example: a linear elastic arch segment $(E = 200000 \text{ N/mm}^2$, $\nu = 0.3)$ is subjected to a constant vertical surface load $(t = 30 \text{ N/mm}^2)$ acting on the upper horizontal boundary. The arch segment is fixed in the vertical direction at the four vertices of the lower horizontal boundary and symmetry boundary conditions are imposed at the four vertical boundaries. The shape optimization aims to minimize the volume of the arch segment. To introduce a coupling to the mechanical response, the optimization is subject to an inequality constraint that restricts the increase of the compliance. Beside the compliance constraint, the optimization is subject to a fictitious energy constraint that allows to control the shape change of the design. Figure (a) shows the initial design and (b) the optimized design of the arch segment. The volume reduction amounts to 55% and the increase of the compliance to 50%. Although the compliance increases, the maximum von Mises stress remains approximately constant since, as shown by the contour plots of the von Mises stress distribution $(N/mm²)$, the shape optimization improves the equal distribution of the stresses.

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Multi-scale modelling of heterogeneous materials

Ulrike Schmidt, Paul Steinmann

The aim of the project E-8 of the cluster 'Engineering of Advanced Materials' is to model and simulate materials which, at a macroscopic scale, seem to be homogeneous, but turn out to be heterogeneous when viewed at a microscopic scale. Although this may be said about all materials, the focus lies on materials, where the microscopic length scale is much larger than the atomistic length scale. Overall constitutive assumptions for materials with heterogeneities often fail to describe material behaviour realistically. Therefore, another approach is considered in this project, namely computational homogenization.

The cooperation with S. Ricker from the University of Kaiserslautern made it possible to start with an existing MATLAB implementation of first order computational homogenization for two scales in 2-D, which is also known as FE^2 . The theory for three dimensions was studied in detail and the implementation was extended to deal with sophisticated three dimensional problems.

Figure 1: The Two Scales of $FE²$

Although the FE²-method suffers from high computational costs, especially for 3-D, it is unavoidable for complex microstructures, such as the ceramic foams treated within the cluster. The cooperation with Prof. Greil and Dr. Fey gave an insight into the complexity of the microstructure of ceramic foam. For calculations of real materials not only the computational time, but also the memory requirements are very high. Therefore, the efficiency of the implementation is investigated and a powerful workstation with large memory capacity has been acquired.

The homogenization of thermo-mechanically coupled problems is currently being investigated, which requires a deeper understanding of thermo-mechanics. In particular, the implementation of a weakly coupled nonlinear microscopic problem was completed. Homogenized tangents for the use in a general macroscopic problem with a scale transition from the literature has been investigated and implemented.

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Mechanical integrators for simulation of contact in elastic multibody systems

Patrick R. Schmitt, Paul Steinmann

When dealing with the simulation of dynamical contact processes several solution methods are commonly used. Constraints imposed by contact/impact events are usually formulated as linear complimentary problem (LCP), which needs to be solved alongside the time-stepping scheme. In order to accurately describe the underlying physical processes time-stepping schemes exactly conserving certain intrinsic properties of the system (energy, linear and angular momentum etc.) are highly desirable. In situations with frictional contact the corresponding dissipative effects need to be accounted for, whereas in the "free-flight" phases between contacts integrators that conserve geometric structures of (velocity-)phase-space exactly can be employed, see e.g. [1]. As an example for frictional contact we consider a billiard table consisting of a hard surface and four hard walls. 28 object balls and the cue ball, all with identical mass and moment of inertia, are arranged on the table as in Fig. 1 (left). The billiard balls are subject to gravity loading and all interactions (ball/surface, ball/wall and ball/ball) are frictional and therefore dissipative. The resulting nonsmooth dynamical system can be described using a augmented quasi-Lagrangian formulation (Alart-Curnier, see e.g. [3]) and solved by Moreau's time-stepping algorithm as implemented in the SICONOS software platform [2].

Figure 1: (left) The initial configuration of billiard balls subject to gravity loading perpendicular to the table's surface. The arrow indicates the initial velocity of the cue ball whereas the object balls are initially at rest. (right) Resulting configuration after 400 time-steps of width $h = 0.005s$ taking into account frictional contact for ball/surface, ball/wall and ball/ball interactions.

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On the Modeling and Simulation of Magneto-Sensitive Elastomers

Franziska Vogel and Paul Steinmann

Magneto-sensitive elastomers are smart materials which are composed of a rubber-like basis matrix filled with magneto-active particles. If matter consisting of such a material is subject to a magnetic field, the body β deforms and its finite deformation is influenced not only by the magnetic field within the body but also by the field in the surrounding free space S .

The coupled system of equations to solve consists of the quasi–static Maxwell's equations on the magnetics side together with the mechanical equilibrium equation in the deformed configuration:

 $\nabla_{\boldsymbol{x}} \times \mathbb{h} = \boldsymbol{0} \quad \nabla_{\boldsymbol{x}} \cdot \mathbb{b} = 0 \quad \text{in} \quad \mathcal{B}_t \cup \mathcal{S}_t, \qquad \nabla_{\boldsymbol{x}} \cdot \boldsymbol{\sigma}_{tot} = \boldsymbol{0} \quad \text{in} \quad \mathcal{B}_t, \qquad \nabla_{\boldsymbol{x}} \cdot \boldsymbol{\sigma}_{\max}^{\mathcal{S}} = \boldsymbol{0} \quad \text{in} \quad \mathcal{S}_t.$

The total stress σ_{tot} is a symmetrized stress tensor which already contains the contributions from the non–symmetric Cauchy stress and the magnetic body forces. The influence of the outer space is taken into account by the Maxwell stress σ_{max}^S . The scalar potential of the magnetic field is used as independent magnetic variable.

In the reference configuration, an augmented energy function Ω is introduced following [1]. Then it is possible to establish constitutive laws for σ_{tot} and b. Additionally, a functional I is defined, which also considers the contribution from the free space modeled by M_0 and whose stationary point is equivalent to the solution of the upper system of equations as shown in [2].

$$
I(\boldsymbol{\varphi}, \Phi) = \int_{\mathcal{B}_0} \Omega(\boldsymbol{F}, \mathbb{H}) \ dV + \int_{\mathcal{S}_0} M_0 \ dV
$$

In order to show the influence of the free space, a unit cube under potential loading is plotted. One can see a difference in considering the exterior of the body, the maximum value and the distribution of the the norm of the displacement. Furthermore, the edges of the cube are slightly bent in contrast to the straight edges of the computational experiment neglecting the outer space.

Figure 1: Magnitude of displacement $\|u\|$.

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A 2-D coupled BEM-FEM simulation of electro-elastostatics at large strain

Duc Khoi Vu and Paul Steinmann

The numerical simulation of nonlinear electro-elastostatics is considered in this work using the coupled boundary and finite element method. The objective of the work is to properly simulate the deformation of an electro-elastic body undergoing large deformation subjected to electric stimulations in the case, where the surrounding space has significant influence on the electric field inside the body. Finite elements are used to model the nonlinear electro-elastic body in which both geometrical nonlinearity and electro-mechanical nonlinearity are taken into account. Boundary elements are used to model the surrounding space and account for the large deformation of the boundary of the body.

Figure 1. Distribution of electric potential (V) in deformed configuration using coupled BEM-FEM (left) and FEM (right)

As numerical example we consider a plate of dimensions $60\mu m \times 60\mu m$. The plate has a hole of the size 30μ m \times 30μ m at the center of the plate. The electric potential is given on the lower and upper edge of the plate as: $\psi_{lower} = -500V$ and $\psi_{upper} = +500V$, respectively. In our simulation, 1200 linear quadrangular 4 node elements are used to model the plate. On the outer boundary of the plate, the outer space is modeled by 160 linear 2 node boundary elements and on the inner boundary the hole is modeled with 80 linear 2 node boundary elements. The simulation results obtained by using both the coupled BEM-FEM and by using only finite elements are presented to demonstrate the necessity of the coupled BEM-FEM.

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Simulation of 3D fatigue crack propagation

Wilhelm Weber, Günther Kuhn

To prevent accidents due to fatigue crack growth, 3D fatigue crack propagation in terms of linear elastic fracture mechanics is simulated. Since the nature of crack growth is nonlinear an incremental procedure has to be applied. Special attention is focused on the continuous change of the stress field within the incremental procedure. In each increment three steps have to be performed: a) a complete stress analysis including the calculation of the stress intensity factors (SIFs) and T-stresses, b) the evaluation of the 3D crack growth criterion to determine the new crack front and c) the update of the numerical model.

The 3D dual boundary element method is applied for the computation of the stress field. This method is especially suitable for stress concentration problems and the update of the discretization. In addition the crack surface contact is considered [5]. In order to reduce the numerical complexity of the stress analysis, fast methods are applied [1,4]. The fracture mechanical parameters are accurately extrapolated from the stress field by a regression analysis optimized by the minimization of the standard deviation.

The crack deflection and the crack extension for every point along the crack front have to be determined in order to define the new crack front relative to the current one. In the present context the cyclic equivalent SIF $\Delta K_{eq}(P)$ is calculated by the criterion of the maximum energy release rate [2]. By the evaluation of a crack propagation rate formulation the local crack extension $\Delta a(P)$ is obtained. The maximum tangential stress criterion has been established for the calculation of the kink angle $\Delta\varphi(P)$. It is extended by the utilization of the T-stresses in order to consider the curvature of the crack path [3].

Since the fact of the changing stress field between the initial and the new crack front is neglected, an analysis of the prediction is required. Therefore, an implicit time integration method in terms of a predictor-corrector scheme is applied [3]. In case of crack surface contact non-proportional mixed mode conditions have to be taken into account. Here, the challenges of changing kink angles during a load cycle and the transition of shear mode to tensile mode crack growth have to be solved [5,6].

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Parameters of implant stability measurements based on resonance frequency and damping capacity - a comparative finite element analysis

Werner Winter, Stefan Möhrle, Matthias Karl

It has been argued that stability both at placement and during function is an important criterion for the success of dental implants. Bone loss can be observed, too (see Fig. 1). Determination of primary implant stability has also been used as an indicator for future osseointegration.

Figure 1: Dental implant and bone loss

The need for a clinically effective noninvasive technique for monitoring implant stability has led to the development of two major diagnostic tools. Whereas the Periotest[®] device (see Fig. 2a)) determines the damping capacity of a tooth or an implant (Periotest[®] value, PTV), the Osstell[®] system (see Fig. 2b)) is based on resonance frequency analysis (Implant stability quotient, ISQ).

Figure 2: Noninvasive technique for monitoring implant stability: a) Periotest[®] device; b) FE-model for Periotest[®]; c) Osstell[®] system; d) FE-modell for Osstell[®] system

Contradictory results have been reported on the comparability of implant stability measurements performed with Periotest[®] or Osstell[®] mentor. The purpose of this Finite Element Analysis (see Fig. 2b) and Fig. 2d)) was to simulate the influence of the parameters implant length, bone quality (cortical thickness and damping factor) bone loss and quality of transducer fixation on resonance frequency (RFA) and damping capacity measurements. Measurements were simulated at four stages of osseointegration.

The results of this investigation are published in [1]. In summery, although both measuring devices react similarly when different parameters of implant stability are changed, good correlation between PTV and ISQ can only be derived when measurement values of implants without bone loss are being considered.

References

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Quality of alveolar bone: Structure dependant material properties and a design of a novel measurement technique

Werner Winter, Thomas Krafft, Matthias Karl, Paul Steinmann

The purpose of this investigation was to describe the mechanical behavior of cortical and trabecular bone in view of bone structure, bone density and stiffness which can be used as a basis for determining bone quality by measuring elastic properties of bone (see Fig. 1) and to design a novel device for the determination of bone quality following implant site preparation.

Figure 1: Dental implant and states of bone qualities

In view of elastic mechanical behavior trabecular bone is a cellular material and cortical bone a material with pores. Thus, we can use the results of cellular material in general as shown in [1]. In Fig. 2 the results of numerical simulation of the material stiffness (Young's modulus) is plotted against the relative density. Some special results for trabecular bone behavior are also shown.

Figure 2: Normalized Young's modulus against relative density

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4 Activities in 2009

4.1 Teaching

- Statik (MB) (video recording http://www.video.uni-erlangen.de/cgi-bin/index.pl/Course/15)
- Elastostatik und Festigkeitslehre (MB)
- Statik und Festigkeitslehre (CBI, LSE, Mech, MT, Wing, WW, ET)
- Dynamik starrer Körper (MB, Mech, Wing)
- Lineare Kontinuumsmechanik (MB, Mech, Wing)
- Nichtlineare Kontinuumsmechanik (MB, Mech)
- Technische Schwingungslehre (MB, Mech, Wing)
- Mehrkörperdynamik (MB, Mech)
- Einführung in die Schädigungsmechanik (MB)
- Mechanik der Materialverbunde (MB)
- Bruchmechanik (MB)
- Methode der Finiten Elemente (MB, Mech, Wing)
- Finite Elemente in der Plastomechanik (MB)
- Introduction to the Finite Element Method (CE)
- Nichtlineare Finite Elemente (MB, CE)
- Finite Elemente Praktikum (MB, Mech)
- Höhere Festigkeitslehre (MB)
- Hauptseminar (MB, Mech)
- Seminar über Fragen der Mechanik
- Number of exams 2078

4.2 Industrial contributions to lectures

4.3 Dissertation theses

• Jürgen Schmidt, *Experimentelle und numerische Untersuchung dynamisch belasteter Verbundstrukturen mit zellularen metallischen Kernen*

Dissertation theses at LTM of University of Kaiserslautern, supervised by P. Steinmann:

- Philippe Jäger, *Theory and numerics of three-dimensional strong discontinuities at finite strains.*
- Holger Meier, *Computational homogenization of confined granular media.*

4.4 Diploma theses

- F. Hauer, *Generierung und Analyse des Kontaktverhaltens anisotroper, nicht-Gaußscher Oberfl¨achen*
- A. Knorr, *Statistische Qualifizierung von Streuungseinfl¨ussen bei Finite-Elemente-Festigkeitsanalysen von Kraftwerkskomponenten*
- T. Götzmann, *Vergleich von gemessener Schallabstrahlung an Fahrzeugtüren mit mittels FEM und BEM berechneten Simulationsergebnissen*
- M. Walter, *Erarbeitung und Analyse eines thermomechanisch optimierten Druckmaschinenlagerkonzeptes*
- S. Schmaltz, *Elastoplastische Spannungsberechnung an rissbehafteten Strukturen mit der Randelementmethode*

4.5 Student research projects theses

- C. Absenger, *Vergleichende Untersuchung der Knochenbeanspruchung bei Implantaten mit unterschiedlichen Oberfl¨achen*
- M. Amann, *Implementierung eines elastischen Materialgesetzes f¨ur große Deformationen basierend auf einem logarithmischen Verzerrungsmaß*
- M. Ammon, *Implementierung eines effizienten Kontaktalgorithmus zur Behandlung des 3D-Risskontakts*
- M. Heckel, *Gestaltoptimierung von Stabwerken*
- P. Heinl, *Identifikation und Regelung eines Axialkolbenverstellmotors*
- R. Prüller, *Vergleich verschiedener Modellierungsmethoden zur Erstellung von Stabwerkskonstruktionen*
- M. Reißner, *Untersuchung der Kopplung der Finiten Elemente Methode mit teilchenbasierten Berechnungsverfahren unter Verwendung von Matlab*
- K. Seiler, *Untersuchung thermischer Einfl¨usse auf das 3D Rissausbreitungsverhalten am Beispiel* $einer\ rotierenden\ Scheibe\ einer\ arialen\ Strömunasmaschine$
- D. S¨uß, *Quer- und Vertikaldynamikuntersuchungen von Kraftfahrzeugen*

4.6 Girls' Day

As every year, aiming to interest young girls in engineering and natural sciences, the Girls' Day (23.04.2009) provided an insight into science and education at the University of Erlangen-Nuremberg. The Chair of Applied Mechanics offered the opportunity to perform interesting experiments in the field of solid mechanics ranging from photoelasticity to finite elements.

4.7 Long Night of Science

Die Lange Nacht der **issenschaften**

Nürnberg·Fürth·Erlangen Sa 24.10.2009 18-1 Uhr

Already for the fourth time since its start in the year 2003, on Saturday, October 24th, Die Lange Nacht der Wissenschaften ('Long Night of Science') took place in the cities of Nuremberg, Erlangen and Fuerth. Between 6 p.m. and 1 a.m. an interested audience had the chance to inform itself at universities, non-university research institutes, companies and other institutions about current trends in sciences and development. The Chair of Applied Mechanics, as in the years 2003, 2005 and 2007 before, shared in this event and opened its doors on Saturday evening to introduce research results in the areas of experimental stress analysis, system dynamics and cellular materials. The extremely high attendance at our chair encourages us to participate also next time in Die Lange Nacht der Wissenschaften, which will be taking place in autumn 2011.

4.8 Ultimate Load Contest - The Student Event

Taking place on the 16th December 2009, the Ultimate Load Contest again attracted more than a dozen of participating groups consisting of students of all engineering disciplines. The object of this contest is an optimization problem in applied mechanics: built out of hard masonite and commercial glue, an engineering structure is loaded until it collapses. The structure is supported at three points and should have a weight of not more than 2 kg. Nearly 200 spectators were thrilled by the events 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.

4.9 Seminar for Mechanics

4.10 Editorial activities

4.10.1 Edited Books

Steinmann, Paul (Editor): Progress in the Theory and Numerics of Configurational Mechanics. Proceedings of the IUTAM Symposium Erlangen, Germany October 20-24, 2008 Band. XII. Berlin : Springer, 2009 (IUTAM Bookseries Band. 17) - pp. 272, ISBN 978-90-481-3446-5

4.10.2 GAMM-Mitteilungen

The GAMM-Mitteilungen (GAMM-Messages) are published by Wiley-VCH Verlag, Berlin twice a year (http://www3.interscience.wiley.com/journal/60500232/home). They are edited by Prof. P. Steinmann

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4.10.3 Advisory/Editorial Board Memberships

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- International Journal of Numerical Methods in Engineering
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5 Talks

- 1. P. Fischer, J. Mergheim, P. Steinmann. C1 continuous discretization of gradient elasticity based on Bernstein-B´ezier patches 80th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM), Gdansk, Poland, 09-13.02.2009
- 2. S. Germain, M. Scherer, P. Steinmann. On Inverse Form Finding for Hyperelasticity in Logarithmic Strain Space. 7th EUROMECH Solid Mechanics Conference (ESMC 2009), Lisbon, Portugal, 7-11.09.2009
- 3. D. Görke, K. Willner. Experimentelle und numerische Untersuchung des Kontaktverhaltens rauer metallischer Oberflächen. VDA Workshop 'Grundlagen der Bremsgeräusche - Industrie trifft Universität', Frankfurt, 18.05.2009
- 4. M. Hossain, G. Possart, P. Steinmann. A Phenomenological Finite Strain Framework for the Simulation of Elastic Curing. Sixth European Conference on Constitutive Models for Rubber (ECCMR VI), Dresden, Germany, 07-10.09.2009.
- 5. M. Hossain, G. Possart, P. Steinmann. Finite Strain Viscoelastic Models to Simulate the Curing Process of Polymers. 1st International Conference on Material Modelling, Dortmund, Germany, 15-17.09.2009.
- 6. A. Javili, P. Steinmann. A Finite Element Framework for Continua with Boundary Potentials. 80th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM), Gdansk, Poland, 09-13.02.2009
- 7. M. Kraus, P. Steinmann. Polygonal finite element formulations for 2d linear-elastic FE problems. 80th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM), Gdansk, Poland, 09-13.02.2009
- 8. J. Mergheim. Multiscale modelling and simulation of failure processes and heterogeneous materials. Seminar for Computational Mechanics, Universität Erlangen-Nürnberg, 19.03.2009
- 9. J. Mergheim. Simulation of failure processes with the variational multiscale method. ESAFORM, Twente, Holland, 28.04.2009
- 10. J. Mergheim. Computational Multiscale Modeling of Solids at Failure. Research Day, Lehrstuhl für Systemsimulation, Universität Erlangen-Nürnberg, 13.08.2009
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- 12. S. Pfaller, P. Steinmann. On Bridging Domain Methods to Couple Particle- and Finite-elementbased Simulations. 80th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM), Gdansk, Poland, 09-13.02.2009
- 13. S. Pfaller, P. Steinmann. On Bridging Domain Methods to Couple Particle- and Finite-elementbased Simulations. 2nd South-East European Conference on Computational Mechanics, Greece, Island of Rhodes, 22-24.06.2009
- 14. G. Possart, M. Hossain, P. Steinmann. Modelling and Simulation of Curing Polymer Adhesives. Seminar für Mechanik, Universität der Bundeswehr München, Neubiberg, Germany, 25.03.2009.
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7 Contributions to Proceedings in 2009

- 1. S. Bargmann, R. Denzer, P. Steinmann. On Configurational Forces within Green-Naghdi Thermo-Hyperelasticity. In *Proceedings of IUTAM Symposium on Progress in the Theory and Numerics of Configuration Mechanics* (peer reviewed), Erlangen, Germany, 20.-24.10.08. 2009.
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