Annual Report
2012

Chair of Applied Mechanics
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Prof. Dr.-Ing. Kai Willner
Prof. Dr.-Ing. Julia Mergheim
University of Erlangen-Nuremberg

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Contents

1 Preface

It is again a good time to look back in order to reflect on the academic achievements and social activities at the Chair of Applied Mechanics. The various summer barbecues, parties and excursions may surely have served as an incentive to fulfil the quite heavy teaching commitments and produce the internationally recognised outputs, but it was of course only the hard work and amazing enthusiasm of all of the member of the Chair that made this possible. This annual report aims to highlight the modus operandi at the Chair of Applied Mechanics at the University of Erlangen-Nuremberg during 2012 and should convince the reader of the high level of dedication and ambition exhibited by all members of the Chair.

Paul Steinmann, Kai Willner, Julia Mergheim

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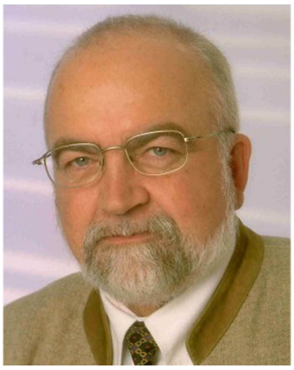

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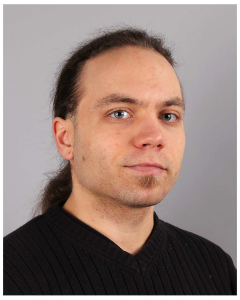
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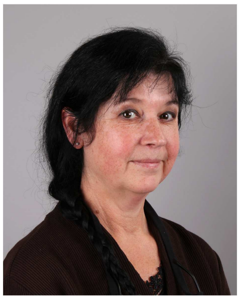
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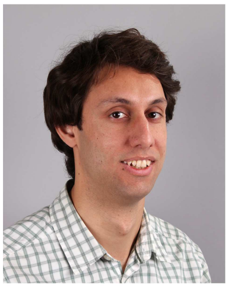
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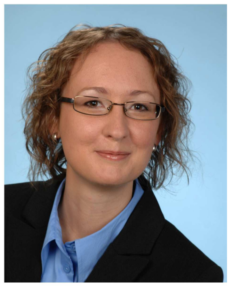
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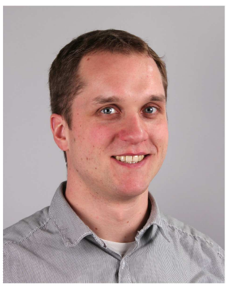
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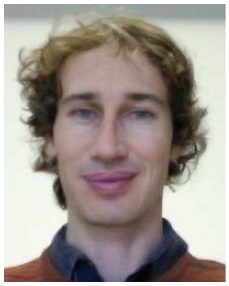
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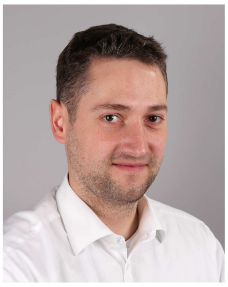
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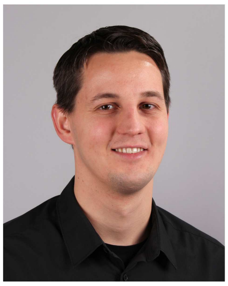
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Student assistants are mainly active as tutors for young students in basic and advanced lectures at the BA- and MA-level. Their indispensable contribution to high quality teaching at the Chair of Applied Mechanics is invaluable, thus financial support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

3 Scientific Reports

The following pages allow a short overview on the various ongoing research projects pursued at the Chair of Applied Mechanics during 2012. These are mainly financed by third-party funding of various (public and industrial) funding sources and are in addition supported by the core support of the university. Topicwise we have a nice mix of continuations of previous projects with projects that started afresh in 2012. Also the complementing expertise as displayed in the three professorships for continuum mechanics, structural mechanics and computational mechanics established at the Chair of Applied Mechanics is reflected by the variety of research that is performed. This spans from atomistic approaches to structural problems, from experimental investigations to computational challenges and from frictional contact to dental mechanics. Of course the research on these topics constantly produces new insights, thus the following reports can only shed a spot-light on the current state of affairs.

Homogenization Framework for Magnetorheological Elastomers

George Chatzigeorgiou, Ali Javili, Paul Steinmann

This work presents a homogenization framework for magnetorheological elastomers under large deformation. The developed framework is general and can be applied for linear and nonlinear material constitutive laws.

Considering a composite consisting of material constituents with general magnetomechanical behavior we define the homogenization process as a two scale approach. Both the macroscale and microscale responses in material and spatial description are presented and the connection between macroscopic and microscopic variables is established through appropriate volume averaging. We introduce appropriate potentials for the deformation gradient, the stress, the magnetic field and the magnetic induction and we identify the conditions for a well established homogenization problem in Lagrangian description that leads to a large deformation process with meaningful space averages [1].

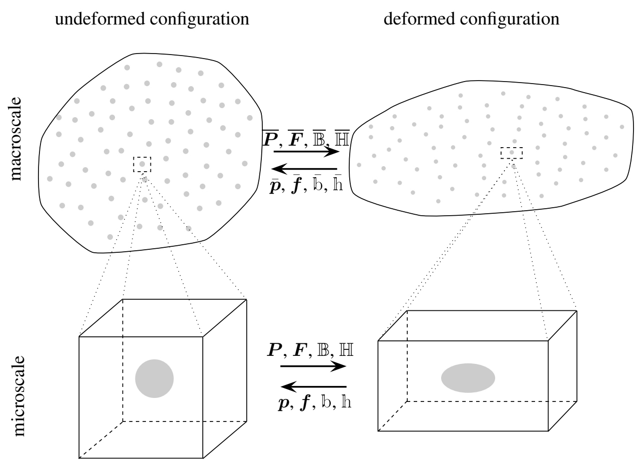


Figure 1: Macro- and microscale of a composite with magnetomechanical behavior in undeformed and deformed configuration

Using the Hill's lemma for large deformations [2] we obtain several magnetomechanical boundary conditions that satisfy the Hill-Mandel property, i.e. the volume average of the increment of the magnetomechanical energy in the representative volume element being equal to the macroscopic energy increment.

The connection between the macroscopic magnetomechanical field variables obtained in Lagrangian description and the volume averaging of the corresponding microscopic variables in the Eulerian description is examined for all combinitions of appropriate mechanical and magnetic boundary condition types. It is shown that the use of kinematic and magnetic field potentials instead of kinetic field and magnetic induction potentials provides a more appropriate homogenization process [3].

References

[1] F. Costanzo, G. L. Gray, P.C. Andia. On the definitions of effective stress and deformation gradient for use in MD: Hill's macro-homogeneity and the virial theorem. *International Journal of Engineering Science* **43**, 533–555 (2005).

[2] R. Hill. On macroscopic effects of heterogeneity in elastoplastic media at finite strain. *Mathematical Proceedings of the Cambridge Philosophical Society*, **95**, 481–494 (1984).

[3] G. Chatzigeorgiou, A. Javili, P. Steinmann. Unified magnetomechanical homogenization framework with application to magnetorheological elastomers. *Mathematics and Mechanics of Solids*, in press.

A coupled MD-FE simulation method accounting for interphases in nanoparticle filled thermoplastics

Denis Davydov, Ali Javili, Paul Steinmann

The aim of this project is to extend a recently developed hybrid MD-FE simulation scheme to describe materials dominated by polymer–solid interphases. In order to bridge the gap between particle-based models (MD) and continuum approaches, as well as to enhance the MD-FE simulation scheme, the basic framework to link the atomistic and the continuum world is introduced [1]. The approach allows a comparison of the MD and surface-enhanced FE solutions. As a benchmark example, a copper plate with a hole was considered in both molecular statics [2] and molecular dynamics [3] case. We compared atomistic fields obtained from the averaging procedure [1] to their counterpart, obtained from numerical approximations to the surface-enhanced continuum (SEC) theory, whereby the surface is equipped with its own constitutive structure. The ability of the SEC formulation to model size effects was shown [2]. The local fields evaluated using both the continuum and discrete approach are in a good agreement [2, 3]. The application of this methodology to the case of polymers with nanoparticles is work in progress. The financial support of the German Science Foundation (Deutsche Forschungs-gemeinschaft, DFG) , grant STE 544/46-1, is gratefully acknowledged.

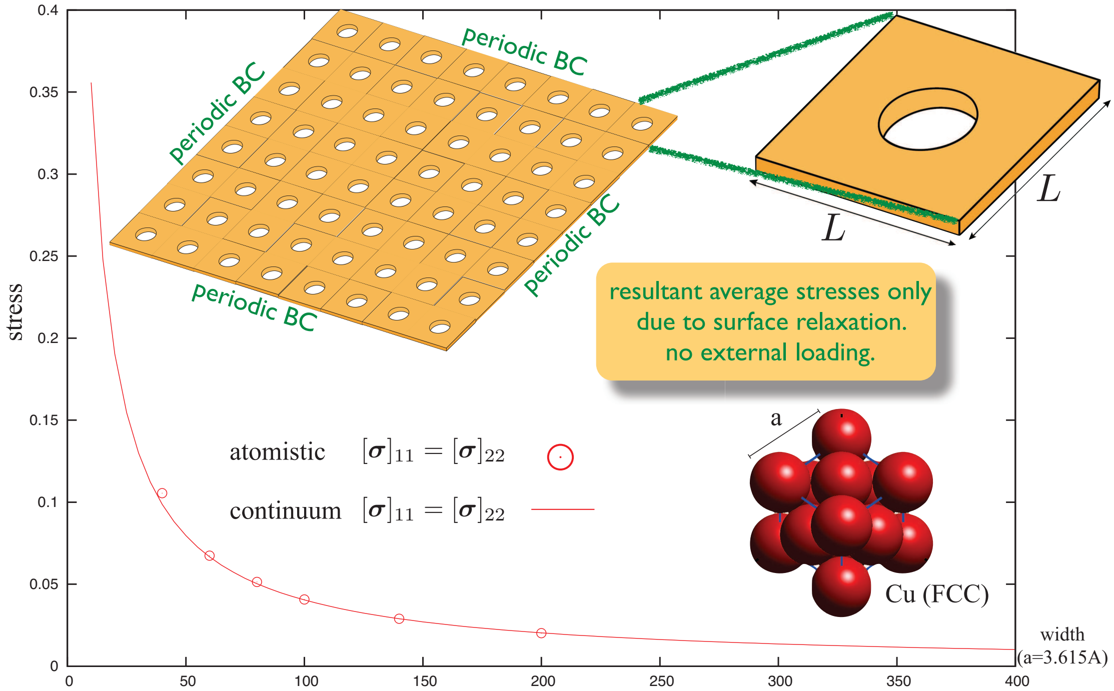


Figure 1: Illustration of the size effect due to the presence of the surface energy. Comparison of the surface enhanced continuum theory and atomistic calculations.

References

[1] D. Davydov, P. Steinmann. Reviewing the roots of continuum formulations in molecular systems. Part I: Particle dynamics, statistical physics, mass and linear momentum balance equations. *accepted.*

[2] D. Davydov, A. Javili, P. Steinmann. On molecular statics and surface-enhanced continuum modeling of nano-structures. *submitted.*

[3] D. Davydov, A. Javili, P. Steinmann, A. McBride. A Comparison of Atomistic and Surface Enhanced Continuum Approaches at Finite Temperature. *accepted*

Molecular static simulation of ferroelectric materials

Florian Endres, Paul Steinmann

Ferroelectric materials are modeled and simulated on different length scales between the electron structure and the continuum description. Especially models and algorithms on the atomistic level have been developed further in the last decade and attain accurate results. Still the computational costs of the established molecular dynamics methods are significant.
The aim of this project is the development of a quasi-static ansatz using the finite element method and the interaction potentials of the core shell model [1]. Using a finite element discretization of a crystal lattice the internal energy of the system can be described by:

$$U_{int} = \sum_{i=1}^{N} \sum_{\substack{j \neq i \\ |\mathbf{r}_{ij}| < R_c}} \frac{1}{4\pi\epsilon_0} \frac{q_i q_j}{|\mathbf{r}_{ij}|} + A\exp\left(-\frac{|\mathbf{r}_{ij}|}{\rho}\right) - \frac{C}{|\mathbf{r}_{ij}|^6} + \frac{1}{2} k_2 |\mathbf{r}_{ij}|^2 + \frac{1}{24} k_4 |\mathbf{r}_{ij}|^4$$

The core shell model describes not only the long range interaction between charged particles but also noncovalent bindings by the Buckingham potential. To this end every atom is described by two particles which represent the atom core and the electron shell of each ion linked by a nonlinear spring. Thus the polarization of the ions within a crystal is may be captured.

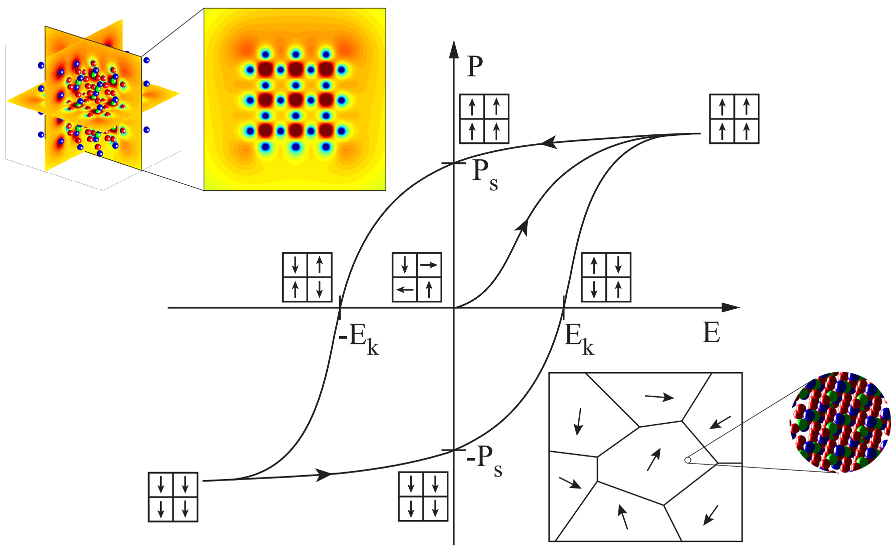


Figure 1: Dielectric hysteresis loop of a ferroelectric crystal

In a next step the molecular static model will be used to analyze polarization processes of barium titanate on an atomistic level. In order to simulate larger structures the quasi-static method will be combined with a continuum mechanics framework e.g. the quasicontinuum method or the FE^2 method.

References

[1] S. Tinte, M. Stachiotty, M. Sepliarsky, R. Migoni and C.O. Rodriguez. Atomistic modelling of $BaTiO_3$ based on first-principles calculations. *Journal of Physics: Condensed Matter* **11**, 9679–9690 (1999)

[2] Yihui Zhang, Ran Xu, Bin Liu, Daining Fang. An electromechanical atomistic-scale finite element method for simulating evolutions of ferroelectric nanodomains. *Journal of the Mechanics and Physics of Solids* **60**, 1383–1399 (2012).

A Novel Cohesive Zone Model Accounting for In-plane Stretch of an Interface

Ali Esmaeili, Ali Javili, Paul Steinmann

Interfaces play an important role in mechanical and thermal responses of a body simply because they can possess different properties than that of the bulk. The numerical modelling of a solid with finite deformation, using the finite element method, including mechanical interfaces, is performed to investigate these effects.
To numerically model a geometrically non-coherent interface, a decohesion element with mixed-mode capability and zero thickness, based on a normal-shear decomposition of displacement discontinuity is used, exploiting two different traction-separation laws: Bi-linear and Exponential [1]. The constitutive equation used, relates the traction vector to the displacement jump and the normal vector to the mid-plane for loading and unloading procedures [1, 2].

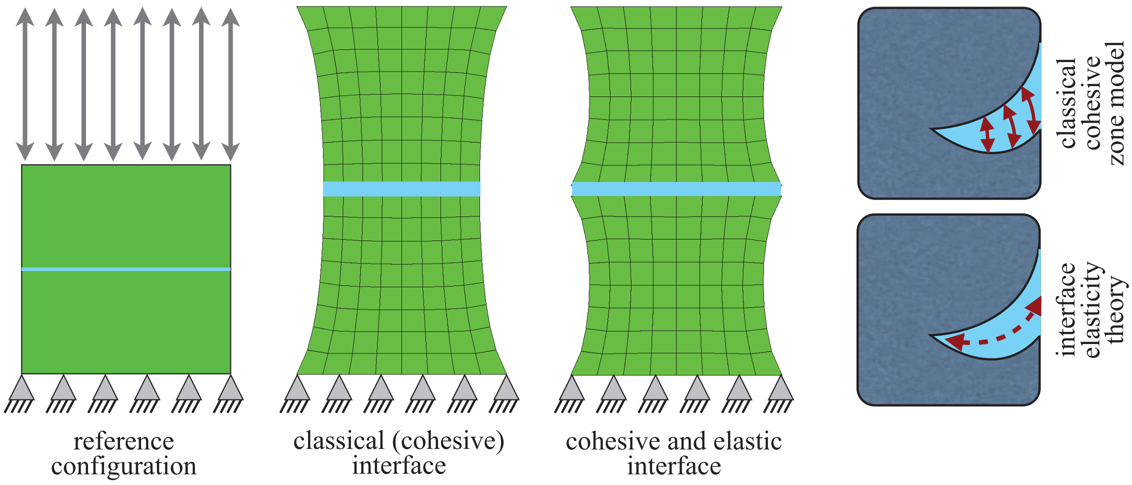


Figure 1: Interface with and without in-plane resistance.

In addition to classical strategies, interfacial elements are allowed to have in-plane stretch resistance by assuming a hyperelastic interface Helmholtz energy $\bar{\Psi}$. Let $\bar{\mathbf{F}}$ denote the interface deformation gradient of the mid-plane, a surface between two faces of interface. Motivated by the surface/interface elasticity theory [3], the interface Helmholtz energy is a function of the interface deformation gradient, $\bar{\Psi}(\bar{\mathbf{F}})$.

References

[1] M. Oritz, I. Pandolfi. Finite-Deformation Irreversible Cohesive Elements for Three-Dimensional Crack-Propagation Analysis. *International Journal for Numerical Methods in Engineering* **44**, 1267–1282 (1999).

[2] G. Alfano, M. A. Crisfield. Finite-Deformation Irreversible Cohesive Elements for Three-Dimensional Crack-Propagation Analysis. *International Journal for Numerical Methods in Engineering* **50**, 1701–1736 (2001).

[3] A. Javili, A. McBride, P. Steinmann. Thermomechanics of Solids with Lower-Dimensional Energetics: On the Importance of Surface, Interface and Curve Structures at the Nanoscale. A Unifying Review. *Applied Mechanics Reviews* (in print).

On the homogenization of technical textiles

Sebastian Fillep, Julia Mergheim, Paul Steinmann

The consideration of the macroscopic behavior of microscopic heterogeneous material can be performed by a multi scale modeling method [1, 2, 3].
Technical textiles conform to that description of materials with a nonlinear behavior that differs from the underlying fiber material and is due to heterogeneities on the micro level. The macroscopic constitutive behavior is strongly influenced by the structural assembly of the fibers and the appearing contact zones.
On the macroscopic level textiles are characterized by a large area-to-thickness ratio, such that a discretization with shell elements is numerically efficient. To capture the contact the representative volume element is explicitly modeled by means of a volumetric micro sample. The challenge is to transfer the information across length scales. Therefore a shell specific homogenization scheme is applied to transfer the microscopic response to the macro level. Therefore the microscopic continuum quantities have to be pre-integrated in thickness direction to create shell specific stress resultants. Afterwards the stress resultants are transferred across the length scales.

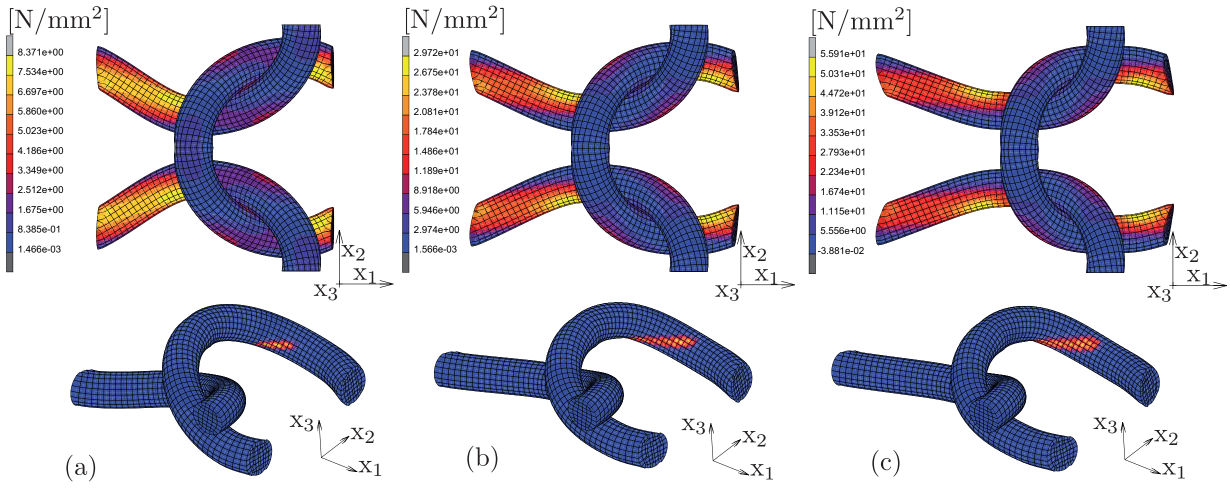


Figure 1: Von Mises plot of a knitted representative volume element for different stretch deformations (top) and display of the contact zone (below) for prescribed macroscopic deformations e_{11} of (a) 0.12, (b) 0.30, (c) 0.40.

The resulting nonlinear material behavior is strongly influenced by the arising micro structural contact zones between the fibers as depicted in Figure 1. Therewith physically motivated constitutive laws can be derived.

References

[1] S. Fillep, J. Mergheim, P. Steinmann. Modelling and homogenization of technical textiles. *(submitted)*

[2] S. Fillep, J. Orlik, Z. Bare, P. Steinmann. Homogenization in periodically heterogeneous elastic bodies with multiple micro contact. *(submitted)*

[3] E.W.T.Coenen, V.G. Kouznetsova, M.G.D. Geers. Computational homogenization for the heterogeneous thin sheets. *International Journal for Numerical Methods in Engineering* **83**, pp. 1180-1205, (2010).

Adaptive h–refinement based on asymptotic expansions for node insertion on finite element meshes

Jan Friederich, Günter Leugering[1], Paul Steinmann

[1] Chair of Applied Mathematics II, University of Erlangen-Nuremberg

We consider h–refinement on finite element discretizations by continuous graph changes such as splitting nodes along edges. A possible scenario is depicted in Figure 1, where the continuous process of inserting the new node $\mathbf{x}_\epsilon$ along edge $E = (\mathbf{x}_0, \mathbf{x}_+)$ is parametrized in the variable $\epsilon > 0$. This approach allows for the calculation of the sensitivity of an objective functional J with respect to the topological mesh change: Considering a linear second-order elliptic PDE with Galerkin solutions u_h and u_h^ϵ corresponding to the finite element mesh $\mathcal{T}_h$ and the refined mesh $\mathcal{T}_h^\epsilon$, respectively, we define

$$D_E J(u_h) = \lim_{\epsilon \to 0} \frac{J(u_h^\epsilon) - J(u_h)}{\epsilon}.$$

For the computation of $D_E J(u_h)$ for a large class of functionals J we rely on the analytical derivation of the first-order asymptotic expansion of u_h^ϵ with respect to $\epsilon > 0$.
In this context, a particular objective functional J of interest is the total potential energy of the given variational problem, minimization of which can be shown to decrease the approximation error $\|u - u_h\|$ in the energy norm [1]. Hence, these sensitivities can be employed as edge-wise indicators for local h–refinement. Analytical as well as numerical examinations prove that this approach leads to an competitive strategy for adaptive refinement in comparison to the well-known error estimation techniques [2].
The details of our method for a model problem in 1d are presented in [3]. More general results are currently prepared for publication. See Figure 2 for a numerical example in 2d.

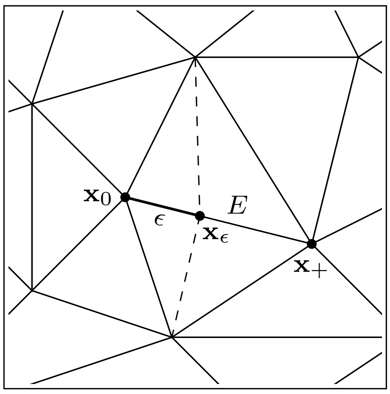


Figure 1: Insertion of the new node $\mathbf{x}_\epsilon$ along edge $E = (\mathbf{x}_0, \mathbf{x}_+)$.

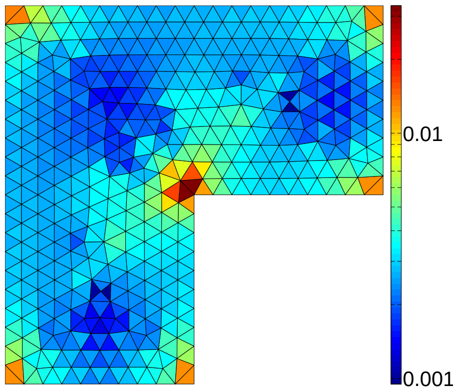


Figure 2: Logarithmic plot of refinement indicator based on topological sensitivities: $-\Delta u = c$, $u|_{\partial\Omega} = 0$ on L-shaped domain.

References

[1] M. Delfour, G. Payre, J.-P. Zolésio. An optimal triangulation for second-order elliptic problems. *Comput. Meth. Appl. Mech. Eng.* **50**, 231-261 (1985).

[2] R. Verfürth. A review of a posteriori error estimation and adaptive mesh refinement techniques. Wiley-Teubner, Chichester (1996).

[3] J. Friederich, G. Leugering, P. Steinmann. Adaptive refinement based on asymptotic expansions of finite element solutions for node insertion in 1d. *GAMM-Mitt.* **35**, 175–190 (2012).

On a recursive algorithm for avoiding mesh distortion in elasto-plastic inverse form finding

Sandrine Germain, Paul Steinmann

A challenge in the design of functional parts is the determination of the initial, undeformed shape such that under a given load a part will obtain the desired deformed shape, i.e. an inverse form finding problem. A gradient-based shape optimisation formulation can be used in the sense of an inverse problem via successive iterations of a direct mechanical problem in order to solve the inverse form finding problem. The objective function of the inverse form finding problem is defined by a least-square minimisation of the difference between the target and the current deformed configuration of the shape. The design variables are defined by the discretized nodes of the functional component with the finite element method (node-based shape optimisation). This choice may however lead to mesh distortions in the undeformed shape. For example, the target deformed configuration of the three dimensional extension of the classical two dimensional Cook's membrane is plotted in Figure 1. After two iterations of the shape optimisation the algorithm gets stuck and the undeformed shape plotted in Figure 2 is obtained, where mesh distortions are well identified. In order to avoid the mesh distortions a recursive algorithm [1] was implemented. Between two operations the current optimised undeformed configuration is used in the computation of the subsequent value of the objective function. The total applied force is then split onto all entities. Figure 3 shows the obtained undeformed Cook's cantilever with the use of the recursive algorithm. A disadvantage of the recursive formulation is the comparatively high computational costs.

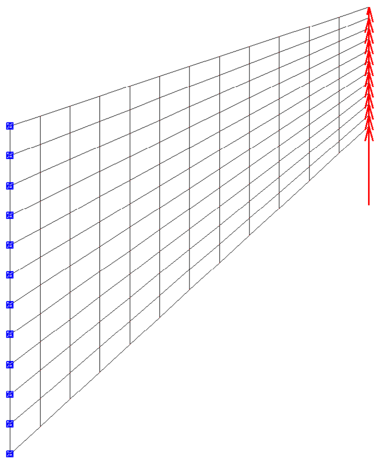


Figure 1: Deformed Cook's cantilever in the spatial configuration in the $[\boldsymbol{x}_1, \boldsymbol{x}_2]$ plane.

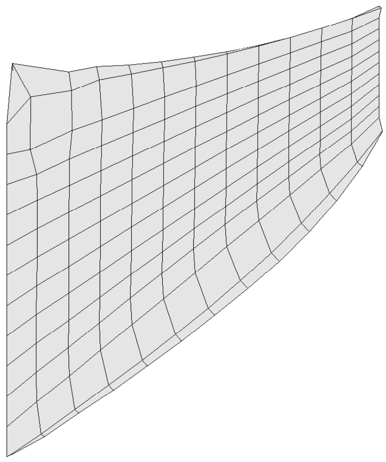


Figure 2: Undeformed Cook's cantilever in the material configuration in the $[\boldsymbol{X}_1, \boldsymbol{X}_2]$ plane after two iterations.

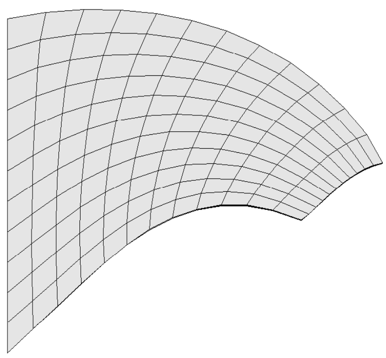


Figure 3: Undeformed Cook's cantilever in the material configuration in the $[\boldsymbol{X}_1, \boldsymbol{X}_2]$ plane.

This work is supported by the German Research Foundation (DFG) within the Collaborative Research Centre SFB Transregio 73.

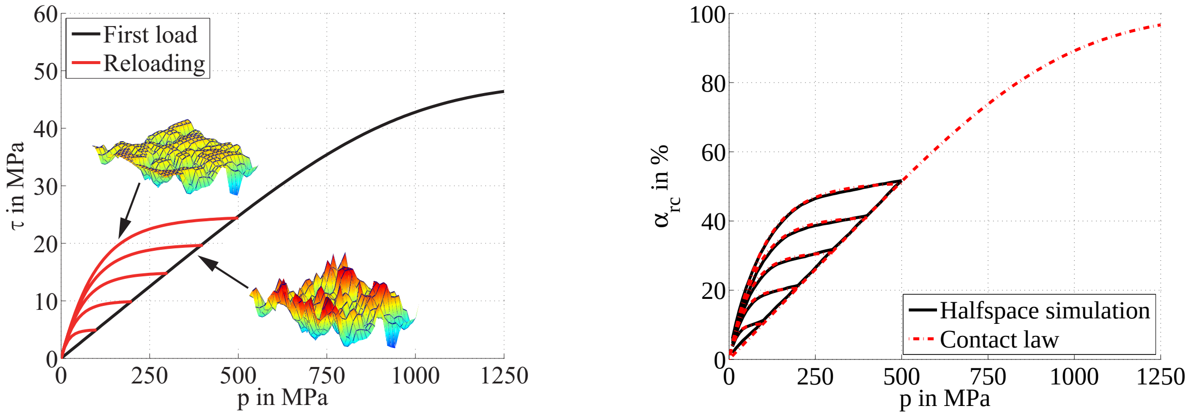
References

[1] S. Germain, P. Steinmann. On a recursive algorithm for avoiding mesh distortion in inverse form finding. *Journal of the Serbian Society for Computational Mechanics* **6**, accepted.

Development of a friction law for sheet-bulk metal forming

Franz Hauer, Kai Willner

Friction has an significant effect on the process and the product quality in metal forming in general. Characteristic of sheet-bulk metal forming are sheet forming operations with moderate contact pressures and bulk forming operations with large contact pressures in one process. Therefore a friction law modelling friction precisely both for low and high contact pressures is necessary for the accurately simulation of the sheet-bulk metal forming process. In order to derive a suitable friction law for this purpose a halfspace contact model has been calibrated and verified experimentally [1]. This halfspace model was used to perform various contact simulations taking into account the plastic smoothing of the surface in contact. Based on these simulation results a contact law was identified. Figure 1 a shows the good agreement between the contact simulations an the real contact ratio α_{rc} predicted by the identified friction law. The maximum shear stress in the contact τ is given by the ratio of the real contact area and the shear strength $m \cdot k_f$ in the real contact area, which is identified from experiments. Characteristic for the developed contact law is the distinction between first loading with an unsmoothed surface and un- and reloading with a smoothed surface. The real contact area ratio and thus the friction stresses are higher in re- and unloading due to the plastic surface smoothing.



a) b)

Figure 1: Contact area in halfspace simulation and contact law (a) and friction law (b).

$$\tau_r = m \cdot k_f \cdot \alpha_{rc} = m \cdot k_f \cdot \sqrt[n_1]{\tanh\left(\frac{p \cdot C_{el}}{H}\right)^{n_1}}$$

$$\tau_r = m \cdot k_f \cdot \sqrt[n_2]{\tanh\left(\frac{p \cdot C_{el} \cdot C_1}{H \cdot \alpha_{rc}\left(p_{hist}\right)}\right)^{n_2}} \cdot \alpha_{rc}\left(p_{hist}\right)$$

The friction law is defined by one equation for first loading and one equation for re- and unloading. Both equations perform a smooth transition to a stationary value for full contact at high contact pressures as defined by the Tresca friction law. The plastic surface smoothing in previous contact is incorporated into the second equation by the factor α_{rc}.

References

[1] F. Hauer, H. U. Vierzigmann, K. Willner, U. Engel. Numerical simulation of friction in metal forming using a halfspace model. *Proc. 14th Int. ESAFORM Conf. on Material Forming. AIP Conf. Proc. 1353*, 1741–1746 (2012).

Degree of cure-dependent modelling for polymer curing processes at small-strain

Mokarram Hossain, Paul Steinmann

The curing process of polymers is a complex phenomenon involving a series of chemical reactions which transform a viscoelastic fluid into a viscoelastic solid during which the thermal, the chemistry and the mechanics are coupled. A physically-based small strain curing model has been developed and discussed in our previous contribution [1] which is extended later for finite strain elasticity and viscoelasticity including shrinkage. The previously proposed constitutive models for curing process are based on the temporal evolution of the material parameters, namely the shear modulus and the relaxation time (in the case of viscoelasticity). A thermodynamically consistent small strain constitutive model is formulated here that is directly based on the degree of cure, a key parameter in the curing (reaction) kinetics. The new formulation is also in line with the earlier proposed hypoelastic approach. To illustrate whether the proposed model simulate the shrinkage during curing, we adopt a setup for a thin three-dimensional plate that has dimension of $40 \times 10 \times 0.5\,mm^3$ which is discretised by eight-hundred linear brick elements. The final volume reduction is considered as ten percent. Figure 2 depicts the bearing specific deformations as well as the Cauchy stresses in x-direction after 10^6 seconds of curing simulated with the newly proposed viscoelastic curing model together with the shrinkage model [2].

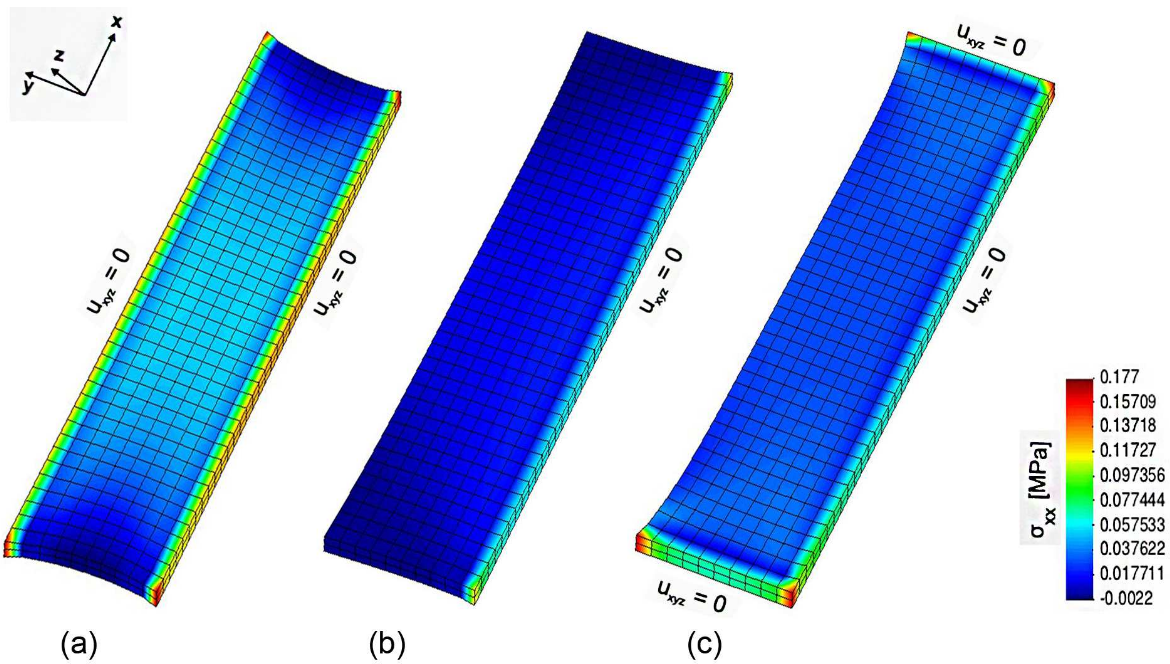


Figure 2: Curing shrinkage of a thin three-dimensional plate subjected to three different bearing conditions, i.e. two longitudinal sides are clamped in all directions, cf. Fig. (a), only one longitudinal side is fixed and rest of the boundaries are free to move, cf. Fig. (b) and only one longitudinal side is free to shrink, cf. Fig. (c); deformation (scaled by two) and Cauchy stress in x-direction.

References

[1] M. Hossain, G. Possart, P. Steinmann, A small-strain model to simulate the curing of thermosets, *Computational Mechanics* 43 (2009) 769-779

[2] M. Hossain, P. Steinmann, Degree of cure-dependent modelling for polymer curing processes at small-strain. Part I: Reformulation, *Submitted* (2012)

Interactions of particles in viscous flows

Simone Hürner, Paul Steinmann

Numerical simulations are widely used to predict interactions of particles in viscous flows under various conditions, like the influence of magnetic fields [1] [2] [3]. Normally, these simulations are executed, assuming a stoke number of zero by implementing the particle behavior into pre-simulated liquid flow profile [4]. However, this approach neglects the influence of particles on the fluid, which has to be considered for stokes numbers unequal to zero. In order to optimize these calculations, this work focuses on developing a numerical simulation tool taking into account both interaction of particles in viscous flows and the impact of particles to the fluid itself.

For implementing the impact of particles to the fluid into such a simulation tool, first of all, it is necessary to predict the properties of the investigated fluid exactly. For this reason, simulations of different fluids in a three dimensional tube are carried out using the FEM-based simulator deal.ii as well as the FVM-based simulator Open-Foam. During the numerical experiments, different current flow profiles are simulated varying velocity, viscosity and density. The result of these experiments are compared and evaluated concerning its contribution to a global simulation tool for particles in fluids. Furthermore, the profiles are used in a particle simulator developed by the University of Maribor. In this simulator, the kinetic reaction of particles in a liquid fluid, caused by a magnetic field in different current flow profiles can be investigated.

On the one hand, these experiments provide a better understanding of the physical principles of particles in liquid fluids. On the other side, these numerical results serve as base and reference for the development of a global simulation tool considering the influence of particles to the current flow profile in fluids with a stoke number unequal to zero.

References

[1] H. Chen, M. Kaminski, X. Liu, Y. Xie, C. Mertz, M. Torno et al. A novel human detoxification system based on nanoscale bioengineering and magnetic seperation techniques. *Med Hypotheses* **68**, 1071–1079 (2007).

[2] G. Hatch, R. Stelter. Magnetic design considerations for devices and particles used for biological high-gradient magnetic seperation (HGMS) systems. *J Magn Magn Mater* **225**, 262–276 (2001).

[3] M. Kaminski, AJ.Rosengart. Detoxification of blood using injectable magnetic nanospheres: a conceptual technology description. *J Magn Magn Mater* **293**, 398–403 (2005).

[4] J. Ravnik, L. Škerget, M. Hriberšek, Z. Žunič Numerical simulation of dilute particle laden flows by wavelet BEM-FEM. *Comput Meth Appl. Mech. Eng* **197** , 789–805 (2007).

Thermomechanics of Solids at the Nanoscale.

Ali Javili, Andrew McBride, Paul Steinmann

Surfaces and interfaces can significantly influence the overall response of a solid body. Their behaviour is well described by continuum theories that endow the surface and interface with their own energetic structures. Such theories are becoming increasingly important when modelling the response of structures at the nanoscale. The objectives of this project are as follows. The first is to summarise the key contributions in the literature. The second is to unify a select subset of these contributions using a systematic and thermodynamically consistent procedure to derive the governing equations. The governing equations describe the fully nonlinear response. Expressions for the energy and entropy flux vectors, and the admissible constraints on the temperature field, all subject to the restriction of non-negative dissipation, are explored. A weak formulation of the governing equations is then presented which serves as the basis for their approximation using the finite element method. The final objective is to elucidate the theory using a series of numerical example problems. Consider a square strip which is partitioned into

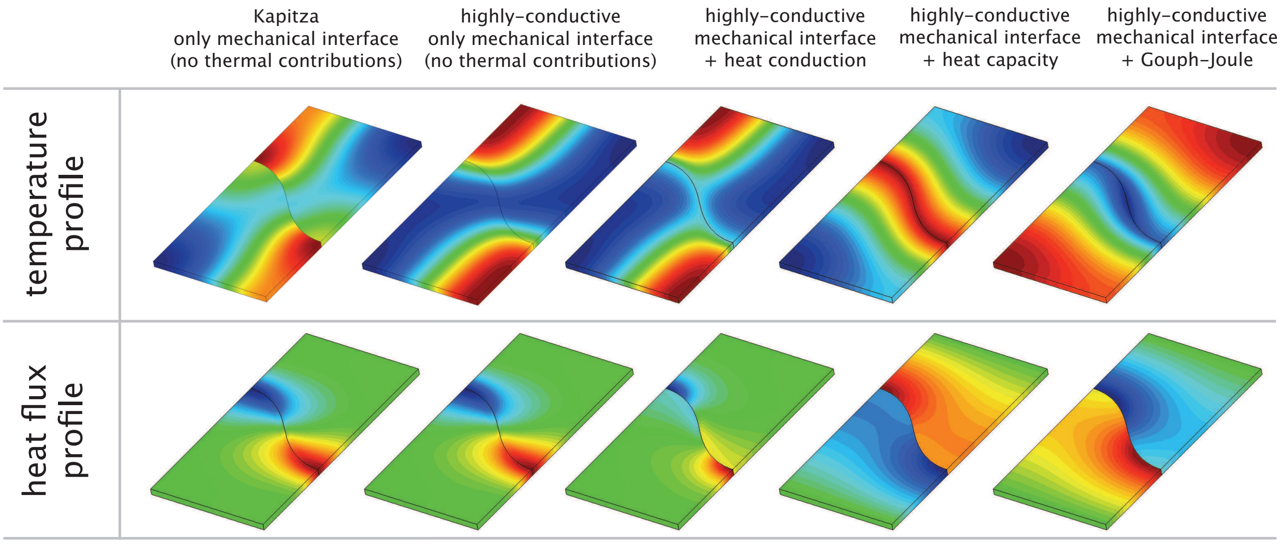


Figure 1: Illustration of the temperature and heat flux profiles for Kapitza and highly-conductive interfaces. For the (only) mechanically energetic interface the normal heat flux across the interface is continuous while for the thermally energetic one is not.

two homogeneous domains by a (thermo-)mechanically energetic interface. A displacement of 100% is prescribed adiabatically, at the specimen level, at the edges resulting in a tensile loading. Lateral deformations as well as change of the thickness are prevented. The mechanical resistance of the interface results in non-homogeneous stress and temperature distributions due to the Gouph-Joule effect. The resulting temperature and heat flux profiles for two cases of the Kapitza and highly-conductive interfaces are illustrated in the Figure. A Kapitza interface, in contrast to a highly-conductive interface, allows the jump of the temperature across the interface while the normal heat flux vanishes.

References

[1] A. Javili, A. McBride, P. Steinmann. Thermomechanics of Solids with Lower-Dimensional Energetics: On the Importance of Surface, Interface and Curve Structures at the Nanoscale. A Unifying Review. *Applied Mechanics Reviews* (in print).

Investigation of a Duffing Oscillator Using the Concept of Nonlinear Normal Modes (NNMs)

Martin Jerschl, Dominik Süß, Kai Willner

Nonlinear normal modes (NNMs) can be seen as a kind of parallel theory to the theory of linear systems but for nonlinear ones. The definition of NNMs can be found in [1].
A first step in this project is to investigate a DUFFING oscillator experimentally, which was built within a student research project. The system consists of an 1-DOF oscillator with a cubic nonlinearity described by the equation of motion

$$J\ddot{\varphi} + c_{lin}\varphi + c_{nl}\varphi^3 = \hat{\varphi}_A \sin(\omega_A t)$$

and is excited harmonically. The cubic nonlinearity is progressive which leads to a hardening effect with increasing excitation amplitude. In contrast to linear systems, it is not possible to decouple the modes of nonlinear vibrations. Therefore the principle of modal superposition is not applicable as in the linear regime. Furthermore extremely complex dynamic behaviour, like jumps, bifurcation, sub- and super-harmonic vibrations, internal resonances, modal interaction and chaos, is not describable with the theory of linear normal modes [2], although the system behaves linearly at low energy levels. This can be seen in Figure 1 – obviously the curve in the configuration space [2] is getting more and more nonlinear or complex with increasing energy (corresponding to the excitation amplitude) in the system. Therefore the concept of nonlinear normal modes is used to investigate the dynamic behaviour of the DUFFING oscillator.
With understanding the structure of NNMs in such small models it shall be possible to forecast and compute the forced responses of nonlinear systems to periodic excitation [1] in large scale models, too.

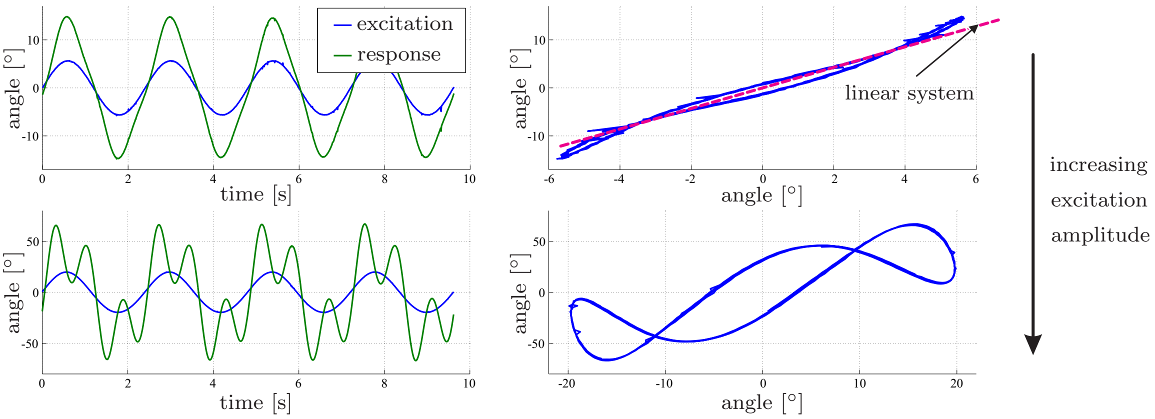


Figure 1: Forced response of the free pendulum ($f = 0.39\,\mathrm{Hz}$). Left plots: measured time series at different excitation amplitudes (5° and 20°). Right plots: corresponding configuration space (horizontal axis: excitation; vertical axis: response).

References

[1] A.F. Vakakis, L.I. Manevitch, Y.V. Mikhlin, V.N. Pilipchuk, A.A Zevin. *Normal Modes and Localization in Nonlinear Systems.* John Wiley & Sons, Inc., New York (1996).

[2] G. Kerschen, M. Peeters, J.C. Golinval, A.F. Vakakis. Nonlinear normal modes, Part I: A useful framework for the structural dynamicist. *Mechanical Systems and Signal Processing* **23**, 170–194 (2009).

Polytope finite elements for orthotropic material behavior

Markus Kraus, Paul Steinmann

The ability to model microstructures is one major motivation for the development of polytope finite elements. These polycrystalline grains often show an orthotropic material behavior, where each grain may posses different principal material axes. In the last year an orthotropic material model was implemented for polytope finite elements, see [1]. For the interpolation in the polyhedral element domains, a polyhedral interpolant has been established that is suitable for any convex and complex polyhedral domain, see [2].
Figure 1 show the view towards the initial beam axis of a deformed orthotropic cantilever simulated with different standard (a-b) and polytope (c-d) finite element formulations, where for comparison reasons the same principal axes were chosen in all element domains and the displacement magnitude is color coded. Besides standard elements, a polytope formulation that is based on an enhanced assumed strain approach is used. These EAS elements show terrific results for both standard and polyhedral meshes. Regarding the maximal deflections and rotations of the front face almost the same absolute values are obtained as by the C3D8I elements of the commercial ABAQUS environment, whereas the linear H_8 elements exhibit only feeble results in this test setup.

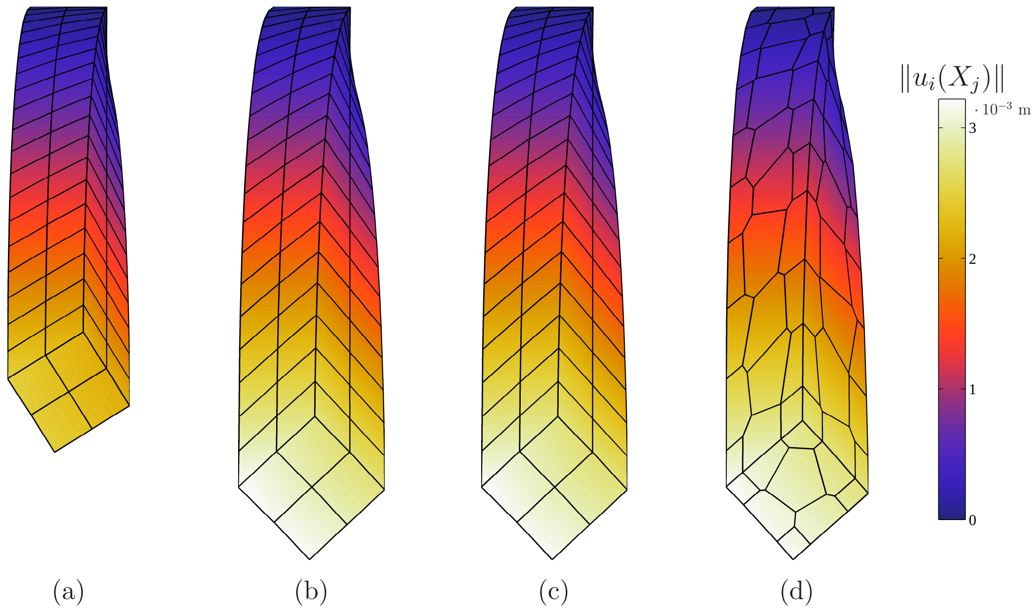


Figure 1: deformation of an orthotropic cantilever: (a) H_8 elements, (b) ABAQUS C3D8I elements, (c) EAS elements on hexahedral mesh, (d) polytope EAS elements on polyhedral mesh.

References

[1] M. Kraus. Entwicklung und Untersuchung polytoper Finiter Elemente für die nichtlineare Kontinuumsmechanik. *Ph.D. thesis*, submitted (in German).

[2] M. Kraus, P. Steinmann. *Finite element formulations for 3d convex polyhedra in nonlinear continuum mechanics*, Computer Assisted Methods in Engineering and Science, **19**, 121–134 (2012).

Analysis of the lamination stack influence onto the damping and stiffness of armature and stator active components

Vera Luchscheider, Kai Willner

For electric motors light weight construction becomes increasingly important. For a proper calculation of the motor it is therefore necessary to know the stiffness and damping behavior of the lamination stack. The stack is a pack of a lot of sheets for strengthening the magnetic field. The behavior of the stack is dependent on the mechanical behavior of the sheets and the contact behavior of the sheets surfaces. In a contact not the whole surface but only single peaks of the roughness are in contact (see Figure 1). Loading the contact with a force the roughness peaks being in contact are deforming and additional peaks are getting in contact. Because of this the behavior of the lamination stack is progressive (see Figure 2). The loading and the unloading curves are not equivalent, because there is a plastic deformation of the highest roughness peaks. So the simulation model has to be elastoplastic. Therefor the Bush-Gibbson-Thomas model [1] and the Bowden-Tabor model [1] are combined. The Bowden-Tabor model is a pure plastic model. The contact pressure $p_{pl.}$ is dependent on the hardness H and the ratio of the real and the nominal contact surface. As the roughness of a technical surface has a Gaussian distribution the ratio is equivalent with the cumulative function of this and the pressure

$$p_{pl.}(z) = H \cdot \frac{1}{\sigma \cdot \sqrt{2\pi}} \int_{-\infty}^{z} exp\left(-\frac{(t-\mu)^2}{2 \cdot \sigma^2}\right) dt$$

is known. The elastic model of Bush-Gibbson-Thomas is based on the theory of fractals. With that theory the surface parameters σ_z and x_T, which are independent of the resolution of measurement, are identified. The contact pressure

$$p_{el.}(z) = \frac{E^*}{2\pi} \frac{\sigma_z^2}{x_T \cdot z} \cdot exp\left(-\frac{z^2}{2 \cdot \sigma_z^2}\right)$$

is dependent on the Hertzian contact modulus E^* and the surface structure.

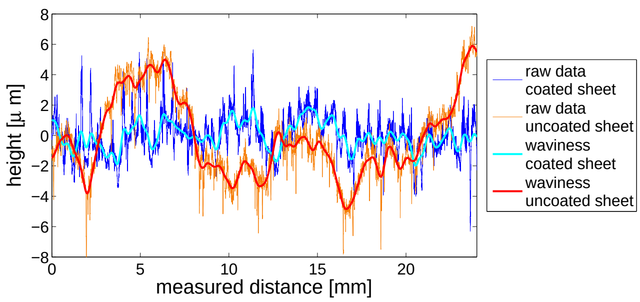


Figure 1: raw data and waviness data of the sheets surfaces

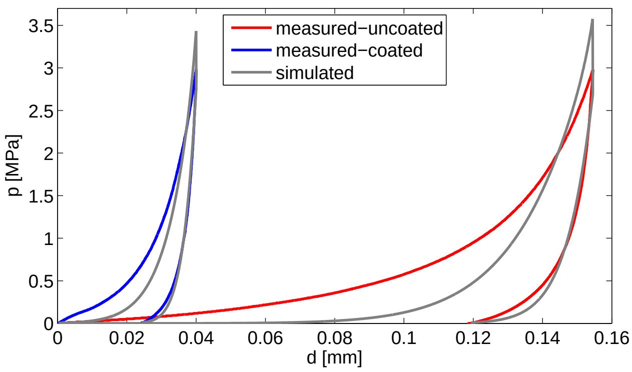


Figure 2: measured and simulated stiffness behavior of the lamination stacks

This project is a cooperation with Siemens AG.

References

[1] K. Willner. Influence of Surface Parameters on the Elastoplastic Contact Behavior of Fractal-Regular Surfaces . *Journal of Tribology* **130**, (2008).

Micro-to-macro transitions for continua with surface structure at the microscale

Ali Javili, Andrew McBride, Julia Mergheim, Paul Steinmann, Ulrike Schmidt

The objective of this presentation is to detail an application of the computational micro-to-macro transition framework that involves the surface elasticity theory of Gurtin and Murdoch. For this application, the microstructure contains voids with additional surface energy. The response of the associated macrostructure is approximated using elasticity theory. Homogenisation, as pioneered by Hill, provides a consistent methodology to link the macroscopic and microscopic scales.

The motivation for endowing the surface of the voids at the microscale with their own structure is to capture the well-documented effect whereby the surface plays an ever-increasing role in the overall macroscopic response as the size of the voids decrease. At the microscopic scale we have a continuum with a surface structure and the constitutive laws are presumed known [1]. At the macroscopic scale the constitutive relations are not explicitly known; they are replaced by the results of the computations on the microscopic scale using numerical homogenisation.

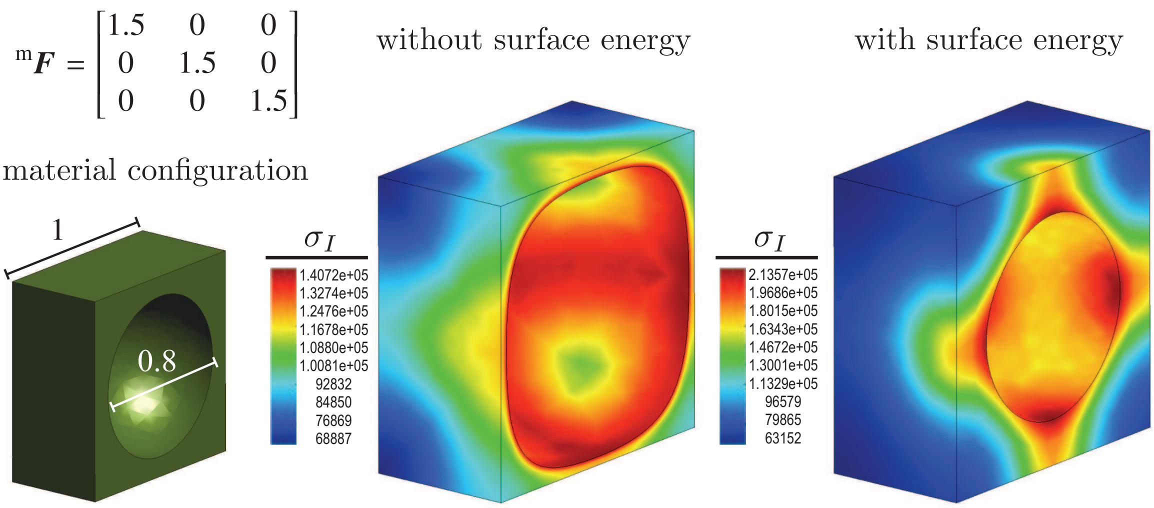


Figure 1: The response of a three-dimensional microstructure to a macroscopic volumetric expansion type loading condition $^{\mathrm{m}}\boldsymbol{F}$. The material and spatial configurations without and with an energetic surface are shown. The distribution of the von Mises stress is indicated.

An interesting outcome of endowing the microstructure with one or more energetic surfaces is that the response of one microstructure relative to another is dependent on the ratio of the area of the energetic surfaces to the volume of the bulk. Our key contribution here is the numerical determination (using the finite element method) of the effective macroscopic material properties as a function of both the microscopic void size and the coupling between the microscopic bulk and surface free energies [2].

References

[1] A. Javili, P. Steinmann. On thermomechanical solids with boundary structures. *International Journal of Solids and Structures* 47, 3245–3253 (2010).

[2] A. Javili, A McBride, J. Mergheim, P. Steinmann, U. Schmidt. Micro-to-macro transitions for continua with surface structure at the microscale. *In Review.*

Damage in thermosetting adhesives

Julia Mergheim, Gunnar Possart, Paul Steinmann

The curing of thermosetting adhesives is a complex polymerization process that involves the transition of a viscous liquid into a viscoelastic solid. The following observations can be made during this process and, consequently, should be reproduced by the curing model, compare [1]: The development of new cross-links increases the stiffness and viscosity of the material, but not its stress-state - unless an externally applied strain-state is modified. Therefore, the model has to include temporally evolving material parameters and it has to be formulated in terms of the rates of stress and strain. Furthermore, the specific volume of the material is decreasing, which is reproduced here by using a curing-dependent volumetric shrinkage strain. This shrinkage and the increase in stiffness can lead to mechanical stresses within the adhesive layer. If the mechanical stresses exceed a critical value, thermosetting materials are known to be prone to the initiation and growth of micro-cracks, which reduce both load-bearing capacity and durability of the adhesive joint. Emergence and evolution of such defects is here modeled in a 'smeared' or homogenized manner by a continuum damage approach. The basic idea consists of the introduction of a damage state variable quantifying the amount of degradation present within the material. This damage variable increases whenever an appropriately chosen equivalent stress-, strain- or energy-measure exceeds a pre-defined threshold and reduces the stiffness. The strain-softening characteristic of such material models leads to severe mathematical problems which are related to the loss of ellipticity of the corresponding governing equilibrium equations. Therefore, a regularization method has to be adopted to obtain meaningful and mesh-independent numerical simulations. Here, an implicit gradient-enhanced damage formulation is combined with the viscoelastic curing model.
A double-lap shear test is simulated, whereby the curing process of the adhesive layers and subsequent loading is taken into account. The influence of the curing shrinkage is compared by adopting three different magnitudes: 0%, −1% and −2%. The figure below shows the geometry of the structure, the load displacement answers for the three cases and damage distributions within the adhesive layer at the end of the curing process.

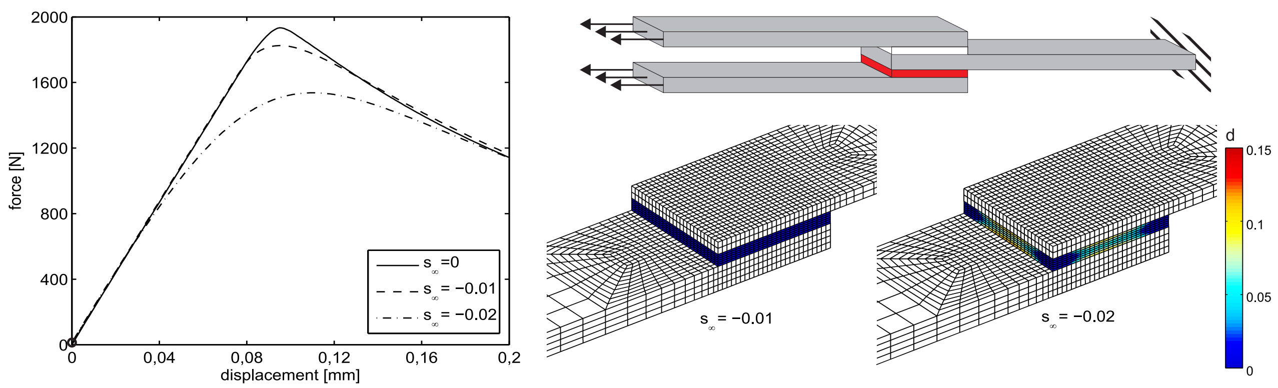


Figure 1: Double-lap shear test: load displacement response, geometry and damage distributions at the end of the curing process for two different shrinkage magnitudes

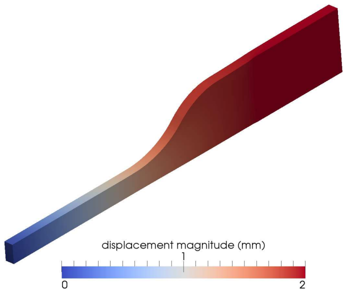
References

[1] J. Mergheim, G. Possart, P. Steinmann. Modeling and simulation of curing and damage in thermosetting adhesives. *The Journal of Adhesion*, accepted (2012).

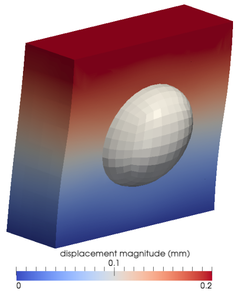
A framework for computational modelling of thermal- and magneto-sensitive polymers

Jean-Paul Pelteret, Paul Steinmann

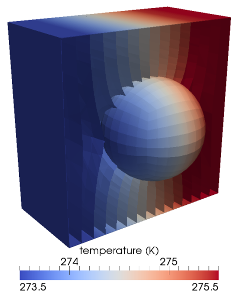
The ERC advanced grant MOCOPOLY (multi-scale, multi-physics modelling and computation of magneto-sensitive polymers) project consists of numerous individual components of research working towards the characterisation of the multi-scale behaviour of magneto-sensitive polymers. Within each field of research exist numerous challenges with respect to the simulation of these materials as their behaviour is highly non-linear and the description of the multi-physics problem is challenging. The polymeric matrix exhibits incompressible, thermal and rate-dependent [1] characteristics and, due to the presence of embedded particles has a dependency on the alignment of these particles and the magnetic field [2] that permeates the material. Additionally, complex chemical interactions between the particles and the matrix render boundary interaction [3] important.



35mm long uniaxial test specimen



A RVE in shear



Particle in thermal field

To this end, a computational framework aimed at connecting the various components of research is in development. The multi-physics framework, based on modern finite-element [4] and auxillary libraries, provides resources to deal with the numerous numerical and computational challenges involved in the development of the phenomenological model of material behaviour. Provision for the use of distributed computing and adaptive mesh refinement, which are critical requirement to resolve the multi-scale physical problem, is made. A suite of robust tools to assist in the development of material models, which couple the numerous fields, have been developed. Direct coupling of the macro- and micro-scale phenomena through the use of representative volume elements (RVEs) is possible. Further developments include the incorporation of metaheuristic algorithms to assist in the determination of the material parameters.

References

[1] S. Reese and S. Govindjee. Theoretical and Numerical Aspects in the Thermo-Viscoelastic Material Behaviour of Rubber-like Polymers. *Mechanics of Time-Dependent Materials* **1**, 357–396 (1998).

[2] A. Dorfmann and R. Ogden. Nonlinear magnetoelastic deformations of elastomers. *Acta Mechanica* **16744**, 13–28 (2004).

[3] A. Javili and P. Steinmann. A finite element framework for continua with boundary energies. Part III: The thermomechanical case. *Comput. Methods Appl. Mech. Engrg.* **200**, 1963–1977 (2011).

[4] W. Bangerth, R. Hartmann and G. Kanschat. deal.II – A general-purpose object-orientated finite element library. *ACM Trans. Math. Softw.* **33**, 24/1–24/27 (2007).

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

Sebastian Pfaller, Paul Steinmann

In continuum mechanics, coupling approaches to simulation techniques that are able to capture processes taking place at lower length and time scales have become a very important field of research. In contrast to the field based continuum mechanics, particle based methods can take into account the specific atomistic and molecular structure of the material under consideration. In our approach the system consists of a particle region that is coupled to a continuum by introducing a bridging domain where both regions overlap. The particle domain is computed by Molecular Dynamics (MD), while the continuum is discretized and solved using the Finite Element Method (FEM). In addition to existing coupling schemes, the particles are tethered to anchor points which transfer displacements and forces between the different domains.
In the recent years we have set up a very close cooperation with the Theoretical Physical Chemistry Group at the Darmstadt University of Technology and the coupling algorithm has been developed. This collaboration is also part of the DFG-priority programme 1369 “Polymer-Solid Contacts: Interfaces and Interphases” that is interested among others in simulating polymers filled with nanoparticles. In Figure 1 the system set up is shown together with plots of the system under tensile load at several load steps. Further simulations show the suitability of this method.

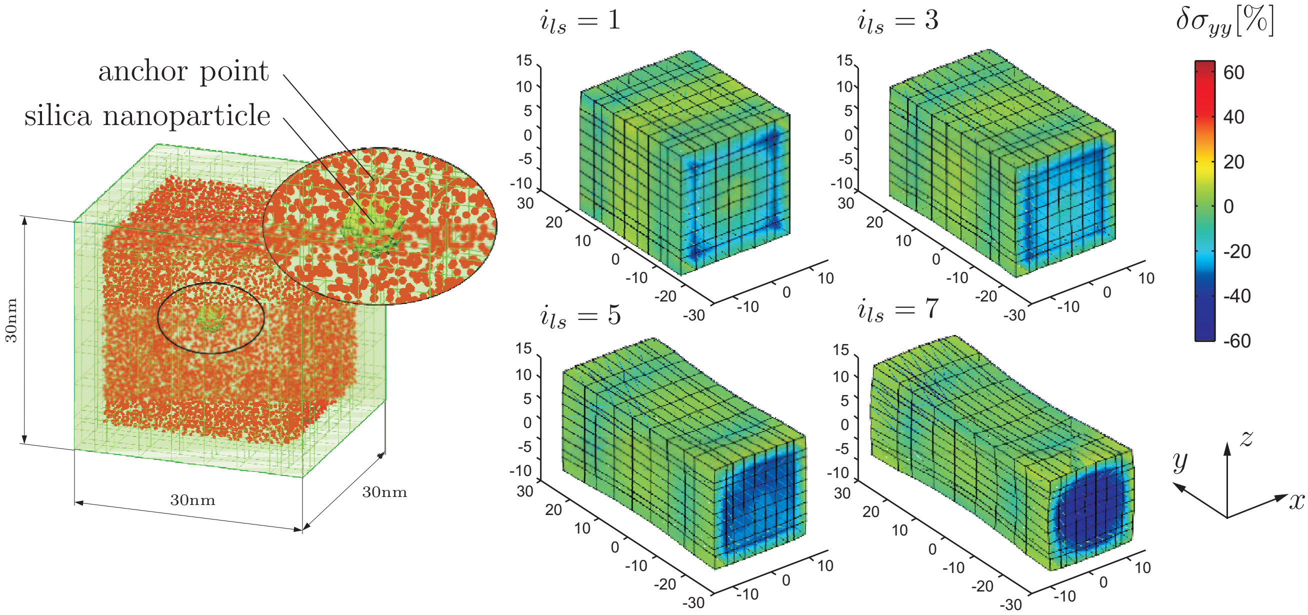


Figure 1: Finite Element domain coupled to polystyrene containing a silica nanoparticle (left), uniaxial tension test in y-direction: deviation $\delta\sigma_{yy}$ in stresses plotted at several load steps, displacements scaled by factor of 15 (right)

References

[1] S. Pfaller, G. Possart, P. Steinmann, F. Müller-Plathe, M. C. Böhm, M. Rahimi: A comparison of staggered solution schemes for coupled particle-continuum systems modeled with the Arlequin method, *Computational Mechanics* **49**, 565-579 (2012).

[2] S. Pfaller, M. Rahimi, G. Possart, P. Steinmann, F. Müller-Plathe, M. C. Böhm: An Arlequin-based method to couple molecular dynamics and finite element simulations of amorphous polymers and nanocomposites, submitted

Thermomechanical modelling and simulation of selective beam melting

Daniel Riedlbauer, Julia Mergheim, Paul Steinmann

The process in which laser or electron beams are used to additively build geometrically complex parts from thin layers of powder material is called selective beam melting. In this process the powder in defined, locally-restricted points in the current layer is fused by the energy of the beam in order to melt the powder into the already fused and recongealed material of the previous layers to construct the part layer-by-layer. Therefore the beam energy causes the powder particles to undergo a phase change from a powder particle to a melt and then to a solid. As the beam has a very high energy the issues of extreme temperatures and temperature gradients occur. The negative side-effects of those are residual stress, deformation and detoriation of the produced component. Hence these quantities shall be precomputed to optimize the mechanical properties of the produced part by adjusting the parameters of the process, e.g. beam scan path or rate of cooling. For the simulation of the process a nonlinear thermomechanical model is used which considers the temperature dependency of the material properties. This model describes the powder material not as single powder particles, but as a continuum. In order to capture the extreme temperature gradients emerging in the area of the beam multiple adaptive mesh refinement strategies are adopted. For reasons of performance, a staggered solution scheme called adiabatic split [1] is applied to the model. This scheme produces, in contrast to the standard monolithic scheme, a symmetric system matrix which reduces the time to solve the system due to the possibility to use faster solvers. Moreover a thermoelastoplastic material model is developed to describe the complex behaviour of the powder material in the process.

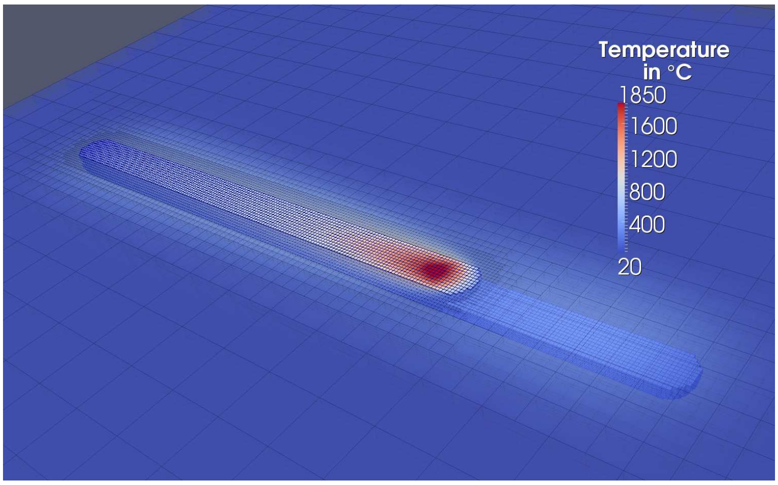


Figure 1: Simulation of the selective beam melting process

References

[1] F. Armero, J. C. Simo. A new unconditionally stable fractional step method for non-linear coupled thermomechanical problems. *International Journal for Numerical Methods in Engineering* **35**, 737–766 (1992).

Shape optimization using stress sensitivities

Stefan Riehl, Paul Steinmann

In a node-based shape optimization approach, the nodal coordinates of a given finite element discretization are directly addressed as design variables. To efficiently solve an optimization task, where the maximum equivalent stress (e.g. the von-Mises stress) is explicitly or implicitly incorporated in the formulation of either the objective function or any constraint function, one has to provide the sensitivities (i.e. the first order derivatives) of the maximum equivalent stress with respect to all design variables.
For the approximation of the maximum equivalent stress in the model problem, we propose the following continous and differentiable formulation

$$f_p\left(\mathbf{X}\right) = \left[\left(\sum_{e=1}^{n_e} V^{(e)} \right)^{-1} \sum_{e=1}^{n_e} V^{(e)} \left(\sigma_{vM}^{(e)} \right)^p \right]^{1/p} .$$

The formulation of f_p allows us to define optimization tasks that aim to reduce locally measured equivalent stresses, where the target area can be specified by defining a corresponding element set. This effect was used to reduce the locally measured maximum equivalent stress at the top side of a piston. Due to the high thermal load in this area, the measured equivalent stresses have to be kept at a minimum to reduce the risk of material failure. Since the geometry of the combustion bowl at the top side of the piston directly affects the flame propagation during the combustion cycle, it must not be changed. Therefore we defined the nodal coordinates of the nodes located at the interior surface as design variables.

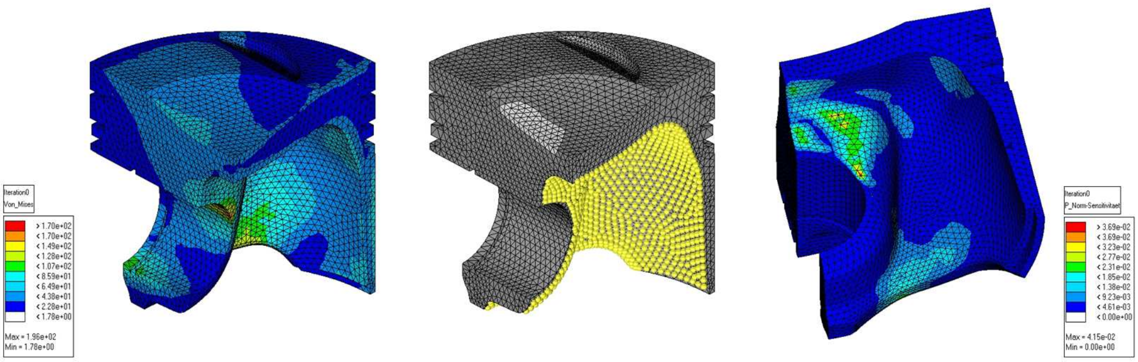


Figure 1: The contour plot on the left shows the von-Mises stresses in the initial piston design. The setup for the shape optimization is shown in the middle: the area highlighted in light gray indicates the target area for the stress reduction, which was then used for the computation of f_p; the nodal coordinates of the nodes highlighted in yellow served as design variables. The contour plot on the right shows the computed sensitivities of f_p with respect to all design variables.

References

[1] M. Scherer. Regularizing Constraints for Mesh and Shape Optimization Problems. Dissertation Thesis. *Schriftenreihe Technische Mechanik, Band 5* (2011).

[2] S. Riehl. Shape optimization using stress sensitivities. *Diploma Thesis* (2012) *(in German).*

Large strain magneto-viscoelasticity with application to magnetorheological polymers

Prashant Saxena, Mokarram Hossain, Paul Steinmann

This work is a part of the European Research Council Advanced Investigators Grant within the project 'Multi-scale, Multi-physics **Mo**delling and **Co**mputation of magneto-sensitive **Poly**meric materials (**Mocopoly**)'.
Magnetorheological polymers are rubber-like materials composed of a polymeric matrix filled with ferromagnetic particles. These elastomers exhibit remarkable properties like tuneable elastic modulus, non-homogeneous deformation, and a quick response to the magnetic field; thus making them useful in a variety of engineering applications such as vibration dampers and robotics. A major aim of this project is to develop mathematical models to analyze the magneto-viscoelastic properties of such materials. Such a model will be useful to experimentally identify various material parameters as well as in the design of 3–dimensional actuators.
Magnetorheological materials do not just show mechanical viscoelasticity but also dissipative effects on the application of a magnetic induction $\mathbf{B}_l$, for example, a gradual change in magnetization due to a sudden change in the applied magnetic induction. These effects are modelled by considering multiple independent internal dampers in the material. We consider a multiplicative decomposition of the deformation gradient into an elastic and a viscous part as $\mathbf{F} = \mathbf{F}_e^k \mathbf{F}_v^k$, $k = 1, ..., n$ (see, for example, [1]), and assume existence of n magnetic-field like internal variables $\mathbf{A}^1, ..., \mathbf{A}^n$. This motivates a split of the strain energy function Ω into an equlibrium and a 'viscous' part as

$$\Omega(\vartheta, \mathbf{F}, \mathbf{B}_l, \mathbf{A}^1, ..., \mathbf{A}^n, \mathbf{F}_v^1, ..., \mathbf{F}_v^n) = \Omega^{\text{eq}}(\vartheta, \mathbf{F}, \mathbf{B}_l) + \sum_{i=1}^{n} \Omega^k \left(\mathbf{F}_{\text{e}}^k = \mathbf{F} \left[\mathbf{F}_v^k \right]^{-1}, \mathbf{B}_l, \mathbf{A}_k \right).$$

Together with the balance laws of magnetoelasticity and the laws of thermodynamics [2], these assumptions provide a set of partial differential equations to solve for an appropriate domain.

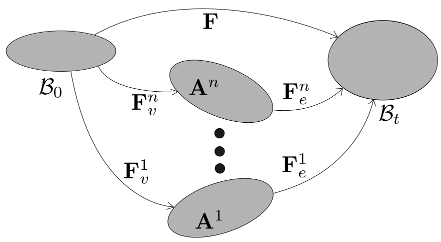


Figure 1: Reference and deformed configurations with n intermediate states

At present, experimental data describing the mechanical properties of such materials is limited. However, significant experimental work is underway at LTM to gain further insights into the physics of the problem. In future the obtained experimental data will be correlated with these mathematical models to obtain various material parameters and to further improve the modelling process itself.

References

[1] S. Reese, S. Govindjee. A theory of finite viscoelasticity and numerical aspects. *International Journal of Solids and Structures* **35**, 3455–3482 (1998).

[2] A. Dorfmann, R. W. Ogden. Nonlinear magnetoelastic deformations. *Quarterly Journal of Mechanics and Applied Mathematics* **57**, 599–622 (2004).

Modelling and Simulation of thermal influences in turning process

Stefan Schindler, Paul Steinmann

During machining mechanical work is dissipated into thermal energy by frictional processes and plastic deformations of the workpiece material. Taking dry cutting into account, the generated heat flows into the tool, the workpiece and the chips. Workpiece and tool are thereby subjected to thermal and mechanical loads that cause thermal expansions and mechanical deformations. These lead to deviations between the nominal and the actual depth of cut. Thus the accuracy of machining is decreased. In order to increase the accuracy, enhanced cutting conditions need to be determined. Finite element (FE) simulations allow for such an optimization prior to machining, whereby this work focuses on turning.
The turning process is split into two models [1]. A local model of the chip formation determines the heat flux into the workpiece and the cutting forces regarding the cutting conditions (Figure 1a). Therefore, the cutting parameters (cutting speed, feed and depth of cut) and the tool geometry need to be allocated to the local model. The results are used as boundary conditions (BC) in a second global model of the whole workpiece (Figure 1b). This global model allows calculating the temperature distribution, the thermal expansions and the deflection of the workpiece in terms of the actual tool position. Since the removal of material is the focus of the machining process, it has to be taken into account. In the FE simulation the removal of material, the process forces and the heat flux into the workpiece are controlled by the NC-code of the lathe. The material removal is done by element deactivation. Because of the thermal expansion and the deflection of the workpiece the element faces do not match the tool path. The technique of adaptive mesh refinement allows dividing elements exactly at the tool path, thus the material above the tool path can be deactivated accurately.
Experiments have been carried out to verify the numerical results, see Figure 1c. The accuracy of machining can be virtually optimized by 70% only through the determination of convenient cutting parameters. The compensation of the dilation during the cutting process could increase the accuracy by further 30%.

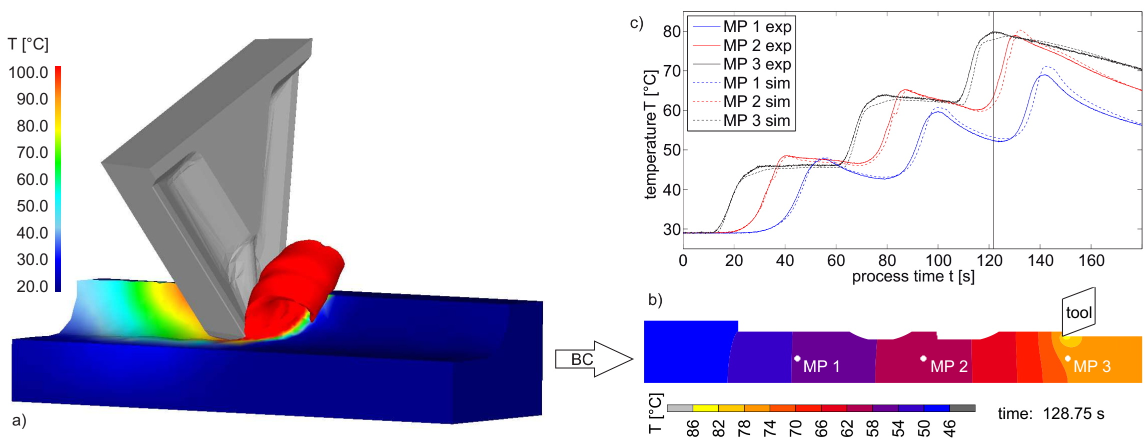


Figure 1: a) chip formation, b) whole turning process, c) temperature distribution

References

[1] S. Schindler, M. Zimmermann, J.C. Aurich, P. Steinmann. Thermo-elastic deformations of the workpiece when turning aluminum alloys - experiments and finite element simulations, submitted (2012).

Identification of material parameters for an anisotropic material model

Stefan Schmaltz, Kai Willner

New production classes and more complex production processes like sheet-bulk-metal forming and orbital cold forming result in a need of more precise material models with adapted parameters. Both of the mentioned forming processes utilize sheet-metal boards, but the usual assumption of having a two-dimensional stress- and strain-distribution does not apply, as in both cases a material flow in thickness direction of the sheet-metal appears. Therefore a three-dimensional anisotropic material model at finite strain is needed. The material behavior is modeled with an additive split of the logarithmic strain tensor $\boldsymbol{E} = \boldsymbol{E}^{\mathrm{e}} + \boldsymbol{E}^{\mathrm{p}} = \frac{1}{2}\ln\boldsymbol{C}$. The elastic part is calculated analogous to the linear model of Hooke and the plastic contribution is represented via a Hill-type criterion $\Phi\left(\boldsymbol{T}, \frac{\partial\psi}{\partial\alpha}\right) = \left(\frac{3}{2}\boldsymbol{T} : \mathbb{H} : \boldsymbol{T}\right)^{\frac{1}{2}} - \sigma_{\mathrm{Y}}(\alpha)$, with the anisotropy tensor $\mathbb{H}$ [1] and a Hockett-Sherby hardening function $\sigma_{\mathrm{Y}}(\alpha) = \sigma_\infty - [\sigma_\infty - \sigma_0] \cdot e^{(A\alpha^B)}$. The flow rule satisfies the associative ansatz $\dot{\boldsymbol{E}}^{\mathrm{p}} = \dot{\gamma}\, \partial\Phi/\partial\boldsymbol{T}$.

For modeling the sheet-metal behavior properly, fitting material parameters are to be found. With direct identification methods several different experiments have to be performed to capture the anisotropy, which is costly and time consuming. The problem is tackled by utilizing an inverse Finite Element Model Updating (FEMU) method and a biaxial tensile test, see Figure 1. In the FEMU procedure a Finite Element simulation of the experimental test is built up and run, while an optimization algorithm varies the material parameters in every iteration until an optimum is found. To verify the finding of an global optimum two different optimization algorithms and different initial starting parameter sets are taken. If the identified parameters of all procedure-runs converge to one value set, a global optimum is found [2].

In our case the optimization values are the Hill parameters of the plastic anisotropy tensor $\mathbb{H}$ and a gradient-based Levenberg-Marquardt (LM) and a gradient-free Nelder-Mead-Simplex (NM) algorithm are used. Figure 2 shows the directly identified initial yield values of a 2.0 mm thick DC04 sheet-steel and the optimized yield surfaces. A good correlation is found showing the capabilities of the identification procedure.

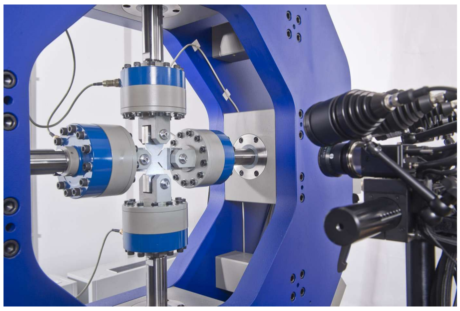


Figure 1: Biaxial testing machine with tensile specimen and optical measurement system.

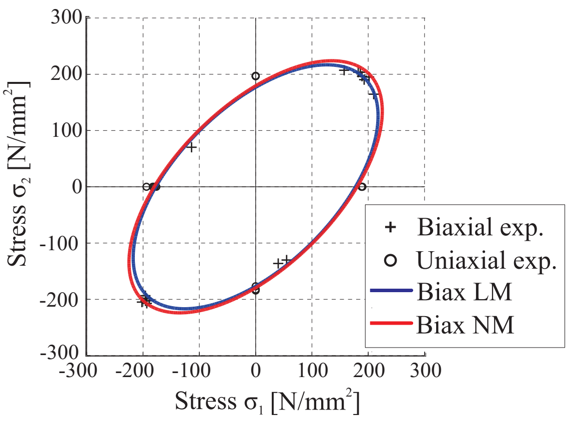


Figure 2: Identified yield surfaces and experimental yield values.

References

[1] R. de Borst, P. H. Feenstra. Studies in anisotropic plasticity with reference to the Hill criterion. *Int. J. Numer. Meth. Eng.* **29**, 315–336 (1990).

[2] B. M. Chaparro, et al. Material parameters identification: Gradient-based, genetic and hybrid optimization algorithms. *Comp. Mater. Sci.* **44**, 339–346 (2008).

Multi-scale modeling of heterogeneous materials

Ulrike Schmidt, Julia Mergheim, Paul Steinmann

Multi-scale modeling can efficiently be used to describe the macroscopic behavior of microscopically heterogeneous material. Based on geometry, material model and parameters of the microscopic structure, a homogenized stress-strain-relation can be calculated and thus the macroscopic response. The discretized homogenization problem is given by the FE^2 method. The inverse problem is fitting the simulation result to the measured macroscopic response by tuning micro material parameters. This parameter identification is formulated as a least squares problem. Natural boundaries of the microscopic parameters range are maintained using optimization constraints. Gradient-based methods are employed to solve the optimization. Analytical and numerical sensitivities of the objective function differ significantly [1] and therefore, a strategy to calculate the analytical sensitivities in the context of elastoplastic multi-scale modeling has been derived. Earlier results for the elastic case can be found in [2]. Since the elastoplastic behavior depends on the load history, the derivatives of the stresses with respect to the material parameters within a FE program are usually calculated recursively [3]. The microscopic displacements at the boundary depend on the macroscopic strain and therefore on the material parameters. This dependency is taken into account when calculating the sensitivities of the multi-scale simulation. The order of the design variables may differ greatly and a negative effect on the reidentification of parameters has been observed. Normalization of the design variables proved to be an easy to implement and effective remedy. The reidentification of the material parameters of two constituents can be difficult, but separate identification of elastic and plastic parameters can be used to get satisfying results.

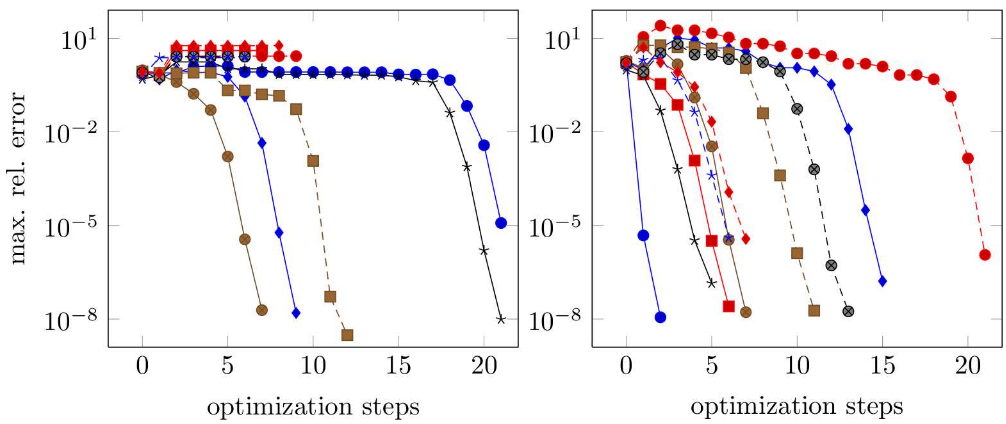


Figure 1: Re-identification failed for all parameters (left), but succeeded for separate re-identification of plastic parameters $(\sigma_{Y,1}, h_1, \sigma_{Y,2}, h_2)$. (right)

References

[1] J. Fish, A. Ghouali. Muliscale analytical sensitivity analysis for composite materials. *Int. J. Numer. Methods Eng.*, **50**(6), pp. 1501–1520 (2001).

[2] U. Schmidt, J. Mergheim, P. Steinmann. Multi-Scale Parameter Identification. *Int. J. Multiscale Comput. Eng.*, **10**(4), pp. 327–342 (2012).

[3] R. Mahnken, E. Stein. A unified approach for parameter identification of inelastic material models in the frame of the finite element method. *Comput. Meth. Appl. Mech. Eng.*, **136**(3-4), pp. 225–258 (1996).

Isogeometric shape optimization using T–splines

Oliver Schmitt, Jan Friederich, Paul Steinmann

Isogeometric shape optimization combines the advantages of both, parameterized and parameter–free shape optimization. Without the need of an additional design model the given domain can be defined accurately using NURBS–based basis functions. Isogeometric analysis can be seen as a special case of the isoparametric finite element method.
A further extension of isogeometric analysis is based on T–splines [1] [2]. T–splines allow to refine the control grid locally. Futhermore, with T–splines two patches can be glued together gapless. The main difference to B–splines is that the so–called T–mesh allows for T–junctions. As a consequence, the basis functions have to be defined on a local knot vector (see figure 1).

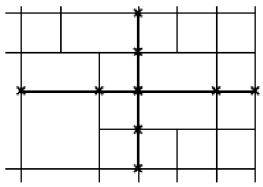


Figure 1: T–mesh with local knot vectors

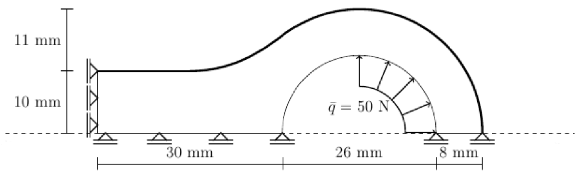


Figure 2: loading condition of the hook

We use the advantages of T–splines to solve shape optimization problems. In the depicted example we minimize the compliance. The loading and boundary conditions are shown in figure 2. Using T–splines we are able to refine the T-mesh locally in places with higher stresses. The optimization results are getting more accurate whereas the computational expense increases only slightly in comparison to global refinement (see figures 3 and 4).

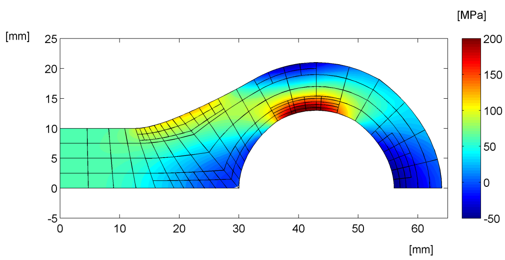


Figure 3: initial shape and v. Mises stress before optimization

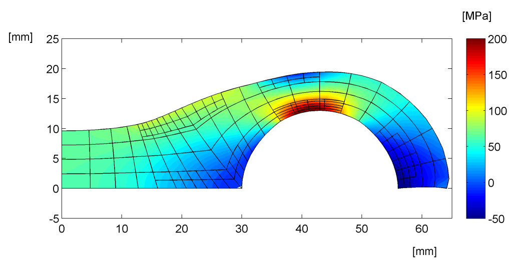


Figure 4: optimized shape and v. Mises stress after optimization

References

[1] T. W. Sederberg, D. L. Cardon, G. T. Finnigan, N. S. North, J. Zheng, and T. Lyche. T–spline Simplification and Local Refinement. *ACM Transactions on Graphics (TOG) - Proceeding of ACM SIGGRAPH,* **23** (2004).

[2] S. H. Ha, KK Choi, and S. Cho. Numerical method for shape optimization using T–spline based isogeometric method. *Structual and Multidisciplinary Optimization,* **42(3)** (2010).

Investigation of a Resonator Using the Multiharmonic Balance Method

Dominik Süß, Kai Willner

The system investigated here is a resonator including a bolted lap joint. In [1] this system is modeled by a simple 3-DOF model and because of the special design of the structure this works very well. But in order to get a way of predicting the stationary dynamic behavior of jointed structures in general, here the Finite Element Method is applied. A part of the mesh of the chosen FEM model is pictured in figure 1 overlaid to a picture of the real system.

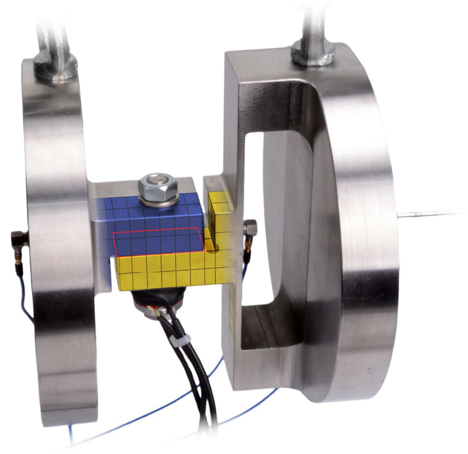


Figure 1: overlay of the real structure and the chosen finite element mesh.

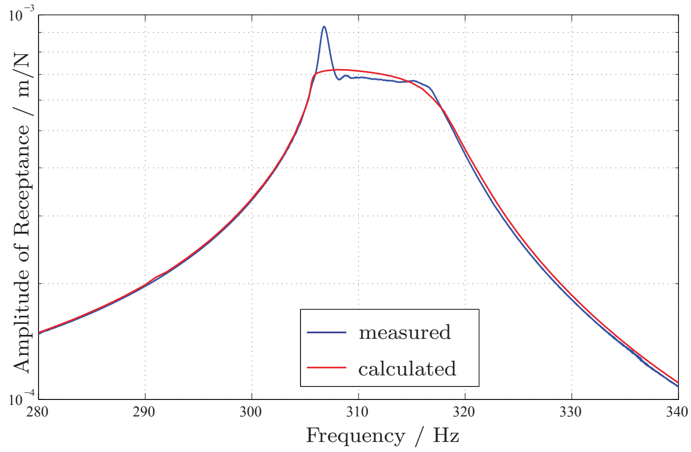


Figure 2: comparison of measured and calculated FRFs.

The two parts of the system are discretized using hexahedral elements. For discretizing the contact plane (red frame in figure 1) Zero Thickness elements are implemented, see e.g. [2, 3]. In order to compute the stationary behavior of the system in the frequency domain the Multiharmonic Balance Method (MHBM) in combination with the Alternating Frequency Time Domain Method (AFT) is applied. For solving the system equations a Newton-Raphson type solver is applied. Using the constitutive law also applied in [4] it is possible to compute the partial derivatives needed for this solver analytically in the framework of the AFT algorithm. The measurements for getting reference FRFs of the real system are recorded using a shaker and performing a swept sine excitation of the structure. Using a least squares model updating algorithm the calculation results are fitted with respect to the measured curves to identify the contact parameters. The good correlation of a measured and a computed FRF calculated accounting for 11 harmonics can be seen in figure 2.

References

[1] D. Süß , K. Willner. Multiharmonic Balance Analysis of a Jointed Friction Oscillator. *Proceedings of the ECCOMAS*, CD-ROM (2012).

[2] J. Geisler, K. Willner. Modeling of jointed structures using zero thickness interface elements. *PAMM*, **7**, No.1: 4050009–4050010 (2007).

[3] D. Süß, J. Geisler, K. Willner. Numerical and experimental investigations on dynamic contact phenomena of jointed structures. *PAMM*, **10**, 263–264 (2010).

[4] J. Geisler. *Numerische und experimentelle Untersuchungen zum dynamischen Verhalten von Strukturen mit Fügestellen.* PHD thesis. LTM Erlangen (2010).

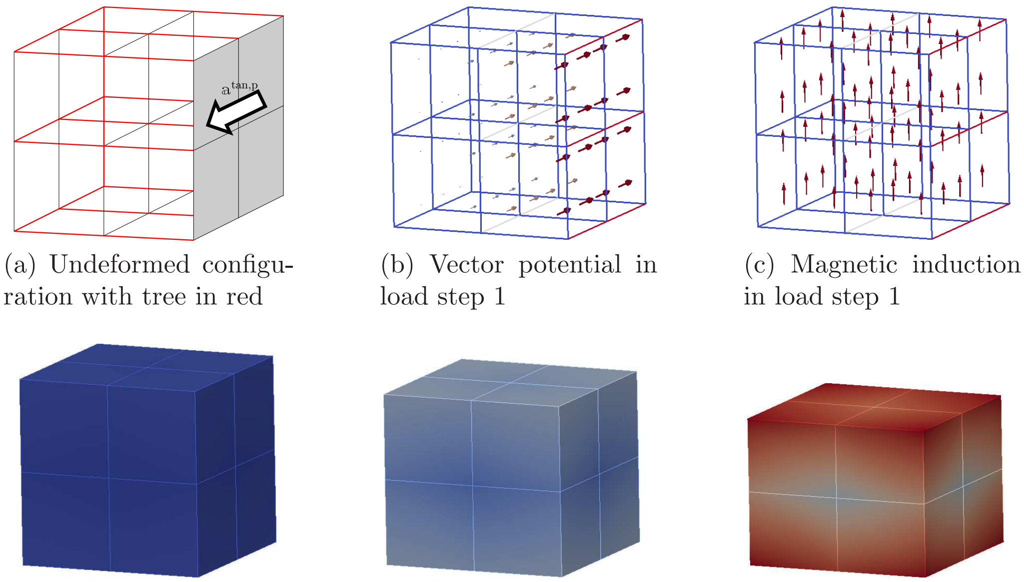
On the Modeling and Simulation of Magneto-Sensitive Elastomers

Franziska Vogel, Paul Steinmann

Magneto-sensitive elastomers are smart materials composed of a rubber-like basis matrix filled with magneto-active particles. Their ability to deform significantly, i.e. geometrically nonlinear, under the stimulation of a magnetic field makes them an interesting tool for the development of novel actuators.

In order to represent the underlying physics correctly within a computational model, we choose a mixed variational framework depending on two unknown fields: the deformation map and the magnetic vector potential. For the balance of linear momentum valid in magnetoelasticity, we follow the formulation in terms of a symmetrized total Cauchy-type stress tensor presented by Dorfmann and Ogden [1]. The solution of the mechanical problem is covered by a nodal-based finite element method, whereas the Maxwell's equations are expressed in terms of the magnetic vector potential and discretized with edge-based finite elements [2].

Since the magnetic vector potential is not defined uniquely, an additional gauge condition is necessary. Within the application of edge elements, this condition can be incorporated elegantly through a tree-cotree gauging technique [3]. A tree is a graph through a mesh that connects all nodes with a minimal number of edges. Setting the tangential components of the magnetic vector potential to zero along the edges that belong to the tree guarantees a unique solution.



(a) Undeformed configuration with tree in red

(b) Vector potential in load step 1

(c) Magnetic induction in load step 1

(d) Deformation in load step 1

(e) Deformation in load step 3

(f) Deformation in load step 5

Figure 1: Unit cube loaded with magnetic vector potential with zero-tree gauging.

References

[1] L. Dorfmann, R. Ogden. Magnetoelastic Modeling of Elastomers. *European Journal of Mechanics – A/Solids*, **22**, 497–507 (2001).

[2] J. Jin. *The Finite Element Method in Electromagnetics.* John Wiley & Sons, Inc., New York (2002).

[3] C.J. Carpenter. Comparison of Alternative Formulations of 3-Dimensional Magnetic Field and Eddy Current Problems at Power Frequencies. *Proceedings of the Institution of Electrical Engineers*, **124(11)**, 1026–1034 (1977).

On the released energy in nonlinear electro-elastostatics with consideration of free space

Duc-Khoi Vu, Paul Steinmann

This work is motivated by the challenging task of computing the so-called released energy, or the energy that is released when the material configuration of a body under electric stimulation is altered. It is a well-known fact that for many materials the surrounding free space can be conveniently ignored because of its negligible contribution. As a consequence of this negligence the electric traction caused by the Maxwell's stress and the electric flux on the boundary of the body are often not considered in simulating the deformation of the body as well as in computing the released energy, for example in the case of crack propagation. With the discovery of new materials like electronic electro-active polymers (EEAPs), it has been observed that the free space may have a significant influence on the electric and deformation field inside the material body [1], and therefore on the released energy.

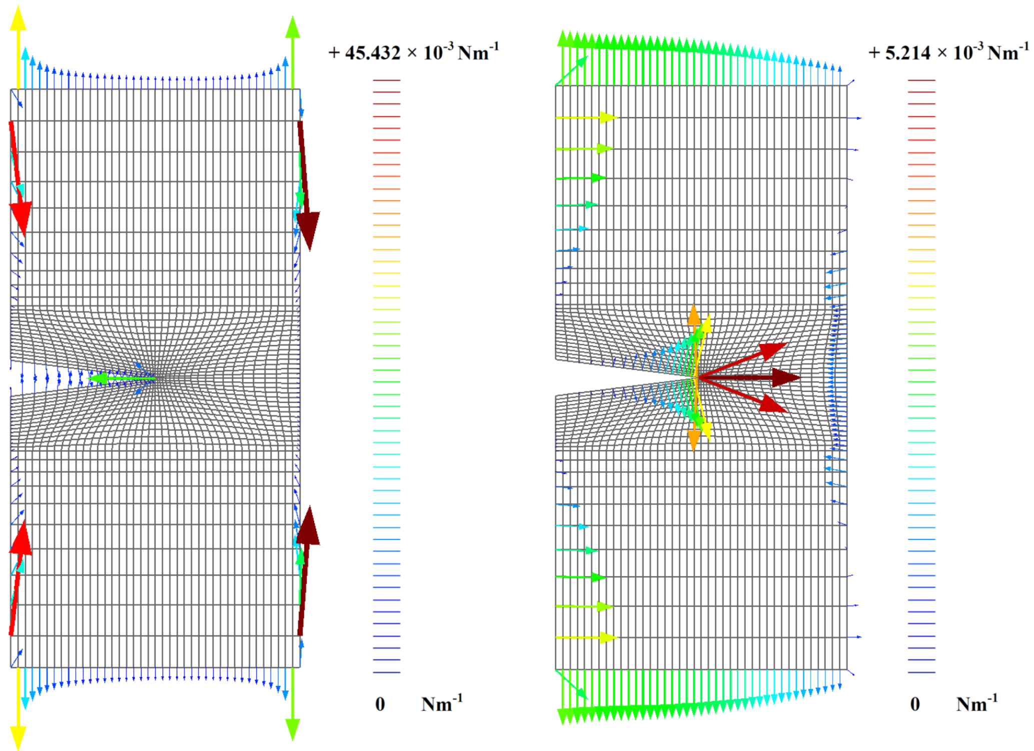


Figure 1: Material forces with (left) and without (right) consideration of free space

By examining the material motion problem in nonlinear electro-elastostatics [2], it can be shown that the released energy can be computed in terms of material forces. In the above figure, an example is presented to demonstrate the necessity to account for the contribution of the free space in computing these forces.

References

[1] D. K. Vu, P. Steinmann. On 3-D coupled BEM-FEM simulation of nonlinear electro-elastostatics. *Computer Methods in Applied Mechanics and Engineering* **201-204**, 82-90 (2012).

[2] D. K. Vu, P. Steinmann. On the spatial and material motion problems in nonlinear electro-elastostatics with consideration of free space. *Mathematics and Mechanics of Solids* **17**, 803-823 (2012).

On the modelling of twin interface movements in single-crystalline MSMA specimens

Jiong Wang, Paul Steinmann

Systematic experiments have revealed that the variant reorientation in single-crystalline magnetic shape memory alloys (MSMAs) is realized by the twin interface movements [1]. In this project, we shall proposed a constitutive model to study the movements of twin interfaces in a MSMA specimen, which is the key point to model the magneto-mechanical response of the specimen. The circumstance of current model is illustrated in Fig. 1a. The transformation between two martensite variants will be considered and the twin interfaces are assumed to be orientated along certain direction. The following constitutive assumption is proposed for the effective magnetization in the two variant regions (cf. Fig. 1b):

$$\mathbf{M}_i(\alpha_i, \mathbf{m}_j^{(i)}) = M_s[\alpha_i \mathbf{m}_1^{(i)} + (1-\alpha_i)\mathbf{m}_2^{(i)}], \quad i,\ j = 1,\ 2.$$

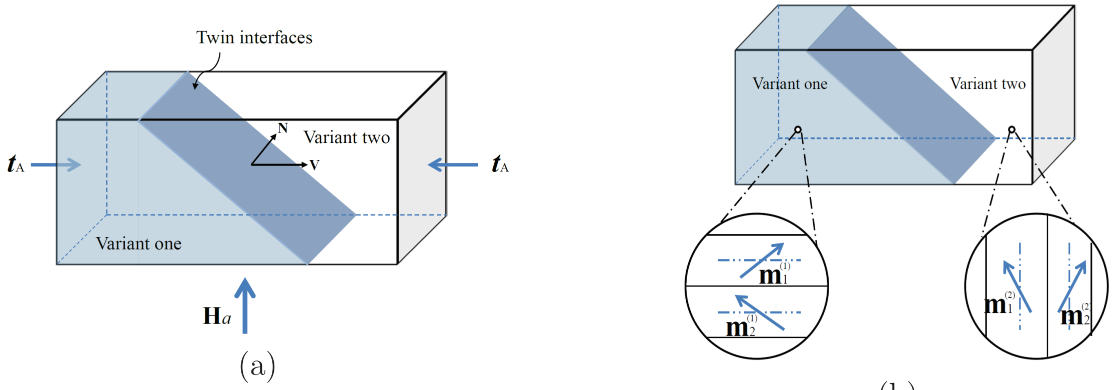


Figure 1: (a) Illustration of the MSMA specimen and the external loading pattern; (b) Constitutive assumption on the effective magnetization vector in the MSMA specimen.

The total energy functional $\mathcal{G}$ for the whole magneto-mechanical system are formulated, which depends on the spatial placement $\mathbf{x}$, the magnetic scalar potential Ψ, the internal variables α_i and $\mathbf{m}_j^{(i)}$ and the variant distribution in the specimen $\{\Omega_r^1, \Omega_r^2\}$. By calculating the variations of $\mathcal{G}$ with respect to the independent variables, we can obtain the governing PDE system for the current model. Especially, the following configurational force on the twin interfaces can be derived:

$$\mathcal{T}_c = [[\int_{\mathcal{S}} \rho_r\{\phi - \mu_0 \mathbf{M}\cdot(\mathbf{H}_a + \mathbf{H}_d) + K_\theta(1 - \alpha(\mathbf{m}_1\cdot\mathbf{e})^2 - (1-\alpha)(\mathbf{m}_2\cdot\mathbf{e})^2) + f^\alpha(\alpha) \\ - ((\frac{\partial\phi}{\partial\mathbb{F}})^T\mathbf{N})\cdot(\mathbb{F}\cdot\mathbf{N})\}ds]].$$

The governing PDE system will be implemented by adopting suitable numerical schemes and it is hoped that the magneto-mechanical response of the MSMA specimen can be predicted at a quantitative level.

References

[1] L. Straka, V. Novák, M. Landa, O. Heczko. Acoustic emission of Ni-Mn-Ga magnetic shape memory alloy in different straining modes. *Mater. Sci. Eng. A* **374**, 263–269 (2004).

Structure - Property - Relationships of Magnetorheological Elastomers

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This work is part of the ERC Advanced Grant "Multi-scale, Multi-physics, **MO**delling and **CO**mputation of magneto-sensitive **POLY**meric Materials" (**MOCOPOLY**), focusing on the manufacturing and characterization of **M**agneto**r**heological **E**lastomers (**MRE**s). MREs are smart materials, whose properties, in particular the rheological and mechanical ones, can be altered significantly, applying an external magnetic field. In general, MREs are composed of a non-magnetic, rubber-like, polymeric matrix filled with magnetically permeable particles of micro meter size (typically ∅ 3-5 μm). By applying a magnetic field, magnetic dipoles are induced. Due to dipole-dipole interactions, the originally randomly distributed particles (Figure 1) build up chain-like structures (Figure 2) oriented in field direction [1]. The properties of the polymeric matrix, the size and size-distribution of the particles as well as their composition and volume filler fraction influence the characteristic response of the MRE [2]. In addition, other fillers present in the rubber (e.g. fumed silica), may have an effect on the resulting MREs as well. A sketch of a MRE with homogeneously dispersed particles without a magnetic field (Figure 1) and the formation of the particle strings under an external magnetic field B (Figure 2) is shown below.

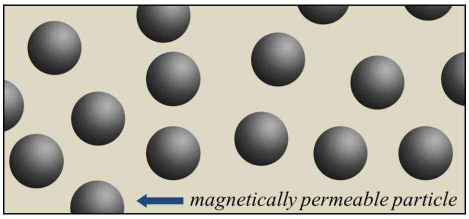

Figure 1: Sketch of particle structure in a MRE without external magnetic field ($B = 0$).

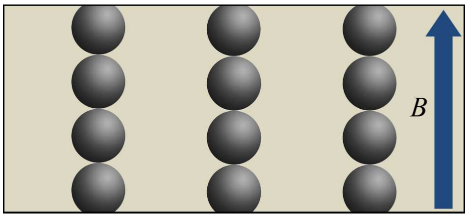

Figure 2: Sketch of particle structures in a MRE with external magnetic field B.

The formation of structures in the MRE causes anisotropy in the properties, which can be used in various applications of MREs as sensor and/or actuator. The project aims to understand the influence of material formulation (e.g. polymer, crosslinking density and filler content, etc.) and processing conditions during crosslinking (e.g. temperature, magnetic field, etc.), to optimize the properties of MREs. Therefore, model systems are studied by means of a rheometer equipped with a magneto-rheological cell (Anton Paar) and a universal testing machine allowing the measurement of mechanical properties in a defined magnetic field. μ-CT and SEM imaging are used to control the homogeneity, structure and reproducibility of the composite. Thus, correlations between microstructure and performance are established. The data generated is used to define a **R**epresentative **V**olume **E**lement (**RVE**) in order to simulate the material behaviour. Finally, the experimental results are used to optimize the simulation of MREs.

References

[1] M.R. Jolly, J.D. Carlson, B.C. Muñoz. A model of the behaviour of magnetorheological material. *Smart Materials and Structures* **5**, 607–614 (1996).

[2] C. Ruddy, E. Ahearne, G. Byrne. A review of magnetorheological elastomers: properties and applications. *Proceedings of the International Manufacturing Conference (IMC)* **24**, 999–1005 (2007).

Modified rainflow counting considering hold times

Paul Wilhelm[1], Paul Steinmann, Jürgen Rudolph[1]

[1] AREVA NP GmbH

Power plant components, like surge line or pressure vessel, are subjected to thermal-mechanical loadings and influence of environmental medium. The corresponding damage accumulation phenomenon, which treats fatigue plus corrosion effects, is also known as Environmentally Assisted Fatigue (EAF). A common procedure for incorporating EAF effects into fatigue evaluation of reactor materials is given by Argonne National Laboratory (ANL) [1].
Recently conducted laboratory tests study the influence of long-term hold times of up to 3 and 30 days in oxygenated high-temperature water. A trend of decreasing cyclic crack growth rates with imposition of hold times is noticed [2].
Many fatigue relevant locations undergo cyclic loading, which is infrequent and is interspersed with long hold times at relatively constant loading. For example, operational loading originate mainly from temperature stratification, see Figure 1. In contrast to laboratory testing, real plant cycles include many small sub-cycles with strain amplitudes less than the given endurance limit from ANL. The parameter hold time will be incorporated into the ANL stress analysis to reduce conservatism. A modified rainflow counting algorithm may be needed as well, since none of the rainflow methods found in literature are adapted to this problem.
The classical computer optimized rainflow counting [3] has to be extended to a modified rainflow counting algorithm considering hold times. Hence, the elementary event and the result parameter have to be redefined in compliance with the constitutive laws of metal-based materials. An efficient algorithm and small data volume are important, too.

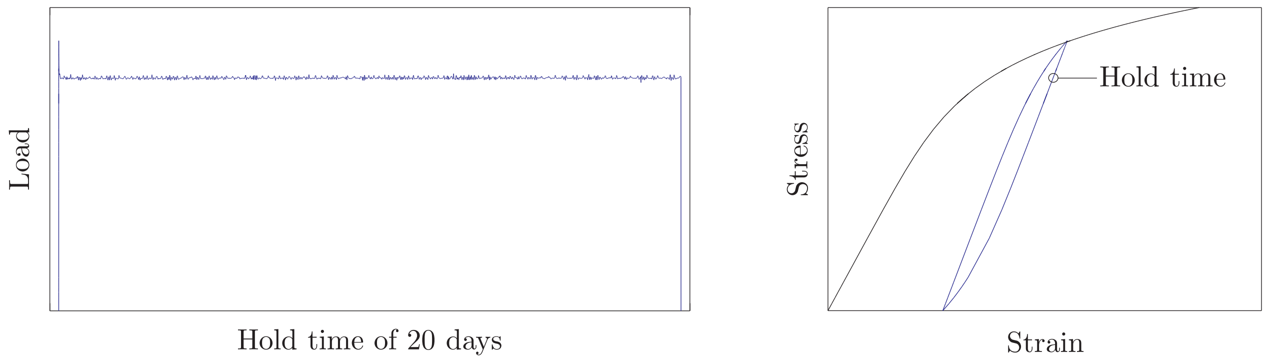

Figure 1: Steady state operation.

References

[1] U.S. Nuclear Regulatory Commission (NRC). Office of Nuclear Regulatory Research: Effect of Light Water Reactor Coolant Environments on the Fatigue Life of Reactor Materials. Final Report. *U.S. NRC* **NUREG/CR-6909; ANL-06/08**, (2007).

[2] A. Roth, B. Devrient. Environmental Effects on Fatigue - Possible Reasons for the Apparent Mismatch between Laboratory Test Results and Operational Experience. **36.** *Materialprüfungsanstalt (MPA)-Seminar, Stuttgart: Werkstoff- und Bauteilverhalten in der Energie- und Anlagentechnik*, (07/08.10.2010).

[3] U. H. Clormann, T. Seeger. Rainflow - HCM: Ein Zählverfahren für Betriebsfestigkeitsnachweise auf werkstoffmechanischer Grundlage. *Stahlbau* **55 Heft 3**, 65-71 (1986).

4 Activities

4.1 Teaching

- Statik (MB)
- Elastostatik und Festigkeitslehre (MB)
- Statik und Festigkeitslehre (CBI, ET, IP, LSE, ME, MT, WING, WW)
- Lineare Kontinuumsmechanik (MB, ME, WING)
- Nichtlineare Kontinuumsmechanik (MB, ME)
- Technische Schwingungslehre (MB, ME, WING)
- Methode der Finiten Elemente (MB, ME, WING)
- Materialmodellierung und -simulation (CE, MB)
- Finite Elemente in der Plastomechanik (MB)
- Nichtlineare Finite Elemente (CE, MB, IP)
- Einführung in die Bruchmechanik (MB)
- Rotordynamik (MB)
- Strukturoptimierung in der virtuellen Produktentwicklung (MB, ME)
- Kontaktmechanik (MB)
- Numerische und experimentelle Modalanalyse (MB, ME, WING)
- Introduction to the Finite Element Method (CE)
- Computational Dynamics (CE)
- Finite-Elemente Praktikum (MB, WING, IP)
- Hauptseminar Technische Mechanik (MB, ME)
- Seminar über Fragen der Mechanik
- Advanced Lecture: On the Roots of Continuum Formulations in Molecular Systems
- Advanced Lecture: Theory and Computation of Geometrically Nonlinear Shell Formulations
- Number of exams - 2674

4.2 Habilitation thesis

- D. K. Vu,
  A Study on Nonlinear Electro-Elastostatics: Theory and Numerical Simulation

4.3 Dissertation thesis

- A. Javili,
  Thermomechanics of Solids Accounting for Surfaces and Interfaces

4.4 Diploma theses

- J. Bredl,
  Zur Ermüdungsfestigkeit gekerbter Bauteile
- S. Buchberger,
  Vibroelastische Analyse von CFK, Aluminium- und Stahlkonstruktionen
- P. Dannhorn,
  Umsetzung eines regelungstechnischen Konzepts zur Parameteridentifikation im Zeitbereich
- G. Hopp,
  Identifikation orthotroper, plastischer Materialparameter anhand von hydraulischen Tiefungsversuchen
- M. Jerschl,
  Numerische Untersuchungen zum dynamischen Verhalten der Fügestelle Bremsscheibe-Radnabe
- J. Rehwald,
  Mikromechanische Modellierung und Simulation von Block-Copolymeren
- S. Riehl,
  Formoptimierung basierend auf Spannungssensitivitäten
- R. Schimpf,
  Analyse und Optimierung des strukturdynamischen Verhaltens von Aluminiumrädern
- O. Schmitt,
  Isogeometrische Formoptimierung mit T-Splines

4.5 Master theses

- D. Geiger,
  Implementierung eines Datenakquisitionsprogramms für hochqualitative Schwingungsmessungen
- F. Meinel,
  Modellierung und Implementierung elasto-plastischer Kontakte im Halbraum
- S. Scheeff,
  Modellierung des Wärmeeintrags und Materialabtrags beim Formdrehen mittels Finite-Elemente-Methode

4.6 Bachelor theses

- A. Fokou,
  Untersuchung der Ausbreitung und Reflexion von Wellen in dünnen Stäben
- M. Jüngling,
  Ritz-Vektoren vs. Modale Reduktion - vergleichende Analyse der Reduktionsverfahren am Beispiel der Schwingung einer Gitarrenseite
- H. Münch,
  Untersuchung des Stabilitätsverhaltens von harmonisch erregten Mehrfachpendeln
- S. Neumann,
  Konstruktion und Inbetriebnahme eines Versuchsaufbaus zur Untersuchung von Saitenschwingungen
- J. Scherer,
  Kopplung von FE-Simulationen mit teilchenbasierten Berechnungen: Erweiterung auf ein nichtlineares Stoffgesetz

4.7 Student research projects theses

- B. Berg,
  Mikromechanische Modellierung gestrickter Textilien
- L. Dobrenizki,
  Eine Finite Elemente Struktur zur Bruchmodellierung
- T. Heimerl,
  Identifikation und Simulation viskoelastischer Materialverhalten am Beispiel einer Tennissaite
- J. Horn,
  Automatisierung und Erweiterung des Magnetmessplatzes "Single Sheet Tester"
- S. Hohls,
  Psychoakustische Beurteilung von Fahrzeugklimatisierungssystemen
- R. Höller,
  Biomechanische Analyse des Kraftflusses von Attachments zur Verankerung abnehmbaren Zahnersatzes
- S. Käßmair,
  Berechnung von magnetischen Kräften auf Partikel im Magnetfeld unter Verwendung von PHOENIX
- J.A. Nguechi,
  Modellbildung und exakte positionierung einer mechanischen Iris in einer Optik
- M. Spahr,
  Biomechanische Analyse plastischer Formänderungen im Interface von Zahnimplantaten
- M. Sweid,
  Auswahl von Designvariablen in der Formoptimierung von umgeformten Funktionsbauteilen

4.8 Seminar for Mechanics

19.01.2012 Dipl. Math.-techn. Philipp Landkammer,
Ingenieurbüro KAE GmbH, Hausen b. Forchheim
Das Antwortspektrenverfahren für Erdbebensimulationen

26.01.2012 Fernando Jiménez Alburquerque,
Instituto de Ciencias Matemàticas ICMAT-CSIC, Madrid, Spain
On Discrete Mechanics for Optimal Control Theory

07.02.2012 M. Sc. Daniel Riedlbauer,
Lehrstuhl für Technische Mechanik, FAU Erlangen-Nürnberg
Thermomechanical Modelling & Simulation of Electron Beam Melting

06.03.2012 Prof. Francesco dell'Isola,
DISG, Università di Roma "'La Sapienza"', Rome, Italy
How contact interactions may depend on the shape of Cauchy cuts in N-th gradient continua: approach "'à la D' Alembert"'

23.03.2012 Prof. Dr.-Ing. Ellen Kuhl,
Computational Biomechanics Laboratory, Stanford University
Computational Optogenetics: A Novel Continuum Framework for the Photoelectrochemistry of Living Systems

03.04.2012 Kim-Henning Sauerland,
Lehrstuhl für Technische Mechanik, Universität Paderborn
Process Simulation and Two Scale Tool Simulation related to Hybrid Forming

09.05.2012 Olivier Verdier,
Department of Mathematical Sciences, NTNU Trondheim, Norwegen
Geometric Generalisations of the Shake and Rattle methods

21.05.2012 Oleg M. Zarechnyy,
Department of Aerospace Engineering, Iowa State University, Ames, IA
Modeling and Simulation of Strain-Induced Phase Transformations in Rotational Diamond Anvil Cell

22.05.2012 Dipl.-Math. Zoufine Bare,
Fraunhofer Institut für Techno- und Wirtschaftsmathematik, Kaiserslautern
Asymptotic dimension reduction for linearized contact of thin fibers and simulation of textiles based on 1D models including large deformation

05.06.2012 B. Röhrnbauer, E. Mazza,
Institute of Mechanical Systems, Swiss Federal Institute of Technology Zurich, Switzerland
Mechanical characterization and modeling of prosthetic meshes at different length scales

12.06.2012 Prashant Saxena,
Department of Mathematics, University of Glasgow
Nonlinear magneto-elasticity: some boundary value problems

26.06.2012 Prof. Valery Levitas,
Departments of Aerospace Engineering, Mechanical Engineering and Material Science and Engineering, Iowa State University, Ames, Iowa 50011, USA
Stress- and Surface-induced Phase Transformations:Phase Field Approach

03.07.2012 Prof. Karali Patra,
Mechanical Engineering, Indian Institute of Technology Patna
Study on mechanical and dielectric behavior of VHB 4910 for sensors and actuators applications

09.08.2012 Wencheng Li,
Northwestern Polytechnic University, China
Introduction of My Research Interesting on Structure Preserving Methods

06.09.2012 Kathrin Flaßkamp,
Deparment of Mathematics, University of Paderborn
Variational Formulation and Optimal Control of Hybrid Lagrangian Systems

21.09.2012 Prof. Roger Bustamante,
Departamento de Ingenieria Mecànica, Universidad de Chile
Implicit constitutive relations for electro-elastic bodies

27.09.2012 Dr.-Ing. Joachim Linn,
Fraunhofer-Institut für Techno- und Wirtschaftsmathematik, Kaiserslautern
Viscoelastic Cosserat rods of KelvinVoigt and generalized Maxwell type

22.10.2012 Prof. Dr. Markus Lazar,
Heisenberg Research Group, Continuum Mechanics, Department of Physics, Darmstadt University of Technology, Germany
Non-singular Dislocations in the Theory of Gradient Elaticity

05.11.2012 Hossein Talebi,
Institute of Structure Mechanics, Bauhaus-University Weimar
Single and Multi Scale Methods for Modeling Fracture and Crack Propagation: Methods, Software and Tools

19.11.2012 Dr. Frank Fischer,
Structure Research Lab, Beiersdorf AG, Hamburg
The detailed structure of human skin layers

20.11.2012 Tobias Gail,
Lehrstuhl für Technische Dynamik, FAU-Erlangen-Nürnberg
Computing time investigations of variational multirate schemes

22.11.2012 Dr. Axel Kohlmeyer,
Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy und Institute for Computational Molecular Simulations (ICMS), Temple University, Philadelphia, USA
Accelerating classical MD for multi-core CPUs and GPUs

4.9 Editorial activities

GAMM-Mitteilungen

The GAMM-Mitteilungen (GAMM-Proceedings) are published by Wiley-VCH Verlag, Berlin twice a year (www.onlinelibrary.wiley.com).

Managing Editor:
N. Kondratieva (Chair of Applied Dynamics)

Editor:
P. Steinmann

- Volume 35 Issue 1 2012
  Variational Methods in Computational Mechanics
  Guest Editor:
  J. Mosler, Dortmund

- Volume 35 Issue 2 2012
  Identification, Optimization and Control for Modern Technologies
  Guest Editor:
  G. Leugering, Erlangen-Nuremberg

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- **Archive of Applied Mechanics**
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- **Computational Mechanics**
- **Computers and Concrete**
- **Computers, Materials and Continua**
- **Computer Assisted Methods in Engineering and Science**
- **Computer Methods in Applied Mechanics and Engineering**
- **International Journal of Numerical Methods in Engineering**
- **International Journal of Solids and Structures**
- **International Journal of Structural Changes in Solids**
- **Journal of the Mechanical Behaviour of Materials**
- **Mathematics and Mechanics of Complex Systems**
- **Meccanica**

4.10 Latest news from the test laboratory of the LTM

(ss) The year 2012 was a very challenging and exciting time for our test laboratory, at least concerning the novelties and changes in equipment. The laboratory at the LTM can be divided into three sections: a dynamic testing area, an electro-mechanical testing area and a quasi-static and surface testing part. A further joint section of the laboratory is located at the Institute of Polymer Materials and is used collaboratively.

The dynamic testing area was completely renewed and improved equipment-wise in the end of 2011 and software-wise in the beginning of 2012. Our institute now holds two modal shaker systems, each with a closed loop shaker control including a data acquisition front end. The signal response can be recorded e.g. via acceleration sensors and/or two different Laser-Doppler-Vibrometers.

The electro-mechanical testing area is well equipped and used for testing electro-active polymers to validate the numerical results of the complex material behavior. This kind of materials can be used in sensor or activator applications, with artificial muscles being the most demonstrative example. This year a new branch research was started in the field of magneto-sensitive polymeric materials. The manufacturing and characterization of these so called Magnetorheological Elastomers is performed in a joint laboratory section located at the Institute of Polymer Materials. For the identification of the specific material characteristics (without and under an external magnetic field) a new rotational rheometer (MCR 502, Anton Paar) equipped with a magneto-rheological cell was purchased.

The most important changes of our laboratory occurred in the quasi-static and surface testing part. For the surface testing a laser scanning microscope was purchased, which enables us to measure and visualize the surface of various materials with a resolution down to 5 nm. Right now it is utilized for quantifying the smoothing of rough metal surfaces through normal contact and therewith for the characterization of the changes in the tribological behavior.

The most challenging modernization was the replacement of the old biaxial testing machine by a new one. The background of the changes is a new focus in the material testing, from the former dynamic testing of materials concerning crack growth with large forces, to a more quasi-static testing of sheet metals and polymers. Therefore the hydraulic driven dynamic testing machines were removed and got replaced by a new electro-mechanical, universal, biaxial testing machine built by Zwick according to our specifications.

Hydraulic biaxial machine

Removal transport

Delivery

Electro-mechanical machine

4.11 From an idea to a device: BoneProbe

(ww) The underlying problem is well known from placing screw anchors in walls: ailing walls won't provide enough support. Oral and maxillofacial surgeons are frequently faced with the same issue when trying to insert dental implants into weak jawbones. According to PD Dr. Dr. Tim Krafft, practicing surgeon from Weiden, this constitutes a major problem which should be solved.

Similarly, Matthias Karl, who is working as an Associate Professor at the Department of Prosthodontics, University of Erlangen-Nuremberg Dental School, claims that bone quality is a decisive factor in implant dentistry for choosing the 'right' implant, the best suited surgical protocol and the optimal loading protocol. However, a clinically applicable diagnostic tool for determining bone quality intraoperatively was not available. Based on the well established interdisciplinary cooperation between the Department of Prosthodontics and the Department of Mechanical Engineering, Dr. Werner Winter, who had extensively been working in the field of bone mechanics, was contacted.

Starting with the clarification of fundamental biomechanical phenomena occurring at an implant osteotomy, a clinically applicable diagnostic device was developed allowing the surgeon to determine bone quality during implant placement. Following the creation of a pilot drill hole in bone, a sensing element consisting of a cylinder with a diameter of 3mm which is split into four segments, is placed in the hole and expanded while the force needed for the expansion is measured what allows for an objective classification of bone quality.

BoneProbe Type III (Photograph: ALVEOSTICS)

The measurement principle was first validated using polyurethan foam materials mimicking the mechanical properties of bone followed by human cadaver as well as animal experiments. For clinical application in humans, two measurements, one at the surface and one at the bottom of the drill hole, will be necessary. The results will be available immediately and guide the dentist in optimizing the surgical protocol. Patients benefit from shorter treatment times, less appointments and a reduced complication rate. Besides cost reduction, the device also makes surgeries more predictable and safer, an important factor especially for young and less experienced surgeons.

This led to the idea of founding a start-up business for marketing the BoneProbe named ALVEOSTICS, an acronym based on the words 'alveolus', 'os' [latin word for bone] and 'diagnostics'. As part of these efforts, Werner Winter and Matthias Karl participated in the 'Business Plan Competition 2012' organized by 'Netzwerk Nordbayern'. Besides winning a cash prize of €10,000.-, the team could be completed by Bernd Einmeier, MBA who has plenty of experience in the fields of marketing and start-up organizing.


Urkunde

Businessplan-Wettbewerb Nordbayern 2012

Hochschul-Gründer-Preis 2012

Businessplan Wettbewerb netzwerknordbayern

Platz 1

Hochschul-Gründer-Preis 2012

Knochensonde – BoneProbe

Für die sehr gute Darstellung des Geschäftskonzepts in Phase 2 des Businessplan-Wettbewerb Nordbayern 2012 und die hervorragende Präsentation im Rahmen der Jury-Endausscheidung zum Hochschul-Gründer-Preis 2012 wird das Team als bestes aus einer nordbayerischen Hochschule oder Forschungseinrichtung ausgezeichnet.

Das netzwerk nordbayern gratuliert zu diesem außerordentlichen Erfolg!

Regensburg, 25. April 2012

WIR MACHEN UNTERNEHMER

Dr. Ronald Mertz
Ltd. Ministerialdirigent
Bayerisches Staatsministerium für Wirtschaft, Infrastruktur, Verkehr und Technologie

Dr. Benedikte Hatz
Geschäftsführerin
f.u.n. netzwerk nordbayern gmbh

Dr. Olaf Rathjen
Leiter Siemens Region Bayern
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Sponsoren

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SIEMENS

LfA FÖRDERBANK BAYERN

The ALVEOSTICS-Team:
Bernd Einmeier,
Dr. Werner Winter,
Dr. Matthias Karl
(Photograph: ALVEOSTICS)

The team plans to launch the BoneProbe next year in order to service a market of roughly 800,000 dental implants placed per year in Germany, 3.1 million in Europe and about twice as many around the world. Based on a network of original equipment manufacturers, distributors and an e-commerce channel, ALVEOSTICS even intends to expand globally.

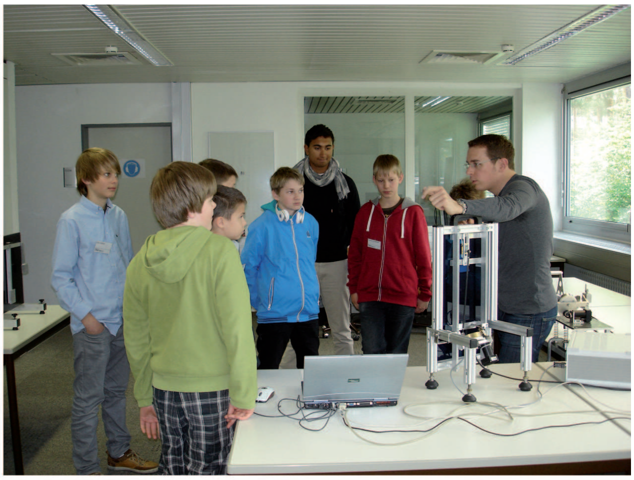
Further developing the BoneProbe, ALVEOSTICS currently evaluates at applications in the field of orthopedic surgery (hip replacements) and traumatology where a first prototype has already been constructed. Prior to application in regular surgeries and marketing, CE certification of the BoneProbe as medical device is required. Given the facts that the experiments conducted so far have been well documented and that comparable devices are missing, CE certification might be possible on the basis of a literature review.

In order to finance CE certification, production of the device as well as global marketing, the team seeks venture capital in the amount of €1.2 million. Besides ambitious plans, the prizes won and the prototypes at hand, the team has convinced Prof. Erich Reinhardt and Prof. Thomas Taylor (USA) to support them.

Having been in charge of Siemens Healthcare for numerous years, Prof. Reinhardt has extensive experience in the medical field while Prof. Taylor is a highly respected pioneer in the field of dental implantology. Both will act as active supporters for ALVEOSTICS granting access to global networks.

4.12 Girls' Day and Boys' Day

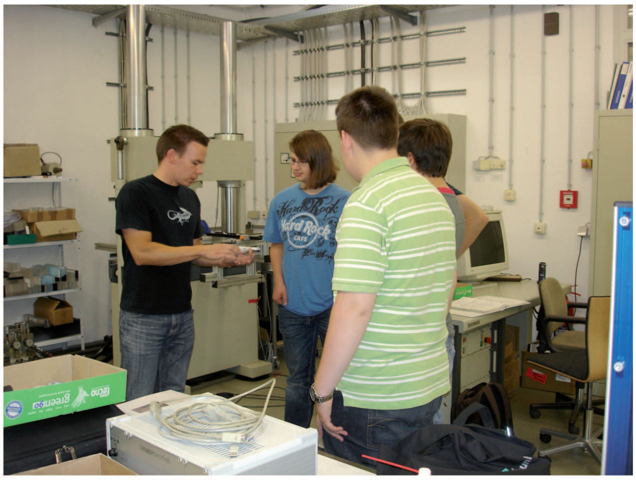
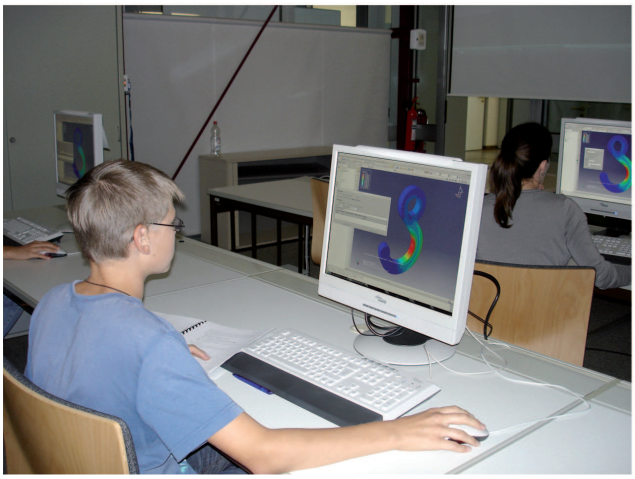
(dp, fv) On Girls' Day (26.04.2012), universities, organizations and companies opened their doors to awaken young girls' interest in engineering, science and trade. This annual event, which was originally designed for girls to provide them with information about non-typical professions for women, is accompanied since 2010 by the corresponding event for boys.
From 5th grade on, the students are encouraged to gain an insight into daily life and education at the University Erlangen-Nuremberg. The Chair of Applied Mechanics contributes to this event with descriptive experiments in the field of dynamics. The students are introduced to the basic principles of free and forced vibrations as well as phenomena like resonance, anti-resonance and resonance catastrophe.



4.13 Practical Course: Girls & Engineering / Youth & Engineering

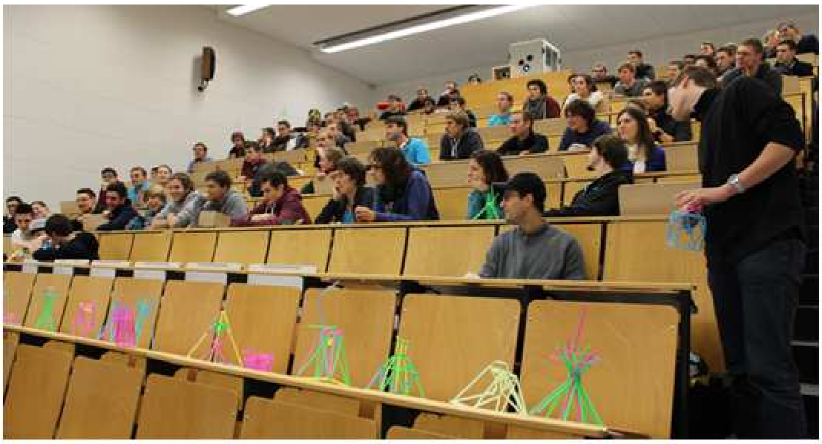
(dp, fv) Forming a long tradition since 1999, the practical course "Girls and Engineering" was held in September during the last week of the Bavarian school summer break. Since 2010, the corresponding course "Youth and Engineering", open for both genders, takes place in parallel. Within these events, students from 8th through 12th grade have the opportunity to learn about engineering and physics from an applied point of view. The students conduct several experiments, which are offered by the departements of the School of Engineering University Erlangen-Nuremberg and the Fraunhofer Institutes located in Erlangen, in order to gain some insight in the diversity of engineering disciplines and to learn more about applied sciences.

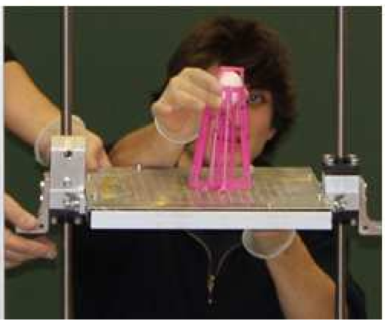
At the Chair of Applied Mechanics, we developed an experiment "Stress Analysis of a Crane Hook" which covers all basic steps in investigating a hook's behavior under loading until failure. The students receive an impression of the stress distribution within the loaded hook with the help of an optical stress analysis. Afterwards they try to extract the material constants of the hook's "unknown" material. With this information, the students perform a finite element analysis in order to reproduce the stress distribution from the optical experiment, to locate the maximal stress and to foresay the maximal possible loading. To verify the results of the numerical simulation, the course concludes with the most popular part among the students: the final destruction of the hook through a tensile test. We are happy, that our experiment was well received by the students and as a result of this good reception we are looking forward to participate also in the next year's event, which will be hosted in September 2013.


4.14 Egg-drop contest

(dkv) Following the successful Egg-Drop Contest organized in the summer semester of 2012 (see section 5.2), the second Egg-Drop Contest was organized in the winter semester (on 06 December of 2012) and attracted more than 30 groups of competing students. The success of the second Egg-Drop Contest not only enriched the teaching activities of the Chair of Applied Mechanics but also demonstrates the interest of many students in solving practical problems.





5 Social events

5.1 Visit of the Bergkirchweih

(us) Going back to the 18th century, the Bergkirchweih is an entrenched fest with residents and students in Erlangen. The fair provides a place for many booths with food and beverages, toys and souvenirs. The tunnels in the beer cellars make a great trip, but are not open during the fest. A big ferris wheel is always one of the great number of rides available for the brave visitor. On Tuesday, the 29th of May, the chair and many other institutes, shops and businesses closed and went for the traditional visit to the Bergkirchweih. With this year's reservation at the Erichkeller we were seated in the Vorderhaus, other chairs of mechanical engineering were seated in close proximity. The weather was warm, sunny and dry. Again, the band "Appendix" played from afternoon until late evening. The atmosphere inspired to do great, but expectations were exceeded.

5.2 Student summer party and egg-drop contest

(dkv) Aiming at attracting the attention of students to challenging problems in simulation and design of machinery and construction works, and as the continuation of four successful Ultimate Load Contests, the first Egg-Drop Contest organized by the Chair of Applied Mechanics took place on the 5th July 2012 in Erlangen together with the student summer party. Participated in the event were 15 groups of competing students. The object of this contest is an optimization problem in applied mechanics: built out of plastic drinking straws and paper staples, an engineering structure is designed to protect an raw egg being dropped from the height of 1 to 2 meters. As a reward for the effort, a prize was handed over to the winners of the contest. Being an exciting supplement to the curriculum of an engineering student, the Egg-Drop Contest deepens and enhances the theoretical part of education in Applied Mechanics by giving it a demonstrative dimension.

5.3 Outing to the ‘Brombachsee’

(fv) After the great success of last year’s event, the reinvention of the chair outing went on August 3rd, 2012, in the second round. Our former colleague, Dr. Winter, who enjoys now his well-deserved retirement, invited us to visit the ‘Franconian Lake District’. Thanks to his perfect organization, we enjoyed an interesting and entertaining day in the recreational area south of Nuremberg.

We started our tour at the information center in the ‘Mandlesmühle’ where we learned about the history and establishment of the artificially created lake district with about 20 km^2 of water surface. Next, we climbed the big embankment dam that delimits the ‘Great Lake Brombach’ to the East. From there we hiked along the northern coast of the lake to the village of Enderndorf where we paused for lunch. Luckily, the only rain drops of the day fell while we were having coffee and cake on the restaurant’s covered patio. In the afternoon, the sun came back and those who didn’t mind the cold temperatures of the lake even went for a swim while others preferred to board the liner for some water activity.

In the early evening we returned to our starting point either by foot or by boat and by then sunny weather and warm temperatures heightened the anticipation of the summer vacations.

6 Contributions to Journals

1. G. Chatzigeorgiou, A. Javili, P. Steinmann. Unified magnetomechanical homogenization framework with application to magnetorheological elastomers. *Mathematics and Mechanics of Solids*, DOI: 10.1177/108128651245810, 2012

2. D. Davydov, A. Javili, P. Steinmann. On molecular statics and surface-enhanced continuum modeling of nano-structures. *Computational Materials Science*, In Press (2012).

3. D. Davydov, P. Steinmann. Reviewing the roots of continuum formulations in molecular systems. Part I: Particle dynamics, statistical physics, mass and linear momentum balance equations. *Mathematics and Mechanics of Solids*, In Press (2012).

4. D. Davydov, A. Javili, P. Steinmann, A. McBride. A Comparison of Atomistic and Surface Enhanced Continuum Approaches at Finite Temperature. Book Chapter, Surface Effects in Solid Mechanics, Altenbach (Edited), Springer-Verlag, 2013

5. S. Diel, O. Huber, H. Saage, P. Steinmann, W. Winter. Mechanical Behaviour of a Cellular Composite under Quasi-Static, Static and Cyclic Compression Loading. *Journal of Materials Science*, **47**, pp. 5635-5645 (2012)

6. J. Friederich, G. Leugering, P. Steinmann. Adaptive refinement based on asymptotic expansions of finite element solutions for node insertion in 1d. *GAMM-Mitt.* 35, No.2, 175–190 (2012). DOI 10.1002/gamm.201210012

7. S. Germain, P. Steinmann. Towards inverse form finding methods for a deep drawing steel DC04 *Key Engineering Materials*, **504-506**, pp. 619-624 (2012)

8. S. Germain, P. Steinmann. On a recursive algorithm for avoiding mesh distortion in inverse form finding. *Journal of the Serbian Society for Computational Mechanics*, **6**, pp. 216-233 (2012)

9. K. Hochradel, S. J. Rupitsch, A. Sutor, R. Lerch, D. K. Vu, P. Steinmann. Dynamic Performance of Dielectric Elastomers Utilized as Acoustic Actuators. *Applied Physics A*, DOI 10.1007/s00339-012-6837-2 (2012)

10. M. Hossain, P. Steinmann. More Hyperelastic models for rubber-like materials: Consistent tangent operators and Comparative Study. *Journal of the Mechanical Behaviour of Materials*, In Press (2012).

11. M. Hossain, D. K. Vu, P. Steinmann. Experimental study and numerical modelling of VHB 4910 polymer. *Computational Materials Science*, **59**, pp. 56-75 (2012).

12. A. Javili, A. McBride, P. Steinmann. Thermomechanics of Solids with Lower-Dimensional Energetics: On the Importance of Surface, Interface and Curve Structures at the Nanoscale. A Unifying Review. *Applied Mechanics Reviews*, In Press (2012).

13. A. Javili, A. McBride, P. Steinmann. Numerical modelling of thermomechanical solids with highly-conductive energetic interfaces. *International Journal for Numerical Methods in Engineering*, DOI: 10.1002/nme.4402, 2012

14. A. Javili, A. McBride, P. Steinmann. Numerical modelling of thermomechanical solids with mechanically energetic (generalised) Kapitza interfaces. *Computational Materials Science*, **65**, pp. 542-551, 2012.

15. A. Javili, A. McBride, P. Steinmann, B. D. Reddy. Relationships between the admissible range of surface material parameters and stability of linearly elastic bodies. *Philosophical Magazine*, **92**, pp. 3540-3563 (2012).

16. S. Klinge, A. Bartels, P. Steinmann. Modeling of curing processes based on a multi-field potential. Single- and multiscale aspects. *International Journal of Solids and Structures*, **49**, pp. 2320-2333 (2012)

17. S. Klinge, A. Bartels, P. Steinmann. The Multiscale Approach to the Curing of Polymers incorporating Viscous and Shrinkage Effects. *International Journal of Solids and Structures*, **49**, pp. 3883-3900 (2012)

18. N. Konchakova, F. Balle, R. Mueller, P. Steinmann, D. Eifler, F.J. Barth. Numerical analysis of the maximum load level in lightweight metal/fibre-reinforced polymer structures. *Advanced Engineering Materials*, accepted (2012)

19. T. Krafft, W. Winter, M. Wichmann, M. Karl. In vitro validation of a novel diagnostic device for intraoperative determination of alveolar bone quality. *International Journal of Oral and Maxillofacial Implants*, **27(2)**, pp.318-328 (2012).

20. T. Krafft, N. Oeßelmann , M. G. Wichmann, W. Winter, S. M. Heckmann, M. Karl. Determination of Bone Quality During Implant Surgery-A Novel Approach. *Implantologia, Parodontologia, Osteologia*, **26(2)**, pp. 24-30. (Ukrainian), 2012

21. T. Krafft, M. G. Wichmann, W. Winter, M. Karl. Applicability of strain measurements on a contra angle handpiece for the determination of alveolar bone quality during dental implant surgery. *Journal of Cranio-Maxillo-Facial Surgery*, **40(5)**, pp. 144-149 (2012).

22. T. Krafft, F. Graef, W. Winter, M. Wichmann, M. Karl. Use of osteotomes for implant bed preparation - effect on material properties of bone and primary implant stability. *Journal of Oral Implantology*, accepted (2012)

23. M. Kraus, P. Steinmann. Finite Element Formulations for 3d Convex Polyhedra in Nonlinear Continuum Mechanics. *Computer Assisted Methods in Engineering Science*,**19**, pp. 121-134 (2012)

24. E. Lehmann, S. Schmaltz, S. Germain, D. Fassmann, C. Weber, S. Löhnert, M. Schaper, P. Steinmann, K. Willner, P. Wriggers. Material model identification for DC04 based on the numerical modelling of the polycrystalline microstructure and experimental data. *Key Engineering Materials*, **504-506**, pp. 993-998 (2012)

25. G. Leugering, M. Prechtel, P. Steinmann, M. Stingl. A Cohesive Crack Propagation Model: Mathematical Theory and Numerical Solution. *Communications on Pure and Applied Analysis*, **12**, pp. 1705-1723 (2012)

26. A. McBride, J. Mergheim, A. Javili, P. Steinmann, S. Bargmann. Micro-to-macro transitions for heterogeneous material layers accounting for in-plane stretch. *Journal of the Mechanics and Physics of Solids*, **60(6)**, pp. 1221-1239 (2012).

27. J. Mergheim, G. Possart, P. Steinmann. Modelling and computation of curing and damage of thermosets. *Computational Materials Science* **53**, pp. 359-367(2012)

28. J. Mergheim, G. Possart, P. Steinmann. Modeling and simulation of curing and damage in thermosetting adhesives. *Journal of Adhesion*, **89(2)**, pp. 111-127 (2013)

29. M. Prechtel, G. Leugering, P. Steinmann, M. Stingl. Optimal Design of Brittle Composite Materials: a Nonsmooth Approach. Journal of Optimization Theory and Applications, **155**, pp. 962-985 (2012)

30. U. Schmidt, J. Mergheim, P. Steinmann. Multi-scale parameter identification. *International Journal for Multiscale Computational Engineering*, **10(4)**, pp. 327-342 (2012).

31. P. Steinmann, A. McBride, S. Bargmann, A. Javili. A deformational and configurational framework for geometrically nonlinear continuum thermomechanics coupled to diffusion. *International Journal of Non-Linear Mechanics*, **47**, pp. 215-227 (2012).

32. P. Steinmann, M. Hossain, G. Possart. Hyperelastic models for rubber-like materials: Consistent tangent operators and suitability for Treloar's data. *Archive of Applied Mechanics* **82(9)**, pp. 1183-1217 (2012).

33. F. Vogel, R. Bustamante, P. Steinmann. On Some Mixed Variational Principles in Magneto Elastostatics *International Journal of Non-Linear Mechanics*, DOI: 10.1016/j.ijnonlinmec.2012.12.005 (2012)

34. D. K. Vu, P. Steinmann. On 3d Coupled BEM-FEM Simulation of Nonlinear Electro-Elastostatics *Comp. Meth. Appl. Mech. Engnrg.*, Vol. 201-204, pp. 82-90 (2012)

35. J. Wang, P. Steinmann. H.-H. Dai. Analytical study on the stress-induced phase or variant transformation in slender shape memory alloy samples. *Meccanica*, accepted (2012)

36. J. Wang, P Steinmann. A variational approach towards the modeling of magnetic field-induced strains in magnetic shape memory alloys. *Journal of the Mechanics and Physics of Solids*, **60**, pp. 1179-1200(2012)

37. W. Weber, P. Steinmann, G. Kuhn. Simulation of 3d Fatigue Crack Propagation Using an Implicit Time Integration Scheme. *International Journal of Fatigue*, accepted (2012)

38. W. Winter, M. Karl. Dehydration-induced shrinkage of dentin as a potential cause of vertical root fractures. *Journal of the Mechanical Behavior of Biomedical Materials*, **14**, pp. 1-6 (2012)

39. W. Winter, D. Klein, M. Karl. Effect of model parameters on finite element analysis of micromotions in implant dentistry. *Journal of Oral Implantology*, accepted (2012)

40. W. Winter, S. Holst, M. Karl. Screw loading and gap formation in implant-supported fixed restorations: Procera implant bridge vs. conventionally cast screw-retained restorations. *Quintessence International*, accepted (2012)

41. W. Winter, D. Klein, M. Karl. Micromotion of dental implants - basic mechanical considerations. *Journal of Medical Engineering*, accepted (2012)

Submitted (2012)

1. G. Chatzigeorgiou, A. Javili, P. Steinmann Multiscale modeling for composites with energetic interfaces at the micro or nano scale

2. H. -H. Dai, F. F. Wang, J. Wang, J. Xu Pitchfork and Octopus Bifurcations in a Hyperelastic Tube Subjected to Compression: Analytical Post-bifurcation Solutions and Imperfection Sensitivity

3. S. Fillep, J. Mergheim, P. Steinmann. Modelling and homogenization of technical textiles
4. S. Fillep, J. Orlik, Z. Bare, P. Steinmann. Homogenization in periodically heterogeneous elastic bodies with multiple micro contact
5. S. Fillep, J. Mergheim, P. Steinmann. On the homogenization of technical textiles. Book Chapter, 2012
6. F. Hauer, K. Willner. Development of a friction law respecting plastic surface smoothing
7. M. Hossain, P. Steinmann. Degree of cure-dependent modelling for polymer curing processes at small-strain. Part I: Consistent reformulation
8. A. Javili, F. dell Isola, P. Steinmann. Geometrically nonlinear higher-gradient elasticity with energetic boundaries
9. A. Javili, A. McBride, J. Mergheim, P. Steinmann, U. Schmidt. Micro-to-macro transitions for continua with surface structure at the microscale
10. N. Konchakova, R. Mueller, P. Steinmann, F. Balle, D. Eifler, F.J. Barth. Simulation of adhesive joint by viscoelastic interface material model
11. M. A. Kraus, A. Rajagopal, P. Steinmann. Investigations on the polygonal finite element method: Constrained adaptive Delaunay tessellation and conformal interpolants
12. J. Mergheim, P. Steinmann. Phenomenological modelling of self-healing polymers
13. A. Papastavrou, P. Steinmann, E. Kuhl. On the Mechanics of Continua with Boundary Energies and Growing Surfaces
14. S. Pfaller, M. Rahimi, G. Possart, P. Steinmann, F. Müller-Plathe M. C. Böhm. An Arlequin-based method to couple molecular dynamics and finite element simulations of amorphous polymers and nanocomposites
15. S. Schindler, M. Zimmermann, J.C. Aurich, P. Steinmann. Thermo-elastic deformations of the workpiece when turning aluminum alloys - experiments and finite element simulations
16. P. Steinmann. On Generalized Crystal-Plasticity based on Defect-Densities in a Second-Order Continuum
17. J. Wang, P. Steinmann. Finite element simulation of the magneto-mechanical response of a magnetic shape memory alloy sample

7 Contributions to Proceedings

1. S. Fillep, J. Mergheim, P. Steinmann. Homogenization and modelling of technical textiles. *ECCOMAS 2012*, Vienna, Austria, (2012)
2. S. Germain, P. Steinmann. On two different inverse form finding methods for hyperelastic and elastoplastic materials. *PAMM*, accepted (2012)

3. F. Hauer, K. Willner. Halfspace Simulation of Rough Surface Contact in Metal Forming, Proc. 10th. World Conference on Computational Mechanics, ISBN 978-85-86686-70-2, (2012)

4. A. Javili, A. McBride, J. Mergheim, P. Steinmann, U. Schmidt. Micro-to-macro transitions for continua with surface structure at the microscale. *PAMM*, DOI 10.1002/pamm.201210007.

5. V. Luchscheider, K Willner Analysis of the lamination stack influence on the stiffness of stator active component *PAMM*, accepted, 2012

6. V. Luchscheider, K. Willner. Development of a contact model for an electric motor lamination stack, In Press (2012)

7. V. Luchscheider. K. Willner, M. Maidorn. Development of a model to describe the stiffness of an electric motor lamination stack. In Press, 2012

8. S. Schmaltz, K. Willner. Material parameter optimization utilizing full-field strain measurement data and the Finite Element Method. *Colloquium on metal forming*, XXXI. Colloquium on metal forming, Donnersbach, Austria, 2012, S. 13-18. ISBN: 978-3-902078-17-9

9. S. Schmaltz, K. Willner. Material Parameter Identification utilizing Optical Full-Field Strain Measurement and Digital Image Correlation. In: *ISEM-ACEM-SEM-7th ISEM 2012*, (2012), Taipei, Taiwan (R.O.C.), accepted.

10. D. Süss, M. Jerschl, K. Willner. Numerical and experimental investigation of jointed structures using the Multiharmonic Balance method *IMAC*, accepted.

11. D. Süss, K. Willner. Multiharmonic Balance Analysis of a Jointed Friction Oscillator. *ECCOMAS*, CD-ROM (2012).

12. M. Zimmermann, S. Schindler, P. Steinmann, J.C. Aurich. Analysis of Thermo-Mechanical Effects on the Machining Accuracy when Turning Aluminum Alloys. *9th International Conference on High Speed Machining*, 7-8.03.2012, San Sebastian Spain.

8 Talks

1. S. Schmaltz. Material parameter optimization utilizing full-field strain measurement data and the Finite Element Method. *XXXI. Colloquium on metal forming*, Donnersbach, Austria, 26.02.2012.

2. P. Steinmann. Continuum Modelling, Molecular and Continuum Modelling of Polymers: Molecular Dynamics Meets Finite Elements, *SPP 1369*, 13.+14.03.2012, Pommersfelden, Germany

3. P. Steinmann. Molecular to Continuum Modeling, Molecular and Continuum Modelling of Polymers: Molecular Dynamics Meets Finite Elements, *SPP 1369*, 13.+14.03.2012, Pommersfelden, Germany

4. S. Germain, P. Steinmann. Towards inverse form finding methods for a deep drawing steel DC04. *ESAFORM 2012*, Erlangen, Germany, 14.03.2012

5. E. Lehmann, S. Germain, D. Fassmann, C. Weber, S. Löhnert, M. Schaper, F. Bach, P. Steinmann, K. Willner, P. Wriggers. Material model identification for DC04 based on the numerical modelling of the polycrystalline microstructure and experimental data. *ESAFORM 2012*, Erlangen, Germany, 14.03.2012

6. P. Steinmann, S. Pfaller, G. Possart, F. Müller-Plathe, M. Rahimi, M. C. Böhm. Coupled Molecular/Continuum Simulation of Polymers *Advanced School on Molecular and Continuum Modelling of Polymers: Molecular Dynamics Meets Finite Elements*,Pommersfelden, Germany, 14.03.2012.

7. P. Steinmann, A. Javili, A. McBride, J. Mergheim. Multiscale Modelling of Continua with Energetic Interfaces and Surfaces *EUROMECH Colloquium 537 on Multiscale Computational Homogenization of Heterogeneous Structures and Materials*, 26.-28.03.2012, Paris,France

8. V. Luchscheider, K. Willner Analysis of the lamination stack influence on the stiffness of stator active component. *83rd GAMM*, Darmstadt, 26.-30.03.2012

9. A. McBride, A. Javili, J. Mergheim, P. Steinmann, U. Schmidt. Micro-to-macro Transitions for Continua with Energetic Surfaces at the Microscale. *83rd GAMM*, Darmstadt, Germany, 26.-30.03.2012.

10. D. K. Vu, P. Steinmann. On the spatial and material motion problems in nonlinear electro-elastostatics with consideration of free space. *GAMM 2012*, Damstadt, Germany, 26-30.03.2012

11. J. Mergheim. Selbstheilende Polymere fuer eine interdisziplinäre Herausforderung. *Gesellschaft der Freunde der Bayerischen Akademie der Wissenschaften*, 28.03.2012.

12. S. Germain, P. Steinmann. On inverse form finding for anisotropic materials. *GAMM 2012*, Darmstadt, Germany, 29.03.2012

13. M. Hossain, P. Steinmann. On Consistent Tangent Operator Derivation and Comparative Study of Rubber-like Material Models at Finite Strains. *GAMM 2012*, Darmstadt, Germany, 29.03.2012

14. S. Fillep, J. Mergheim, P. Steinmann. Modelling and homogenization of technical textiles. *7th International Conference on Computational Mechanics for Spatial Structures*, Sarajevo, Bosnia and Herzegovina, 02-04.04.2012

15. A. Javili, A. McBride, P. Steinmann. Thermomechanics of Continua with Energetic Surfaces/Interfaces. *SPP1480*, Karlsruhe, Germany, 11.04.2012.

16. M. Jerschl, D. Süss, S. Kruse, K. Willner. Investigation of the Dynamic Behavior of Braking Disk Joints. *Euro Brake 2012*, Dresden, 16-18.04.2012

17. D. Davydov, A. Javili, P. Steinmann. Atomistic and Continuum Modelling of Nanostructures. *YIC 2012*, Aveiro, Portugal, 24-27.04.2012.

18. J. Mergheim. Towards the Modelling of Self-Healing Polymers. *Abschlusskolloquium Graduiertenkolleg 814*, TU Kaiserslautern, 26.04.2012.

19. M. Hossain, D. K. Vu, P. Steinmann. Experimental Investigation and Numerical Modelling of VHB 4910 Polymer. *EuroEAP 2012*, Potsdam, Berlin, Germany, 28-30.05.2012.

20. P. Steinmann, N. Konchakova, F.J. Barth,R. Müller. Modellierung und Simulation flächig geschweißter Metall/Faser-Kunststoff Verbunde. *Abschlusskolloquium FOR 524*, Kaiserslautern, Germany, 28.+29.06.2012

21. F. Hauer, K. Willner. Halfspace Simulation of Rough Surface Contact in Metal Forming. *WCCM 2012*, Sao Paulo, Brasil, 8-13.07.2012

22. F. Vogel, P. Steinmann. Non-Linear Modeling of Magneto-Sensitive Elastomers within a Mixed-Finite-Element Framework. *ESMC*, Graz, Austria, 9-13.07.2012

23. D. Davydov, A. Javili, A. McBride, P. Steinmann. A Comparison of Atomistic and Enhanced Continuum Approaches for Modelling Surface Effects in Solids. *ESMC 2012*, Graz, Austria, 9-13.07.2012

24. M. Hossain, D. K. Vu, P. Steinmann. Mechanical Behaviour of VHB 4910 Polymer: Experiments, Modelling and Validation. *ESMC 2012*, Graz, Austria, 9-13.07.2012

25. P. Steinmann, A. Javili, A. McBride, B. D. Reddy. The Admissibility of Negative Material Parameters for Surface Elasticity Theory. *ESMC 2012*, Graz, Austria, 9-13.07.2012

26. D. K. Vu, P. Steinmann. On the formulation of the spatial and material motion problem in nonlinear electro-elastostatics. *ESMC 2012*, Graz, Austria, 9-13.07.2012

27. D. Süß, K. Willner. Multiharmonic Balance Analysis of a friction oscillator including a bolted joint. *ICTAM*, Beijing, China, 19.-24.08.2012

28. A. Javili, A. McBride, P. Steinmann. Micromechanics, Interfaces and Multi-scale Modelling. *SolMech 2012*, Warsaw, Poland, 27-31.08.2012.

29. J. Wang, P. Steinmann. A variational approach towards the modeling of the magneto-mechanical responses of a magnetic shape memory alloy sample. *International Workshop on Mathematical and Mechanical Modelling for Materials*, City University of Hong Kong, Hong Kong, 28-31.08.2012

30. P. Steinmann. On the Transition from Molecular Descriptions to Continuum Formulations. *Workshop Multiscale Material Modeling*, 2.-7.09.2012, Bad Herrenalb, Germany

31. A. McBride, A. Javili, J. Mergheim, P. Steinmann, U. Schmidt. Micro-to-macro Transitions for Continua with Energetic Surfaces at the Microscale. *8th SACAM*, Johannesburg, South Africa, 3-5.09.2012.

32. D. Riedlbauer, J. Mergheim, A. McBride, P. Steinmann. Performance considerations for a nonlinear thermomechanical model for the selective beam melting process. *Numerical Heat Transfer 2012*, Wroclaw, Poland, 04-06.09.2012

33. M. Karl, T. Taylor, M. Wichmann, W. Winter. Finite Element Analysis on bone adaptation induced by non-passively fitting implant superstructures *European Prosthodontic Association (EPA), 36th Annual Congress Rotterdam*, Netherlands, 06-08.09.2012

34. A. F. M. S. Amin, M. Hossain, M. Kabir. Eight-chain Model and Its Variants for Hyperelastic Rubber-like Materials: A Comparative Study. *ECCOMAS 2012*, Vienna, Austria, 10-14.09.2012.

35. D. Davydov, A. Javili, P. Steinmann. Atomistic to Continuum Modeling of Materials. *ECCOMAS 2012*, Vienna, Austria, 10-14.09.2012.

36. S. Fillep, J. Mergheim, P. Steinmann. Homogenization and modelling of technical textiles. *ECCOMAS 2012*, Vienna, Austria, 10-14.09.2012

37. M. Hossain, D. K. Vu, P. Steinmann. Micromechanical Modelling for Viscoelastic Electroactive Polymers. *ECCOMAS 2012*, Vienna, Austria, 10-14.09.2012.

38. A. Javili, A. McBride, P. Steinmann, D. Davydov. Multiscale Modelling of Continua with Energetic Surfaces at the Microscale. *ECCOMAS 2012*, Vienna, Austria, 10-14.09.2012.

39. V. Luchscheider, K. Willner Development of a contact model for an electric motor lamination stack. *ECCOMAS 2012*, Vienna, Austria, 10.-14.09.2012

40. J. Mergheim, G. Possart, P. Steinmann. Modelling and simulation of curing and damage of thermosetting adhesives. *ECCOMAS 2012*, Vienna, Austria, 10.-14.09.2012

41. P. Steinmann, A. Javili, A. McBride. On the Modelling and Computation of Nano-Sized Solids with Surface and Interface Thermomechanics. *ECCOMAS 2012*, Vienna, Austria, 10-14.09.2012.

42. D. Süß, K. Willner. Multiharmonic Balance Analysis of a jointed friction. oscillator, *ECCOMAS*, Vienna, Austria, 10.-14.09.2012

43. U. Schmidt, J. Mergheim, P. Steinmann. Identification of Microscopic Material Parameters Within Nonlinear Computational Homogenization Using Gradient-based Optimization Algorithms *IWCMM 2012*, Baltimore, USA, 24-26.09.2012

44. W. Winter, D. Klein, M. Karl. Effect of model parameters on finite element analysis of micromotions in implant dentistry. *American Academy of Implant Dentistry (AAID), 61st Annual Meeting*, Washington DC, USA, 03.-06.10.2012

45. V. Luchscheider, K. Willner, M. Maidorn Development of a model to describe the stiffness of an electric motor lamination stack. *2nd International Electric Drives Production Conference and Exhibition 2012 (E—DPC)*, Nuremberg, Germany, 15.-18.10.2012

46. S. Schmaltz. Material Parameter Identification utilizing Optical Full-Field Strain Measurement and Digital Image Correlation, *ISEM-ACEM-SEM-7th ISEM 2012*, Taipei, Taiwan (R.O.C.), 8-11.11.12

47. F. Endres, P. Steinmann. Towards molecular statics simulation of ferroelectric materials. *First Seminar on Ferroic Functional Materials*, Dortmund, Germany, 21-22.11.2012

48. P. Steinmann, J. Wang. A Variational Approach to the Modelling of Magnetic Shape Memory Alloys *Uni Kassel*, 30.11.2012, Kassel, Germany

49. M. Hossain, P. Steinmann. Degree of Cure-dependent Modelling for Polymer Curing Processes at Small-strains. *ICCMS 2012*, Hyderabad, India, 8-12.12.2012

50. P. Steinmann, J. Mergheim, P. Fischer, A. Rajagopal. C1-Continuous Methods in Computational Continuum Modelling *4th International Congress on Computational Mechanics and Simulation*, Hyderabad, India, 8.-12.12.2012

51. J. Mergheim. Two-scale modelling of material failure through diffusive damage and sharpe discontinuities *Seminar WW1, FAU Erlangen-Nürnberg*, Erlangen, Germany, 13.12.2012.