

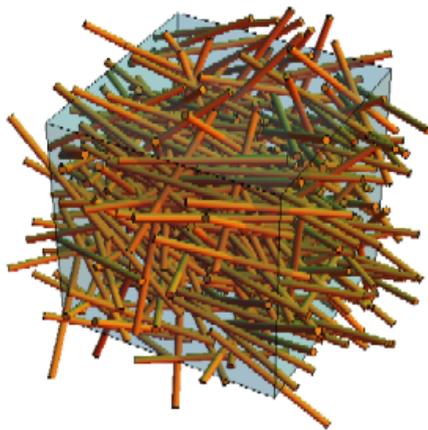
Karlsruhe Institute of Technology
Institute of Engineering Mechanics



University of Paderborn
Chair of Engineering Mechanics



**27th International Workshop
Research in
Mechanics of Composites**



**Bad Herrenalb, Germany
December 11-12, 2014**

Objective of the Workshop

Modern fiber reinforced polymers (FRP) show a macroscopic material behavior depending sensitively on the fiber orientation distribution and arrangement as well as the generally nonlinear material behavior of the constituents. Additionally, the overall composite behavior is influenced by fluid-structure interaction, by curing during the production process as well as by the interface properties. Understanding the correlation of both the microstructure and the micromechanical behavior on the one side, and the macroscopic composite behavior on the other side, is of fundamental interest for the design of materials, the optimization of production processes as well as the dimensioning and optimization of construction parts. In this workshop, new approaches for the material modeling of fiber reinforced composites, corresponding numerical solution strategies, and experimental techniques are discussed.

Prof. Dr.-Ing. habil. Thomas Böhlke

Prof. Dr.-Ing. habil. Rolf Mahnken

PD Dr. Heiko Andrä (Guest Organizer)

Dr. Matthias Kabel (Guest Organizer)

Program for Wednesday, December 10, 2014

Time	Registration and Welcome, Informal Meeting
from 18:00 on	

Program for Thursday, December 11, 2014

Time	Authors	Title of Lecture
09:00 - 09:30	<u>A. Lion</u> and <u>M. Johlitz</u>	Thermodynamic modeling and simulation of semicrystalline polymers
09:30 - 10:00	<u>R. Cuntze</u>	Material properties and model parameters, necessary for the analysis of static, cyclic, dynamic stress states and impact
10:00 - 10:30	Coffee break	
10:30 - 11:00	<u>H. Andrä</u> , <u>J. Spahn</u> , <u>M. Kabel</u> , <u>R. Müller</u> , and <u>C. Linder</u>	The Lippmann-Schwinger-type integral equation for progressive damage in composites
11:00 - 11:30	<u>J. Simon</u> , <u>B. Bednarczyk</u> , <u>B. Stier</u> , and <u>S. Reese</u>	Multi-scale modeling of damage in textile composites
11:30 - 12:00	<u>V. Müller</u> and <u>T. Böhlke</u>	How do microstructural parameters affect the prediction of elastic properties of materials with particulate microstructures?
12:00 - 12:30	<u>A. Dridger</u> , <u>I. Caylak</u> , and <u>R. Mahnken</u>	Uncertainty quantification for linear elastic bodies with two fluctuating parameters
12:30 - 13:30	Lunch	
13:30 - 14:00	<u>B. Bertram</u> and <u>K. A. Weidenmann</u>	μ CT-based characterization of the fibrous microstructure in $\text{Al}(\text{OH})_3$ -filled SMC
14:00 - 14:30	<u>B. Brylka</u> , <u>V. Müller</u> , <u>T. Böhlke</u> , <u>M. Hohberg</u> , and <u>F. Henning</u>	Microstructure-based modeling of temperature-dependent stiffness of SMC
14:30 - 15:00	<u>L. Schulenberg</u> , <u>D.-Z. Sun</u> , and <u>T. Seelig</u>	Micromechanical modeling of long fibre reinforced thermoplastics
15:00 - 15:30	<u>T. Leismann</u> and <u>R. Mahnken</u>	Comparison of hyperelastic micromorphic, micropolar and microstretch continua - Constitutive models and computation
15:30 - 16:00	Coffee break	
16:00 - 16:30	<u>M. Kabel</u> , <u>T. Böhlke</u> , and <u>M. Schneider</u>	FFT-based homogenization of elasticity at large deformations
16:30 - 17:00	<u>M. Schneider</u> , <u>F. Ospald</u> , and <u>M. Kabel</u>	Computational homogenization on a staggered grid
17:00 - 17:30	<u>D.H. Pahr</u>	CT-based FE simulations of composite materials: Possibilities, trends, and applications
17:30 - 18:00	<u>J. Vondřejc</u> , <u>J. Zeman</u> , and <u>I. Marek</u>	From FFT-based homogenization to guaranteed bounds on effective linear properties
19:30	Workshop Dinner	

Program for Friday, December 12, 2014

Time	Authors	Title of Lecture
08:30 - 09:00	<u>H. Finckh</u> , <u>F. Fritz</u> , and <u>G.T. Gresser</u>	Use of high resolution CT for fibre based materials
09:00 - 09:30	<u>F. Buck</u> , <u>B. Brylka</u> , <u>V. Müller</u> , <u>T. Müller</u> , <u>A. N. Hrymalk</u> , <u>F. Henning</u> , and <u>T. Böhlke</u>	Coupling of mold flow simulations with two-scale structural mechanical simulations for long fiber reinforced thermoplastics
09:30 - 10:00	<u>F. Ospald</u> and <u>M. Schneider</u>	Effective viscosity of fiber suspensions
10:00 - 10:30	<u>A. Bernath</u> and <u>F. Henning</u>	Comparison of finite volume and finite element methods for the prediction of process induced residual stresses during resin transfer molding
10:30 - 11:00	Coffee break	
11:00 - 11:30	<u>M. Tort</u> , <u>P. Trimby</u> , <u>G. Sha</u> , <u>K. Xia</u> , and <u>Y. Lapusta</u>	Microstructure and yield strength modeling in a severely deformed Al ₂ 5Cu1.5Mg alloy
11:30 - 12:00	<u>S. Berbenni</u> , <u>F. Dinzart</u> , and <u>H. Sabar</u>	A new internal variables homogenization scheme for linear viscoelastic materials based on an exact Eshelby interaction law
12:00 - 12:30	<u>M. Düsing</u> and <u>R. Mahnken</u>	A phase-field approach for lower bainitic transformation considering carbide formation
12:30 - 13:00	Final discussion	
13:00	Lunch	

The Lippmann-Schwinger-type integral equation for progressive damage in composites

Heiko Andrä¹, Johannes Spahn¹, Matthias Kabel¹, Ralf Müller², and Christian Linder³

¹ Fraunhofer Institute for Industrial Mathematics (ITWM)
Fraunhofer-Platz 1, 67663 Kaiserslautern, Germany

² Institute of Applied Mechanics, TU Kaiserslautern,
Gottlieb-Daimler-Straße, 67653 Kaiserslautern, Germany

³ Department of Civil and Environmental Engineering
Stanford University, 473 Via Ortega, Stanford, CA 94305, USA

Abstract. Conventional macro mechanical models and closed form estimates are in many cases not sufficient to appropriately predict the stiffness and strength of composite materials. Composite failure occurs as a result of complex microstructural damage mechanisms, which arise simultaneously with other nonlinear effects in the microstructure. In this contribution we propose an approach, where nonlinear material effects caused by progressive damage behavior are captured directly on a finer scale. The microstructural constituents are spatially resolved and modeled explicitly. A periodic boundary value problem on a volume element of the microstructure is solved in the numerical homogenization procedure. Because of the highly complex microstructure a fine regular grid is used instead of a boundary aligned mesh to avoid the mesh generation. The periodic boundary value problem is reformulated into a volume integral equation of the Lippmann-Schwinger type and solved efficiently using Fast Fourier Transforms (FFT). In the work at hand, a glass fiber reinforced composite is considered and a ductile damage model is applied for the polymer matrix. The numerical method is validated with experimental data for the considered thermoplastic composite material.

References

- [1] J. Spahn, H. Andrä, M. Kabel, R. Müller: A multiscale approach for modeling progressive damage of composite materials using fast Fourier transforms. *Comp. Meth. Mech. Engrg.*, **268**, 871–883 (2014).

A new internal variables homogenization scheme for linear viscoelastic materials based on an exact Eshelby interaction law

Stéphane Berbenni¹, Florence Dinzart², and Hafid Sabar²

¹ Laboratoire d'Etude des Microstructures et de Mécanique des Matériaux, UMR CNRS 7239, Université de Lorraine, 57045 Metz, France

² Laboratoire de Mécanique Biomécanique Polymères Structures, Ecole Nationale Ingénieurs de Metz, 57078 Metz, France

Abstract. A new time-incremental internal variables homogenization scheme for Maxwellian linear viscoelastic heterogeneous materials is proposed. This scheme is based on the exact solution of the ellipsoidal Eshelby inclusion problem obtained in the time domain. In contrast with current existing methods, the effective behavior as well as the evolution laws of the averaged stresses per phase are solved incrementally in the time domain without need to analytical or numerical inverse Laplace-Carson transforms. This is made through a time-differential equation in addition to the more classic strain rate concentration equation. In addition, the new derived interaction law for the Eshelby inclusion problem is provided in a compact matrix form. It is proved that this is an exact formulation for an arbitrary anisotropic ellipsoidal Maxwellian inclusion embedded in an isotropic Maxwellian matrix. In order to show the interest of the present approach, the results are reported and discussed with a Mori-Tanaka homogenization scheme for two-phase composites in comparisons with other exact or approximate methods.

Comparison of finite volume and finite element methods for the prediction of process induced residual stresses during resin transfer molding

Alexander Bernath and Frank Henning

Institute of Vehicle System Technology, Chair of Lightweight Technology,
Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Abstract. Resin transfer molding (RTM) shows huge potential for the economical large batch production of structural parts made of high performance composite materials. However, during manufacturing residual stresses arise due to temperature driven expansion or contraction and chemical induced shrinkage of the matrix material. As a consequence, final parts show significant geometrical deviations (warpage) and therefore often violate tolerance requirements. Strategies exist which aim to reduce warpage but proper application usually requires extensive experimental knowledge. Therefore, reliable prediction of deviations by using simulation methods is one promising approach for reducing development times and risks while at the same time avoiding the need for comprehensive experimental studies. Up to now, available simulation tools, which are able to solve this type of problem, are solely based on the finite element method (FEM).

This work aims on using the finite volume method (FVM) for this purpose as it offers similar accuracy but higher memory efficiency compared to the FEM and shows good scaling in case of parallel computing [1,2]. Moreover, various open source libraries exist which enable researchers to easily tailor the software to their specific needs [3]. This approach has been followed in this work. Mathematical models were implemented in order to describe the material behavior of both, the matrix itself and the resulting composite. The same has been done for the FEM in order to compare these two discretization techniques. For this purpose both have been applied to generic geometries.

References

- [1] N.A. Fallah, C. Bailey, M. Cross, G.A. Taylor: Comparison of finite element and finite volume methods application in geometrically nonlinear stress analysis, *Applied Mathematical Modelling*, **24**, 439–455 (2000).
- [2] H. Jasak, H.G. Weller: Application of the finite volume method and unstructured meshes to linear elasticity, *International Journal for Numerical Methods in Engineering*, **48**, 267–287 (2000).
- [3] P. Cardiff, A. Karac, A. Ivankovic: A Large Strain Finite Volume Method for Orthotropic Bodies with General Material Orientations, *Computer Methods in Applied Mechanics and Engineering*, **268**, 318–335 (2013).

μ CT-based characterization of the fibrous microstructure in Al(OH)₃-filled SMC

Benjamin Bertram¹ and Kay André Weidenmann¹

Institute for Applied Materials – WK,
Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Abstract. The sheet molding compound (SMC) process is applied in the automotive industry to form a discontinuous fiber-reinforced polymer. The complex microstructure of SMC materials encompasses pores, filler particles and fibers, whose random orientation is caused by the flow and disaggregation of fiber bundles during molding and is likely affected by the large variety of SMC process parameters in use.

Micro X-ray computed tomography (μ CT) is widely used to investigate 3D-fiber orientation distributions; however, CaCO₃ filler particles inhibit μ CT because it has a linear X-ray attenuation that is similarly high as that of glass fibers. Al(OH)₃ is therefore investigated as an alternative filler, which allows for tomography in absorption-mode lab-based μ CT systems. Homomorphic filtering and a cylindrical μ CT specimen shape are used to further optimize the fiber-matrix-contrast and to compute orientation distributions encoded as 4th order orientation tensors introduced by Advani and Tucker [1], which can be directly used for micro-mechanical modeling.

The fiber volume content is a further important input parameter for the micro-mechanical modeling of the effective modulus. An incineration method is adapted to the specific oxidation of the Al(OH)₃-filled matrix. Incineration is time-consuming and limited in spatial resolution, but can be used as a ground truth for the regression of the fiber content from 2D-xray image features, allowing for a non-destructive application to sections of the SMC plate.

The tensile stiffness and strength of the Al(OH)₃-filled SMC are similar to those of the corresponding CaCO₃-filled versions, while facilitating the X-ray-based analysis of the fibrous microstructure and volume content.

References

- [1] S. G. Advani, C. L. T. Iii: The Use of Tensors to Describe and Predict Fiber Orientation in Short Fiber Composites, *J. Rheol.*, **31,8** 751-784 (1987).

Micro structure based modeling of temperature dependent stiffness of SMC

Barthel Brylka¹, Viktor Müller¹, Thomas Böhlke¹, Martin Hohberg², and Frank Henning²

¹ Institute of Engineering Mechanics, Chair for Continuum Mechanics
Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

² Institute of Vehicle System Technology (FAST),
Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Abstract. In many applications, sheet moulding compounds (SMC) are used if class A surface is required. Especially the possibility of forming complex structures leads to an increase of applications in the last few years. Compression moulding as manufacturing process for SMC leads to manufacturing related anisotropic as well as inhomogeneous material properties. These material properties like stiffness, thermal extension, damage and fracture are strongly anisotropic as well as temperature dependent and related to the local fiber orientation distribution which is influenced by flow of the melt. Dimensioning strategies need to take, therefore, the manufacturing process into account by simulation of the compression moulding process. Especially in automotive applications, material models for these inhomogeneous and anisotropic as well as temperature and strain-rate dependent materials are needed. For this reason, homogenization schemes are used based on the micro structure information from mould filling simulation as well as computer tomography, to predict the effective anisotropic, temperature dependent stiffness of SMC. The temperature dependent stiffness of the resin-filler composite matrix as well as the effective SMC has been measured by dynamic mechanical analysis (DMA). A comparison of the effective stiffness predicted by Mori-Tanaka approximation [1] based on mould filling simulation results as well as computer tomography will be presented. These results will be compared to the effective anisotropic stiffness and their scatter investigated in DMA measurements.

References

- [1] Y. Benveniste: A new approach to the application of Mori-Tanaka's theory in composite materials, *Mech. Mat.*, **6**, 147–157 (1987).
- [2] Z. Jendli, F. Meraghni, J. Fitoussi, D. Baptiste: Multi-scales modelling of dynamic behaviour for discontinuous fibre SMC composites, *Comp. Sci. Technol.*, **69**, 97–103 (2009).

Coupling of mold flow simulations with two-scale structural mechanical simulations for long fiber reinforced thermoplastics

Fabian Buck¹, Barthel Brylka¹, Viktor Müller¹, Timo Müller², Andrew N. Hrymak³, Frank Henning², and Thomas Böhlke¹

¹ Institute of Engineering Mechanics,
Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

² Institute of Vehicle Systems Technology,
Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

³ Department of Chemical & Biochemical Engineering,
University of Western Ontario, London, Canada

Abstract. Due to their great weight-related strength and stiffness characteristic values and their versatile usability for complex molding, long fiber reinforced thermoplastics (LFT) become more important in industrial applications. For the calculation of the mechanical properties, which are mainly influenced by the manufacturing induced fiber orientation, the entire simulation process including flow and fiber orientation analysis [1], mapping of the obtained fiber orientation information, homogenization and FE structural simulations has to be investigated. Examination parts are compression molded polypropylene plates with 30 wt.-% glass fibers as reinforcement. The filling of the mold during compression is examined with the commercial software *Moldflow* and the obtained fiber orientation is validated with μ CT data of selected samples. To calculate the effective stiffness properties based on simulated and measured μ CT fiber orientation data three different homogenization schemes are used and compared: a two step scheme, a Mori-Tanaka approach and the self-consistent method [2]. The numerical results of FE calculations are validated with dynamic mechanical analysis (DMA) results of tensile and three point bending tests with static and dynamic load at different positions of the LFT plates. The obtained results identify that the combined methods allow a prediction of the essential mechanical properties and make clear that exact knowledge of the fiber orientation gradients induced by the different charge positions is essential for the entire simulation process.

References

- [1] J. H. Phelps, C. L. Tucker III: An anisotropic rotary diffusion model for fiber orientation in short- and long-fiber thermoplastics, *Journal of Non-Newtonian Fluid Mechanics*, **156(3)**, 165–176 (2009).
- [2] V. Müller, T. Böhlke, F. Dillenberger, S. Kolling: Homogenization of Elastic Properties of Short Fiber Reinforced Composites Based on Discrete Microstructure Data, *PAMM*, **13(1)**, 269–270 (2013).

Material properties and model parameters, necessary for the analysis of static, cyclic, dynamic stress states and impact

Ralf Cuntze

Markt Indersdorf,
retired from industry, linked to Carbon Composites e.V., Augsburg

Abstract. Industry looks for robust and reliable analysis procedures in order to replace the expensive 'Make and Test Method' as far as reasonable. Virtual tests shall reduce the amount of physical tests.

In this context: Structural Design Development can be only effective if realistic input information is available for Design Dimensioning and for Manufacturing, as well.

Reliable material properties are an essential key to achieve this effectiveness accompanied by the necessary high fidelity analyses.

Topics here are high performance laminates and associated structural properties.

The talk is structured according to:

1. Design dimensioning in structural design, some definitions
2. Modeling of materials (elasticity, strength) and analysis
3. Material properties (matrix, fiber, interphase, composite)
4. Special material properties and model parameters
5. Test methods and material sheets
6. Design verification and certification
7. Conclusions with Annex

Uncertainty quantification for linear elastic bodies with two fluctuating parameters

Alex Dridger, Ismail Caylak, and Rolf Mahnken

Chair of Engineering Mechanics,
University of Paderborn, Paderborn, Germany

Abstract. Nowadays the uncertainty quantification becomes an important factor in many physics and engineering applications and should be taken into account. Stochastic partial differential equations (SPDEs) are commonly used to treat these kind of issues.

In this paper, we study a numerical method to solve a linear elastic system with stochastic coefficients. We introduce the strong form of the SPDE and the corresponding weak form. To solve this problem it is necessary to discretize the equation in the spatial and the stochastic area. The spatial discretization is performed by ordinary finite element methods whereas the stochastic discretization uses WIENER'S polynomial chaos [2] to expand the coefficients in deterministic and stochastic parts. Similar to the spatial discretization there are *shape* functions (so-called *Hermite polynomials* [1],[2]) for the stochastic discretization.

We consider a material behavior with two parameters. Two different approaches are presented: The first one presupposes the knowledge of the distribution of the random variables *modulus of elasticity* E and the *shear modulus* G . The second one assumes the distribution of *Poisson's ratio* ν instead of the distribution of G to be known. Computational approaches involving polynomial chaos are used to expand these variables. Therefore, GALERKIN projection [1] can be applied to reduce the stochastic PDE into a system of deterministic PDEs.

This work considers normally distributed random variables. Thus the number of stochastic dimensions is equal to the number of independent input parameters. Subsequently, the resulting equation system is solved iteratively. Finally, our method is applied in a numerical example for a plate with a ring hole.

References

- [1] H. G. Matthies and A. Keese. Galerkin methods for linear and nonlinear elliptic stochastic partial differential equations. *Comput. Methods Appl. Mech. Engrg.*, **194**:1295-1331, 2005.
- [2] R. G. Ghanem and P. D. Spanos. *Stochastic Finite Elements: A Spectral Approach*. Springer-Verlag, New York, 1991.

A phase-field approach for lower bainitic transformation considering carbide formation

Martin Düsing¹ and Rolf Mahnken¹

Chair of Engineering Mechanics (LTM),
University of Paderborn, Paderborn, Germany

Abstract. The phase-field method is a widely used tool to model the material behaviour on a mesoscale [1]. Especially for steel there are many approaches describing the different transformations using this method [2]. Yet there are few phase-field models for the bainitic transformation [3], because it is one of most complex transformations in steel. Bainite consists of carbides, bainitic ferrite and may have residual austenite. In recent reports the formation of carbides has not been considered.

A phase field model to simulate the transformation of lower bainite including carbon diffusion und carbide formation has been developed. To model the evolution of the carbides it is necessary to simulate the diffusion of the carbon. Therefore the model which is based on a classical phase-field approach, is coupled with a viscous Cahn-Hilliard equation to simulate the typical coarsening of the carbon concentration. During the isothermal process a sheaf of bainitic ferrite grows. The carbon starts coarsening because the bainitic ferrite can only contain a fraction of the carbon which was stored in the austenite. At the peaks of the carbon concentration carbides are excreted. The simulations show the described growth characteristics of the lower bainite transformation including carbide formation successfully.

References

- [1] I. Steinbach: Phase-field models in materials science, *Modelling Simul. Mater. Sci. Eng.*, **17**, (2009).
- [2] A. Yamanaka, T. Takaki, Y. Tomita: Phase-Field Simulation of Austenite to Ferrite Transformation and Widmanstätten Ferrite Formation in Fe-C Alloy, *Materials Transactions*, **47(11)** 2725–2731 (2006).
- [3] T.T. Arif, R.S. Qin: A phase-field model for bainitic transformation, *Computational Materials Science*, **77**, 230–235 (2013).

Use of high resolution CT for fiber based materials

Hermann Finckh, Florian Fritz, and Goetz T. Gresser

German Institutes of Textile and Fiber Research (DITF), Institute of Textile Technology and Process Engineering (ITV), Denkendorf, Germany

Abstract. Fiber-reinforced plastics (FRP) have outstanding properties for lightweight construction as they possess very high mass specific strength and stiffness. For a long time numerical methods are applied in automotive, aerospace etc. to compute mechanical properties using idealizations. With increasing efficiency of computer more detailed and precise simulation models have been used, also allowing complex material models. Main focus in FRP is laid on considering correct fiber orientation, fiber distribution and fabric structure to optimize fabric layout. The quality of the FRP part strongly depends on the individual stages of the production processes. In the Resin Transfer Molding (RTM) process the reinforcement fabrics are draped into a mold, the tool is closed and resin is injected at one or several injection points to infiltrate the fabric. The draping of the fabric into the mold results in local reorientation of the fibers. Additionally, by closing the tool the fiber volume content is changed locally. This has a strong influence on the infiltration process as flow resistance is changed by compression of the fibers resulting in a variation of resin velocity and therefore changing the flow direction. Because of many unknown parameters, process simulation gains importance. Simulation of textile processes using micro/meso models have been a key research topic at the ITV, e.g. braiding, weaving, warping, knitting [1]. Now numerical simulation is supplemented with state of the art μ -computer tomography (CT) which proved to be a very valuable experimental technique. μ -CT is not only used for quality assurance (imperfections, air pockets) and damage detection (cracks) but for generating detailed simulation models as well as the validation of numerical simulations. For CFD simulation (e.g. RTM - infiltration) the input data "local permeability" of fabrics can be computed on voxel-data with latest analysis-software. This presentation gives an overview of detailed models gained by process simulation and the novel possibilities with high-resolution computer tomography for more precise numerical simulations of FRP.

References

- [1] H. Finckh: Numerische Simulation der mechanischen Eigenschaften textiler Flächengebilde - Gewebeherstellung. In: 3. LS-DYNA Anwenderforum 2004, 15 p., Germany, Bamberg, 2004

FFT-based homogenization of elasticity at large deformations

Matthias Kabel¹, Thomas Böhlke² and Matti Schneider³

¹ Department of Flow and Material Simulation
Fraunhofer ITWM, Kaiserslautern, Germany

² Institute of Engineering Mechanics,
Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

³ Department of Lightweight Structures and Polymer Technology
Chemnitz University of Technology, Chemnitz, Germany

Abstract. We will present a Newton-Krylov solver for the FFT-based homogenization method of Moulinec and Suquet [4] for elasticity problems at large deformations [2]. Compared to earlier solvers, cf. [3] and [1], which rely upon gradient descent, our method is significantly faster, reducing the computational times by factors of 20 to 100 for some test examples.

Exploiting the special structure of Green's operator, we deduce an algorithmic variant reducing the memory requirements by 40%. For validation we present results for both simple microstructures with analytically known solution fields and complex microstructures of glass fiber reinforced polymer structures (GFRP).

References

- [1] P. Eisenlohr, M. Diehl, R.A. Lebensohn, and F. Roters: A spectral method solution to crystal elastoviscoplasticity at finite strains, *International Journal of Plasticity*, **46**(0), 37–53 (2013)
- [2] M. Kabel, T. Böhlke, and M. Schneider: Efficient fixed point and Newton-Krylov solver for FFT-based homogenization of elasticity at large deformations *Computational Mechanics*, accepted
- [3] N. Lahellec, J. C. Michel, H. Moulinec, and P. Suquet: Analysis of inhomogeneous materials at large strains using fast fourier transforms. In: *IUTAM Symposium on Computational Mechanics of Solid Materials at Large Strains* (ed. C. Miehe), pp. 247–258, Springer Netherlands, 2003
- [4] H. Moulinec and P. Suquet. A numerical method for computing the overall response of nonlinear composites with complex microstructure. *Computer Methods in Applied Mechanics and Engineering*, **157**(12),69 – 94 (1998)

Comparison of hyperelastic micromorphic, micropolar and microstretch continua - Constitutive models and computation

Thorben Leismann¹ and Rolf Mahnken¹

Chair of Engineering Mechanics (LTM),
University of Paderborn, Paderborn, Germany

Abstract. Micromorphic continua are equipped with additional degrees of freedom in comparison to the classical continuum, representing micro deformations of the material points of a body. Therefore, they are able to account for material size-effects and to regularize the boundary value problem, when localization phenomena arise.

Micromorphic continua allow for arbitrary micro deformations, while the special cases micropolar continuum and microstretch continuum only allow for micro rotation and microstretch respectively, see [1]. Only the micropolar case has been covered extensively in the literature, e.g. [2].

One goal of this presentation is to make the transition from a full micromorphic continuum, as presented in [3], to a micropolar or microstretch continuum, by varying the constitutive equations. To this end two different possibilities are presented for hyperelasticity with large deformations. This leads to four different material models, which are then compared using simple numerical examples.

Another goal is to present a constitutive model encompassing the micromorphic, micropolar and microstretch continuum as special cases and arbitrary mixtures of micropolar and microstretch parts, enabling the representation of versatile material behaviour.

References

- [1] A. C. Eringen: *Microcontinuum Field Theories*. Springer, 1999
- [2] W. Ehlers, W. Volk: On theoretical and numerical methods in the theory of porous media based on polar and non-polar elasto-plastic solid materials, *Int. J. Solids Structures*, **35**, 4597–4617 (1998).
- [3] C. B. Hirschberger, E. Kuhl and P. Steinmann: On deformational and cofigurational mechanics of micromorphic hyperelasticity - Theory and computation, *Comput. Methods Appl. Mech. Engrg.*, **196**, 4027–4044 (2007).

Thermodynamic modeling and simulation of semicrystalline polymers

Alexander Lion¹ and Michael Johlitz¹

Institute of Mechanics,
University of the Federal Armed Forces Munich, Neubiberg, Germany

Abstract. In order to simulate production processes or the long-term behaviour of technical components which are made of semi-crystalline polymers, constitutive models describing the crystallisation behaviour in combination with the glass transition are needed. These polymers exhibit amorphous and crystalline regions which are coupled by an interface layer, i.e. by the rigid amorphous fraction. The mass fractions of the phases are essentially determined by the temperature process that the material has experienced.

To represent the thermomechanical behaviour of such polymers, the constitutive model for the specific free energy is based on a hybrid formulation as proposed in: the volumetric part of the total free energy is described by an energy function of the Gibbs type whereas the isochoric part is modelled by an energy function of Helmholtz type. In this contribution, the Gibbs free energy per unit mass of a semicrystalline polymer is assumed to be the sum of five terms. The first term is the chemical potential of the thermoviscoelastic glass-forming amorphous phase, the second term is that of the thermoelastic crystalline phase and the third contribution is the temperature-dependent chemical potential of the rigid amorphous fraction. The two remaining contributions are the enthalpy and the entropy of mixing. The degree of crystallinity is related to the mass fraction of the crystalline phase and is an internal state variable of the model, the mass fraction of the rigid amorphous fraction is assumed to be proportional to the mass of the crystalline phase and the model for the entropy of mixing is developed. When the model for the specific Gibbs free energy is inserted into the Clausius-Duhem inequality, evolution equations for the degree of crystallinity and for the second internal variable describing the glass transition are derived in combination with an algebraic equation for the temperature- and crystallization-induced changes in the specific volume.

The properties of the theory are demonstrated by a series of simulations. The constitutive model is able to represent the characteristic behaviour of the isobaric specific heat of semi-crystalline polymers during heating and cooling. The pronounced dependence of the exothermic crystallisation peak on the temperature rate is described as well as endothermic melting. The equilibrium solution of the constitutive model delivers an expression in closed form for the equilibrium degree of crystallisation which depends on both the pressure and the temperature.

Effective viscosity of fiber suspensions

Felix Ospald¹ and Matti Schneider²

¹ Research Group Numerical Mathematics (Partial Differential Equations),
TU Chemnitz, Chemnitz, Germany

² Department of Lightweight Structures and Polymer Technology,
TU Chemnitz, Chemnitz, Germany

Abstract. Exact knowledge of the effective viscosity of a fiber suspension is of paramount importance for accurate simulations of injection molding. Due to its strong anisotropy, the full viscosity tensor is very difficult to determine by measurements alone. Therefore, we make use of micromechanical simulations. In this talk we discuss a finite difference discretization on a Cartesian staggered grid, whose solution can be accelerated by use of Fast Fourier Transform. Our method enjoys similar benefits as the method proposed by Moulinec and Suquet [1, 2]. In particular, our approach permits a matrix-free implementation and can handle several hundred million unknowns on a single workstation. To deal with the infinite viscosities of the fibers, we work with a dual scheme acting on the fluidities (i.e. the inverse of the viscosities) of the constituents. The numerical results are compared to existing numerical solutions. We will further discuss some aspects of the implementation, parallelization and scalability of the method.

Acknowledgements

Felix Ospald and Matti Schneider gratefully acknowledge financial support by the German Research Foundation (DFG), Federal Cluster of Excellence EXC 1075 “MERGE Technologies for Multifunctional Lightweight Structures”.

References

- [1] H. Moulinec, P. Suquet: A fast numerical method for computing the linear and nonlinear mechanical properties of composites, *Comptes rendus de l'Académie des sciences. Séries II, Mécanique, physique, chimie, astronomie*, **318(11)**, 1417-1423 (1994).
- [2] H. Moulinec, P. Suquet: A numerical method for computing the overall response of nonlinear composites with complex microstructure, *Comp. Meth. Appl. Mech. Engng.*, **157**, 69-94 (1998).

CT-based FE simulations of composite materials: Possibilities, trends, and applications

Dieter H. Pahr¹

Institute of Lightweight Design and Structural Biomechanics,
Vienna University of Technology, Vienna, Austria

Abstract. 3D imaging systems are widely used in the field of biomedical engineering to obtain patient-specific simulation models. Similar methodologies are getting popular in the field of composite engineering.

Three-dimensional image data build the basis of CT-based simulation models. Usually, they are taken by computer tomography but any kind of imaging technique is possible which yields a 3D array of gray-values. The image resolution i.e. the size of a 3D pixel (so called voxel) determines the possible FE model types [1]. High resolution micro FE models showing a detailed microscopic architecture. In general such models need specialized FE solver on powerful computer clusters [2]. Low resolution homogenized FE models are based on a material mapping (gray-value to elasticity) and can be solved on standard PCs [2]. Materials or structures can be analysed by using such models. Typical tasks are material characterization (homogenization, material laws), material calibration (multi-scale gray-value mapping functions), and structural multi-scale analysis. For practical applications automated software tools are needed for an efficient generation, analysis, and results evaluation [3].

In future, 3D images based simulation models will change the classical design philosophy from a standardized modelling concept to a component specific modelling concept. The talk will highlight possibilities, trends, and applications. Methodologies from the biomechanical field will be presented and it will be shown how they could be applied in the field of composite engineering.

References

- [1] D. H. Pahr and P. K. Zysset: From high-resolution CT Data to Finite Element Models: Development of an Integrated Modular Framework, *Comp Meth Biomech Biomed Eng*, **12**, 45–57 (2009).
- [2] D. H. Pahr and P. K. Zysset: A comparison of enhanced continuum FE with micro FE models of human vertebral bodies. *J Biomech*, **42**, 455–462 (2009).
- [3] D. H. Pahr: Medtool User Manual www.dr-pahr.at.

Computational homogenization of elasticity on a staggered grid

Matti Schneider¹, Felix Ospald², and Matthias Kabel³

¹ Department of Lightweight Structures and Polymer Technology,
TU Chemnitz, Chemnitz, Germany

² Research Group Numerical Mathematics (Partial Differential Equations),
TU Chemnitz, Chemnitz, Germany

³ Department of Flow and Material Simulation,
Fraunhofer ITWM, Kaiserslautern, Germany

Abstract. We propose to discretize the problem of elastic homogenization by finite differences on a staggered grid, and introduce fast and robust solvers.

Our method shares some properties with the FFT-based homogenization technique of Moulinec and Suquet [1], which has received widespread attention recently due to its robustness and computational speed. These similarities includes the use of FFT, and the resulting performing solvers.

The staggered grid discretization however, offers three crucial improvements.

First, solutions obtained by our method are completely devoid of the spurious oscillations characterizing solutions obtained by Moulinec-Suquet's discretization.

Second, the iteration number of our solvers are bounded independently of the mesh spacing and the contrast. In particular, our solvers converge for three-dimensional porous structures, which cannot be handled by Moulinec-Suquet's method.

Third, the finite difference discretization allows for algorithmic variants with lower memory consumption. More precisely, it is possible to reduce the memory consumption of the Moulinec-Suquet algorithms by 50%.

Applications include the computation of effective elastic properties of fiber reinforced porous structures and plastification of long fiber thermoplastics.

Acknowledgements

Felix Ospald and Matti Schneider gratefully acknowledge financial support by the German Research Foundation (DFG), Federal Cluster of Excellence EXC 1075 'MERGE Technologies for Multifunctional Lightweight Structures'.

References

- [1] H. Moulinec, P. Suquet. A fast numerical method for computing the linear and nonlinear mechanical properties of composites, *Comptes rendus de l'Académie des sciences. Série II, Mécanique, physique, chimie, astronomie*, **318**(11), 1417-1423 (1994).

Micro-mechanical modeling of long fiber reinforced thermoplastics using local fiber orientation distribution from mold filling simulation

Lukas Schulenberg¹, Thomas Seelig², and Dong-Zhi Sun¹

¹ Fraunhofer Institute for Mechanics of Materials (IWM), Freiburg, Germany

² Institute of Mechanics, Karlsruhe Institute of Technology (KIT),
Karlsruhe, Germany

Abstract. Long fiber reinforced thermoplastics (LFT) combine the advantages of short-fiber reinforcements and those of infinitely long fibers which results in excellent material properties, e.g. high strength and toughness. These are important quantities for automotive crash applications and for that reason it is necessary to correctly predict the material behavior in numerical crash simulations.

In this study, the spatial heterogeneity of LFT made of polypropylene with 30 wt% glass fibers has been analyzed in plate shaped structures. Tensile tests on specimens taken from different positions in the plate have been performed, showing significant variations of the measured local stiffness with position.

The approach by Mori and Tanaka [1] has been used to micro-mechanically approximate the composite stiffness in the linear elastic range. The method, originally suitable only for aligned fiber configurations, is extended to account for the local fiber orientation distribution (FOD) with the approach of Advani and Tucker [2]. The latter is provided from mold filling simulations performed at the Fraunhofer Institute for Industrial Mathematics (ITWM).

The homogenized material model for LFT has been implemented as a user routine in a commercial finite element code. Two different methods to homogenize the orientation distribution have been analyzed. Strengths and weaknesses of the implemented methods have been elaborated especially under the consideration of a feasible CPU time. The gained knowledge has been used to introduce a set of parameters which are able to adjust the material behavior. Finally, experimental tests were reproduced by numerical simulations.

References

- [1] T. Mori, K. Tanaka: Average Stress in the Matrix and Average Elastic Energy of Materials with Misfitting Inclusions. *Acta Metallurgica* **21**, 571-574 (1973).
- [2] S. Advani, C. Tucker: The Use of Tensors to Describe and Predict Fiber Orientation in Short Fiber Composites. *Journal of Rheology* **31 (8)**, 751-784 (1987).

Multi-scale modeling of damage in textile composites

Jaan-W. Simon¹, Brett Bednarczyk², Bertram Stier¹, and Stefanie Reese¹

¹ RWTH Aachen University, Institute of Applied Mechanics, Aachen, Germany

² NASA Glenn Research Center, Cleveland, OH, U.S.A.

Abstract. Textile composites have become very popular in industrial applications due to their ease of manufacture, damage tolerance, and relatively low cost. However, physics-based modeling of the mechanical behavior of textile composites is challenging because additional geometric complexities are introduced, which cause significant local stress and strain concentrations. These internal concentrations are primary drivers of nonlinearity, damage, and failure within textile composites, and thus must be captured in order for the models to be predictive.

The macroscale approach to modeling textile-reinforced composites treats the composite as an effective, homogenized material, with properties typically determined experimentally. This approach is very computationally efficient and can be sufficient in the linear elastic regime, but, because it does not explicitly consider the complex microstructural geometry of the composite, it cannot be considered predictive. In contrast, the mesoscale approach to modeling textile composites explicitly considers the internal geometry of the reinforcing tows, and thus their interaction, and the effects of their curved paths can be modeled. The tows, which are themselves anisotropic, are treated as effective (homogenized) materials, requiring use of anisotropic material models to capture their behavior. The microscale approach goes one level lower, modeling the individual filaments that constitute the textile composite tows.

This paper will compare meso- and micro-scale approaches to modeling the deformation and damage of textile-reinforced polymer matrix composites. For the meso-scale approach, the woven composite architecture will be modeled using the finite element method, and an anisotropic damage model for the tows will be employed to capture the local nonlinear behavior. This same global finite element model will be used in a micro-scale approach, but an embedded semi-analytical micromechanics model will be employed to represent the tows. The homogenized tow behavior, as predicted by this micromechanics model, will be passed to the finite element model at the tow integration points. Finally, a third, more computationally efficient, micro-scale approach will be examined, wherein both the global architecture of the woven composite and the tows are modeled using the aforementioned semi-analytical micromechanics model, without the use of the finite element method. The goal will be the comparison and evaluation of these three approaches to modeling textile-reinforced composites in terms of accuracy, efficiency, and utility.

Microstructure and yield strength modeling in a severely deformed Al_{2.5}Cu_{1.5}Mg alloy

Morgan Tort^{1,2}, Patrick Trimby³, Gang Sha⁴, Yuri Lapusta², and Kenong Xia¹

¹ Department of Mechanical Engineering, University of Melbourne, Victoria 3010, Australia

² French Institute Advanced Mechanics, IFMA, LAMI, F-63175 Aubiere, France

³ Australian Key Centre for Microscopy & Microanalysis and School of Aerospace, Mechanical & Mechatronic Engineering, University of Sydney, NSW 2006, Australia

⁴ Chinese Center of Excellence in Atom Probe Tomography, Gleiter Institute of Nanoscience, Nanjing University of Science and Technology, Jiangsu, 210094 China

Abstract. Establishing microstructure/property relationships is a fundamental task for the design of new materials. In the present work, the study focuses on one ternary Al-Cu-Mg alloy, which is the base system of the 2xxx aluminium series, including 2024 and 2014 alloys. A yield strength model for undeformed and severely deformed Al-Cu-Mg based alloys is proposed, taking into account the intrinsic strengthening, cluster/GPB zones strengthening, S phase strengthening, grain boundary strengthening, solid solution hardening and dislocation hardening. A set of 8 different microstructures, corresponding to different states of precipitation and deformation via equal channel angular pressing (ECAP), was fully characterized using cutting edge characterization techniques. In particular, atom probe tomography (APT) was used to resolve and quantify the clusters constituted of only several atoms and transmission Kikuchi diffraction (TKD) was employed to resolve grains as small as 10 nm. It is shown that a very good agreement is found between the experimental yield strength coming from tensile testing and the yield strength calculated using the microstructure's parameters in the model developed. The model is also used to examine the major contributors to the yield strength.

From FFT-based homogenization to guaranteed bounds on effective linear properties

Jaroslav Vondřejc¹, Jan Zeman², and Ivo Marek³

¹ New Technologies for the Information Society, Faculty of Applied Sciences, University of West Bohemia, Plzeň, Czech Republic.

² Department of Mechanics and ³Department of Mathematics Faculty of Civil Engineering, Czech Technical University in Prague, Prague 6, Czech Republic.

Abstract. FFT-based homogenization algorithms belong to fast numerical methods for evaluating homogenized (effective) properties of periodic heterogeneous materials. Originally, the method was based on a solution of the Lippmann-Schwinger type of an integral equation including the Green function for an auxiliary homogeneous problem. A numerical solution proposed by Moulinec and Suquet [1] is based on the Neumann series expansion corresponding to a simple iteration procedure. We explain the algorithm by the Galerkin method of corresponding variational formulation with an approximation space composed of trigonometric polynomials [2]. Techniques of numerical integrations are discussed and corresponding algorithms are supported by convergence of their approximate solutions to the solution of weak formulation [2]. Moreover, the primal and the dual variational formulations, according to Dvořák [3], allow for evaluating arbitrary accurate guaranteed bounds on the homogenized coefficients [4]. All theoretical results are confirmed with numerical examples.

Acknowledgement. This work has been supported by project EXLIZ-CZ.1.07/2.3.00/30.0013 which is co-financed by the European Social Fund and the national budget of the Czech Republic and by the Czech Science Foundation through project No. P105/12/0331.

References

- [1] H. Moulinec, P. Suquet: A fast numerical method for computing the linear and nonlinear mechanical properties of composites. *Comptes rendus de l'Académie des sciences. Série II, Mécanique, physique, chimie, astronomie*, **318**(11):1417-1423, 1994.
- [2] Vondřejc, J. Zeman, I. Marek: An FFT-based Galerkin method for homogenization of periodic media. *Computers and Mathematics with Applications*, 68(3):156-173, 2014.
- [3] J. Dvořák: Optimization of Composite Materials. Master's thesis, Charles University, 1993.
- [4] Vondřejc, J. Zeman, I. Marek: Guaranteed bounds on homogenized properties by FFT-based Galerkin method. *arXiv:1404.3614*, 2014.

Participants

Title, Name	Institution	E-Mail-Address
Priv.-Doz. Dr. Heiko Andrá	Fraunhofer Institute for Industrial Mathematics ITWM Kaiserslautern, Germany	heiko.andrae@itwm.fraunhofer.de
Dr. Stéphane Berbenni	Laboratoire d'Étude des Microstructures et de Mécanique des Matériaux Université de Lorraine Metz, France	stephane.berbenni@univ-lorraine.fr
Dipl.-Ing. Alexander Bernath	Institute of Vehicle System Technology Karlsruhe Institute of Technology (KIT) Karlsruhe, Germany	alexander.bernath@kit.edu
M.Sc. Róbert Bertóti	Institute of Engineering Mechanics Karlsruhe Institute of Technology (KIT) Karlsruhe, Germany	robert.bertoti@kit.edu
Dipl.-Inform. Benjamin Bertram	Institute for Applied Materials IAM-WK Karlsruhe Institute of Technology (KIT) Karlsruhe, Germany	benjamin.bertram@kit.edu
Prof. Dr.-Ing. Thomas Böhlke	Institute of Engineering Mechanics Karlsruhe Institute of Technology (KIT) Karlsruhe, Germany	thomas.boehlke@kit.edu

Title, Name	Institution	E-Mail-Address
Dipl.-Ing. Barthel Brylka	Institute of Engineering Mechanics Karlsruhe Institute of Technology (KIT) Karlsruhe, Germany	barthel.brylka@kit.edu
cand. M.Sc. Fabian Buck	Institute of Engineering Mechanics Karlsruhe Institute of Technology (KIT) Karlsruhe, Germany	thomas.boehlke@kit.edu
Prof. Ralf Cuntze	Head of CcE V-AG Engineering Carbon Composites e.V. (CCeV) Augsburg, Germany	Ralf_Cuntze@T-Online.de
Dipl.-Math. Alexander Dridger	Chair of Engineering Mechanics University of Paderborn Paderborn, Germany	dridger@itm.upb.de
M.Sc. Martin Düsing	Chair of Engineering Mechanics University of Paderborn Paderborn, Germany	duesing@itm.upb.de
Dipl.-Ing. Hermann Finckh	Institute of Textile Technology and Process Engineering (ITV) German Institutes of Textile and Fiber Research (DITF) Denkendorf, Germany	hermann.finckh@itv-denkendorf.de
Dr. Matthias Kabel	Fraunhofer Institute for Industrial Mathematics ITWM Kaiserslautern, Germany	matthias.kabel@itwm.fraunhofer.de
M.Sc. Loredana Kehr	Institute of Engineering Mechanics Karlsruhe Institute of Technology (KIT) Karlsruhe, Germany	maria.kehrer@kit.edu

Title, Name	Institution	E-Mail-Address
M.Sc. Thorben Leismann	Chair of Engineering Mechanics University of Paderborn Paderborn, Germany	thorben.leismann@ltm.upb.de
Dipl.-Ing. Chris Leistner	Institute of Applied Mechanics TU Clausthal Clausthal-Zellerfeld, Germany	chris.leistner@tu-clausthal.de
Univ.-Prof. Dr.-Ing. Alexander Lion	University of the Federal Armed Forces Munich Neubiberg, Germany	alexander.lion@unibw.de
Prof. Dr.-Ing. Rolf Mahnken	Chair of Engineering Mechanics University of Paderborn Paderborn, Germany	mahnken@ltm.upb.de
Dipl.-Ing. Viktor Müller	Institute of Engineering Mechanics Karlsruhe Institute of Technology (KIT) Karlsruhe, Germany	viktor.mueller@kit.edu
Dipl.-Math. Felix Ospald	Department of Mathematics Chemnitz University of Technology Chemnitz, Germany	felix.ospald@mathematik.tu-chemnitz.de
PD DI. Dr. Dieter H. Pahr	Institute of Lightweight Design and Structural Biomechanics Vienna University of Technology Vienna, Austria	pahr@lsb.tuwien.ac.at

Title, Name	Institution	E-Mail-Address
M.Sc. Céline Röhrig	Chair of Applied Mechanics Saarland University Saarbrücken, Germany	celine.roehrig@uni-saarland.de
Dipl.-Ing. Johannes Ruck	Institute of Engineering Mechanics Karlsruhe Institute of Technology (KIT) Karlsruhe, Germany	johannes.ruck@kit.edu
M.Sc. Malte Schemmann	Institute of Engineering Mechanics Karlsruhe Institute of Technology (KIT) Karlsruhe, Germany	malte.schemmann@kit.edu
Dr. Matti Schneider	Lightweight Structures and Polymer Technology Chemnitz University of Technology Chemnitz, Germany	matti.schneider@mb.tu-chemnitz.de
Dipl.-Ing. Lukas Schulenberg	Fraunhofer Institute for Mechanics of Materials IWM Freiburg, Germany	lukas.schulenberg@iwmm.fraunhofer.de
Dr.-Ing. Jaan Simon	Institute of Applied Mechanics RWTH Aachen University Aachen, Germany	jaan.simon@rwth-aachen.de
M.Sc. Morgan Tort	IFMA - French Institute of Advanced Mechanics Campus de Clermont-Ferrand les Cezeaux Aubiere Cedex, France	tort.morgan@gmail.com
Mgr. Ing. Jaroslav Vondřejc, Ph.D.	Faculty of Applied Sciences University of West Bohemia in Pilsen Pilsen, Czech Republic	vondrej@ntis.zcu.