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GAMM e.V.

GAMM Activity Group

Data-driven modeling and numerical simulation of microstructured materials (GAMM AG DATA)

Kick-Off Workshop

26/27 September 2016, Stuttgart, Germany

University of Stuttgart
Germany

SimTech
Cluster of Excellence

UNIVERSITÄT
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Contents

1 Scope

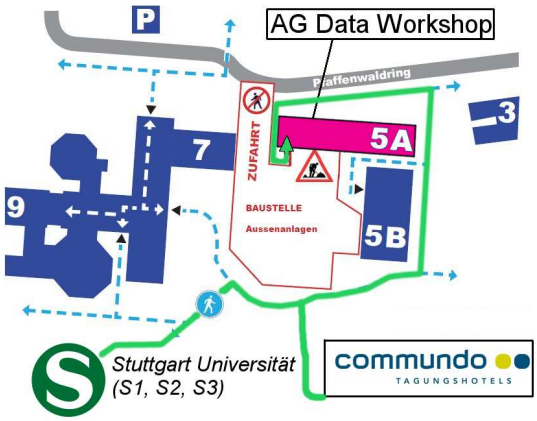
The GAMM activity group Data-driven modeling and numerical simulation of microstructured materials (AG Data) was founded in 2016 by Felix Fritzen (Universität Stuttgart) and Prof. Stefan Diebels (Universität des Saarlandes). The AG Data is the successor of the successful GAMM Activity Group Multiscale Material Modeling which officially terminated at the end of 2015 after a variety of interesting events.

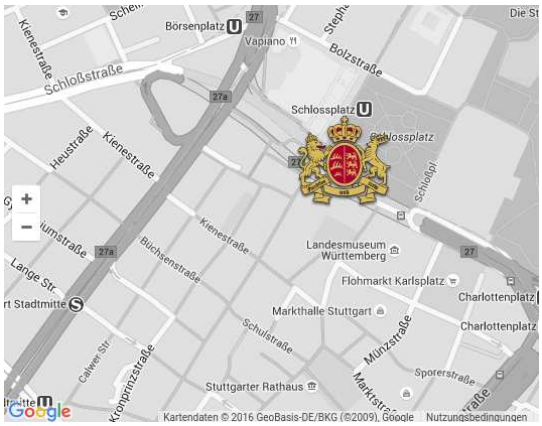
In the new AG Data, novel aspects linked to massive data sets associated with microstructured materials are considered. A motivation for this was the rapid gain of significance of data-driven methods in academia and industry in recent years. For example, modern computed tomography devices can deliver three-dimensional images comprising up to 8000^3 voxels (and possibly more, soon). The processing of these large data sets leads to challenges in mathematics (e.g. characterization of microstructures), computer science (data processing) and mechanics (exploitation of the information in modeling and simulation). Other data-intensive applications involve long-term experiments and simulations, detailed statistical studies, high-resolution space-time information and multi-rate problems exhibiting several concurrent timescales that differ by several orders of magnitude. The processing of large datasets, the simulation of large statistical setups and direct computations on voxel grids are some of the key topics that the new GAMM activity group would like to address.

Felix Fritzen
Stefan Diebels

2 General Information

- The presentations take place in Pfaffenwaldring 5a which is in walking distance from both, the S-Bahn stop *Stuttgart Universität* and the Commundo Tagungshotel.
- The workshop banquet takes place in the restaurant *Alte Kanzlei* which is found in the very center of Stuttgart. The stress address is *Schillerplatz 5A, 70173 Stuttgart* (tel. +49-711-294457).





- Wireless internet access is available via `eduroam`.
- Coffee breaks (Monday afternoon and Tuesday morning) will be held next to the lecture room.

3 Timetable

Monday, September 26	
13:00–13:10	Opening (F. Fritzen, S. Diebels)
13:10–13:40	Johannes Hötzer
13:40–14:10	Frederik Scherff
14:10–14:40	Konrad Schneider
14:40–15:10	Volker Schmidt
15:10–15:45	Coffee break
15:45–16:15	Matti Schneider
16:15–16:10	Jörg Hohe
16:45–17:15	Claudia Redenbach
17:15–17:45	Ralf Jänicke
17:50–18:45	Activity Group Meeting
20:00	Workshop Banquet

Tuesday, September 27	
09:00–09:30	Holger Steeb
09:30–10:00	Heiko Andrä
10:00–10:30	Michael Roland
10:30–11:00	Coffee break
11:00–11:30	Axel Klawonn
11:30–12:00	Benjamin Klusemann
12:00–12:30	Matthias Leuschner
12:30–13:00	Felix Fritzen
13:00–13:10	Closing (F. Fritzen, S. Diebels)
13:10–14:30	Farewell Lunch

4 Abstracts

In the following all abstracts follow in the order of appearance according to the schedule (see Section 3).

The presentations are partitioned into four slots with three or four presentations each. Thematically, four main domains are covered:

- *Monday (1^{st} session):* Microstructural modeling and mesh generation
- *Monday (2^{nd} session):* Microstructural modeling and stochastic/statistical effects
- *Tuesday (1^{st} session):* Large scale simulations
- *Tuesday (2^{nd} session):* Efficient simulation methods

4.1 Large scale phase-field simulations of pattern formation during ternary eutectic directional solidification

J. Hötzer [1,2], P. Steinmetz[1], M. Kellner[1], M. Bauer[3], H. Köstler, U. Rüde[3], A. Dennstedt[4], A. Genau[5], B. Nestler[1,2]

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Materials with defined properties are crucial for the development of new and the optimization of existing applications. These properties are a result of the evolving microstructure which is controlled by the processes conditions and the chemical composition. During the directional solidification of ternary eutectic alloys a wide range of patterns in the microstructure form. These patterns lead to different mechanical properties. To study the underlying physical processes and the complex spatial interplay during the microstructure evolution, phase-field simulations have been established, besides experiments. To conduct large scale simulations, a highly optimized phase-field solver, based on the Grand-potential approach is implemented in the massive parallel waLBerla framework. The solver was optimized on various levels starting from the model and parameters, down to the hardware, reaching 27% peak performance on a single SuperMUC (Phase 1) node. With this solver, large scale simulations of up to $4\,116 \times 4\,088 \times 4\,325$ cells on $171\,696$ cores are conducted for studying the pattern formation **[1]**. Large scale simulations are required to minimize the effect of the boundary conditions **[2]**. In simulations of the ternary eutectic system Al-Ag-Cu a good visual and quantitative accordance with experiments, obtained from 2D micrographs and 3D synchrotron tomography **[3]**, **[4]**. For the quantitative comparison, nearest-neighbors, shape factors and phase fractions as well as novel 3D graph methods and principle component analysis based on two point correlations are used. We show the influence of variations in the melt composition **[5]** as well as of different growth velocities on the pattern formation.

References

[1] M. Bauer, J. Hötzer, M. Jainta, P. Steinmetz, M. Berghoff, F. Schornbaum, C. Godenschwager, H. Köstler, B. Nestler, U. Rüde [2015]: “Massively parallel phase-field simulations for ternary eutectic directional solidification” in Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, ACM

[2] P. Steinmetz, Y.C. Yabansu, J. Hötzer, M. Jainta, B. Nestler, S.R. Kalidindi [2016]: “Analytics for microstructure datasets produced by phase-field simulations”, Acta Materialia **103**, 192–203

[3] A. Dennstedt, L. Helfen, P. Steinmetz, B. Nestler, L. Ratke [2015]: “3D Synchrotron Imaging of a Directionally Solidified Ternary Eutectic”, Metallurgical and Materials Transactions A, 1–4

[4] J. Hötzer, M. Jainta, P. Steinmetz, B. Nestler, A. Dennstedt, A. Genau, M. Bauer, H. Köstler, U. Rüde [2015]: “Large scale phase-field simulations of directional ternary eutectic solidification”, Acta Materialia **93**, 194–204

[5] P. Steinmetz, M. Kellner, J. Hötzer, A. Dennstedt, B. Nestler [2016]: “Phase-field study of the pattern formation in Al-Ag-Cu under the influence of the melt concentration”, Computational Materials Science **121**, 6–13

4.2 Material modeling of dual-phase steel based on 3D microstructures

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Modern dual-phase (DP) steels are composed of a very hard martensite phase embedded in a relativly soft ferritic matrix. This microstructure induces material properties characterized by a combination of an elevated level of ductility, high strength and high work hardening **[1]**[**2**]. Therefore DP steel is used for example in energy absorbing, strength-relevant structures in automotive industry and it is desireable to also accomplish these properties in heavy plate steel.

In the presented work the deformation behavior of DP steel is modeled with an elasto-plastic, microstructure based FEM simulation **[3]**, implemented in the open source code *deal.II*. Because of the widespread stress-strain fields inherent in the microstructure, it is necessary to implement a fully three-dimensional model **[4]**. In this context, the microstructures are acquired by serial section tomography. The three-dimensional simulation induces considerably higher computation times, which makes a data reduction reasonable.

In this contribution the aforementioned numerical model is introduced, with special emphasis on the properties of the interphase between martensite and ferrite. Furthermore, its ability to reproduce DP steel flow curves is shown.

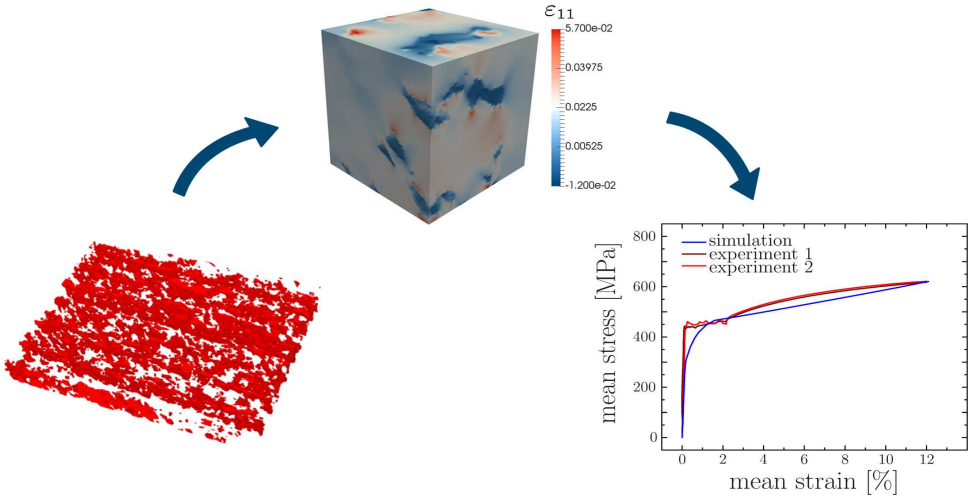

Figure 1: Simulation of flow curves based on 3D microstructures

References

[1] W.M. Kaluza [2003]: “Modellierung der mechanischen Eigenschaften und der lokalen Dehnungen von Dualphasen-Stählen”, Dissertation, Institut für Eisenhüttenkunde, RWTH Aachen.

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[3] F. Scherff, F. Goldschmidt, S. Scholl, S. Diebels [2016]: “High-resolution simulation of microstructures in dual-phase steel”, Proceedings in Applied Mathematics and Mechanics **16**, *submitted*.

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4.3 Automatic generation and meshing of periodic representative volume elements for matrix-inclusions composites

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Modern lightweight structures often feature composite materials to meet the requirements of todays engineering applications. The underlying microstructures of these heterogeneous materials have a vital influence on the mechanical properties and deformation behavior. From a computational viewpoint it is necessary to incorporate this information for most exact simulations. To gain deeper insides in the micromechanical behavior state of the art methods arising from the field of computational micromechanics typically utilize representative volume elements (RVE). The efficiency and trustworthiness regarding numerical homogenization heavily depends on the choice of the RVE and its discretization in terms of quality and representativeness.

Concentrating on matrix-inclusion composites (e.g. polymer blends or short fiber reinforced materials) we demonstrate a novel method for the automatic generation of high quality periodic RVEs up to the finite element discretization. Kernel of the generation process is a random sequential adsorption algorithm that yields the geometry of the microstructure. It incorporates a successive build up of geometric entities employing admissibility checks on the inclusions to meet the non-overlapping constraint. For the purpose of numerical homogenization in the framework of finite element simulations we seek a high quality discretization of the RVE geometry with as few elements as possible while maintaining a high element quality. Special emphasis is put into generating a periodic mesh topology for application of the favourable periodic boundary conditions. The developed meshing algorithm features an individual treatment of all inclusions and a hierarchical mesh generation. Furthermore, systematic comparisons to standard tools show the benefits of the suggested approach.

References

[1] K. Schneider, B. Klusemann, S. Bargmann: “Automatic three-dimensional geometry and mesh generation of periodic representative volume elements for matrix-inclusion composites”, Advances in Engineering Software **99**, 177–188, 2016

4.4 Stochastic microstructure modeling of particle-based materials in 3D and 4D – A powerful tool for virtual materials testing –

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The microstructure of particle-based materials has a strong influence on their macroscopic physical properties, e.g., with respect to mass, charge and heat transport, mechanical strength, or degradation effects. Thus, optimizing the microstructure with respect to functionality is a main goal in materials research. Doing so experimentally in the laboratory causes high costs with regard to time and resources. One way to overcome this problem is the usage of stochastic microstructure models, which allow the realization of virtual microstructures on the computer. The functionality of microstructures generated with such models can be investigated by means of numerical simulations. The results of this combination of stochastic and numerical methods, which is called virtual materials testing, can be used to design materials with improved microstructures that lead to better macroscopic functionalities.

In this talk we consider spatial stochastic models for the microstructure of three types of particle-based materials. First, we show how models of stochastic geometry (point processes, random networks, germ-grain models) can be used to describe the 3D microstructure of electrodes in Lithium-ion batteries **[1]** and how the microstructure of electrodes influences their electrochemical performance and degradation effects **[2]**. Second, we consider the internal 3D microstructure of single agglomerates and show that it has a great influence on their stability and breakage characteristics. To see this, spatial stochastic modeling of spherical agglomerates is combined with numerical DEM simulations for better understanding the breakage behavior of spherical agglomerates under uniaxial compression **[3]**. Finally, we consider a (dynamic) stochastic simulation model for 3D grain morphologies undergoing a grain coarsening phenomenon known as Ostwald ripening. For low volume fractions of the coarsening phase, the classical LSW theory predicts a power-law evolution of the mean particle size and convergence toward self-similarity of the particle size distribution; experiments suggest that this behavior holds also for high volume fractions Using this information we developed a stochastic simulation model for the 3D morphology of the coarsening grains at arbitrary time steps. Our stochastic model is based on random Laguerre tessellations and is by definition self-similar, i.e., it depends only on the mean particle diameter, which in turn can be estimated at each point in time **[4]**. Furthermore, a stochastic model is proposed that describes the statistical evolution of the ”typical” individual grain size as a function of neighborhood characteristics **[5]**. This extends the existing 3D model to 4D.

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[2] S. Hein, J. Feinauer, D. Westhoff, I. Manke, V. Schmidt, A. Latz [2016]: “Stochastic microstructure modelling and electrochemical simulation of lithium-ion cell anodes in 3D", Journal of Power Sources (submitted).

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4.5 Generating fiber-filled volume elements with high volume fraction and prescribed fourth order fiber orientation tensor

Matti Schneider[1]

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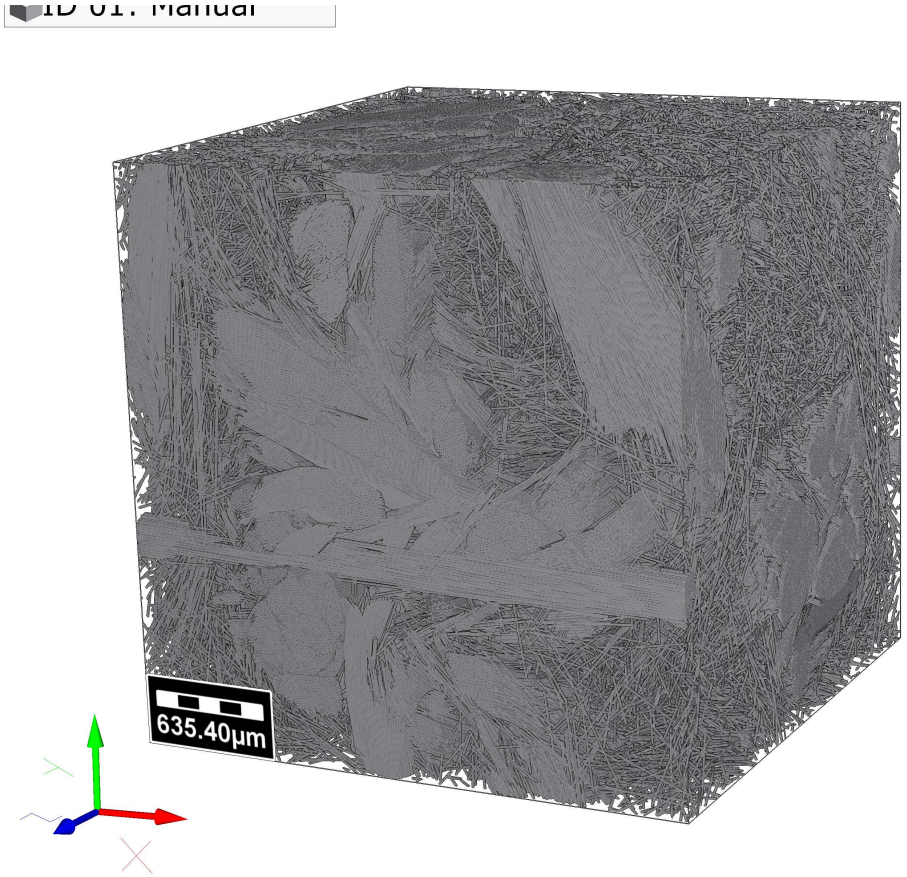

Figure 1: A volume element with aspect ratio of 150, volume fraction $\phi = 20\%$ and isotropic fourth order fiber orientation tensor

The digital material cycle for fiber reinforced plastics crucially depends on microstructures capturing the fiber volume fraction and the fiber orientation. Short fiber composites used in the industry generally feature a large volume fraction and high fiber aspect ratio.
In this talk I will introduce a fast and robust method to generate volume elements including straight cylindrical fibers of equal length. It is based on a reformulation of the microstructure generation problem for prescribed fourth order fiber orientation tensor in terms of an energy minimization problem, which is then solved numerically.
In contrast to existing methods, high accuracy (five significant digits for the fiber orientation tensor), large fiber aspect ratios (up to 150) and large volume fractions (50 volume$-\%$ for isotropic orientation and aspect ratio of 30) can be reached. The talk closes with a small study on the effective linear elastic properties of the resulting microstructures, depending on fiber orientation, volume fraction as well as aspect ratio.

4.6 Probabilistic modelling of long fiber reinforced thermoplastics from micro to macro scale

J. Hohe[1], S. Fliegener[1], C. Beckmann[1]

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Long fiber reinforced thermoplastic composites (LFT) are a new class of composites combining the advantages of short fiber reinforced plastics and continuously fiber reinforced materials. Due to the limited fiber length, LFT materials may be processed by many standard technologies for thermoplastic materials, such as injection or compression molding. On the other hand, the increased fiber length results in superior stiffness, strength and toughness properties.

Due to their production process, long fiber reinforced materials feature an uncertain disordered and process dependent microstructure. Both, the fiber length and the local fiber orientation are subject to distinct variabilities. Depending on the length of the flow path, different degrees of fiber alignment may develop, ranging from complete disorder in the strand inlay or gate areas to preference orientations in the flow ranges.

Objective of the present contribution are strategies for the numerical modelling considering these uncertainty effects. In a first part, a strategy for modelling of the disordered microstructure of LFT material, based on stochastic descriptors is presented. In a second step, this strategy is employed for a microstructural simulation and homogenization of the material response of LFT materials. Finally, probabilistic approaches for including the material uncertainty on the macroscopic level are developed.

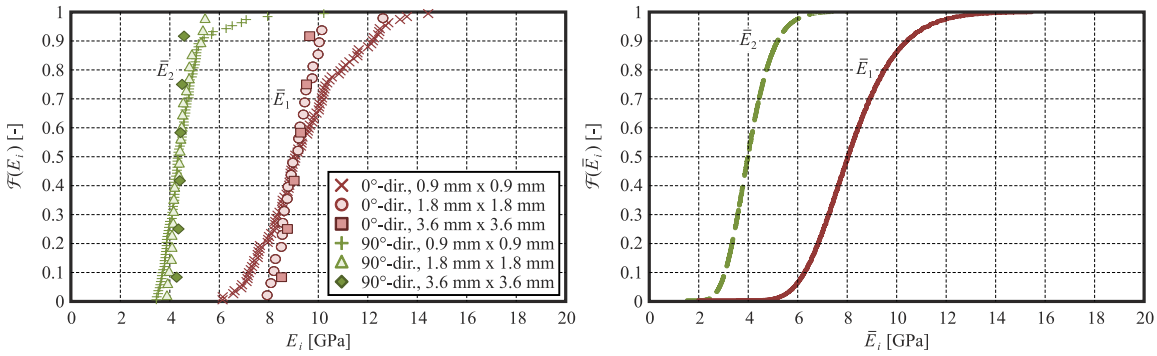

Figure 1: Probability distributions for the Young's modulus - experimental results and numerical prediction

References

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4.7 Geometric characterization and stochastic modelling of microstructures

C.Redenbach [1]

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Macroscopic properties of materials, e.g. the permeability of a filter or the mechanical strength of a fiber composite, are highly influenced by the microstructure. Therefore, an understanding of the reaction of these properties to changes of the microstructure is crucial for the optimization of materials for given applications. Geometric and topological microstructure characteristics such as volume density, fiber orientation or cell sizes can be estimated from tomographic images of the material. The estimated values allow for a characterization and a comparison of material samples.

Subsequently, the microstructure of the material can be described using a model from stochastic geometry. Examples for such models are Boolean models (for porous materials), cylinder processes (for fiber composites) or random tessellations (for cellular materials). These models are fitted to the real microstructure using the geometric characteristics estimated from the image data.

The talk presents these techniques giving some examples from recent projects of our group which are concerned with the investigation of foams and fiber composites.

4.8 Artificial microstructures for the numerical modeling of asphalt concrete

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In the present contribution we establish a methodological framework to numerically investigate the effective mechanical properties of asphalt concrete on the basis of morphological X-ray Computed Tomography (XRCT) data **[1]**, **[2]**, see Fig. 1 a). To this end, we consider asphalt concrete as a multi-scale and multi-phase material with spatially varying constituents on the small scale and with rather homogeneous properties on the large scale. Whereas a typical asphalt concrete consists of mineral aggregates (crushed rock), a bituminous binding agent, pores and further additives, we simplify the system towards a biphasic mastic asphalt consisting of mineral aggregates and bituminous binder neglecting pores. The partial microscopic bulk properties of the particular constituents are well accessible by physical testing and well investigated. Our efforts, therefore, focus on a proper morphological description of the solid aggregate particles. Gaining information about the aggregates' volume fraction and their particle size distribution from XRCT data we create artificial Statistical Volume Elements for our numerical investigations. We first apply a discrete particle simulation to generate a densely packed sphere model with an appropriate particle size distribution. In a second step, we use this dense sphere model to execute a weighted Voronoi tessellation. Finally, the volume fraction of the mineral aggregates is adjusted by a stochastic shrinkage process of the resulting Voronoi cells, see Fig. 1 b). The complete algorithm is is executed in a periodic manner, and the resulting artificial structures can be used for computational homogenization with periodic boundary conditions.

In our presentation, we describe in detail our algorithm to generate artificial Statistical Volume Elements and comment on the constitutive description of the bituminous (viscoelastic) binding agent. Finally, we investigate the upscaling properties of asphalt concrete in a geometrically linear as well as in a geometrically nonlinear framework. An outlook on ongoing research (open-porous asphalt) is given.

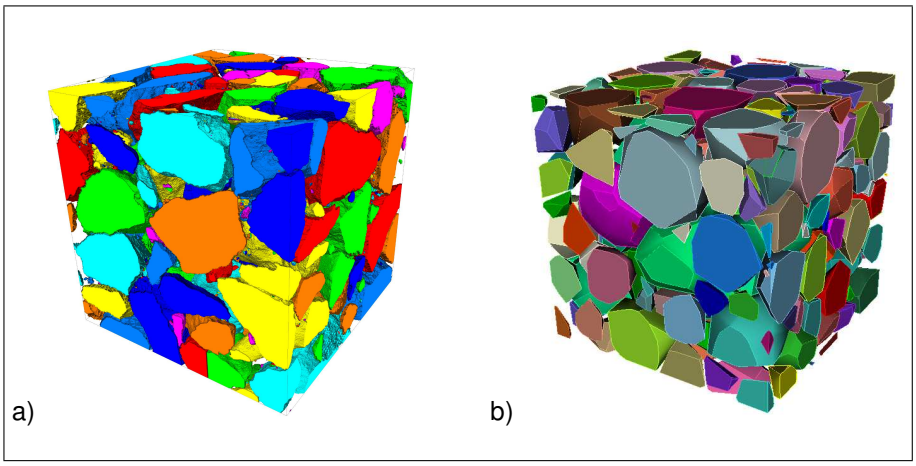

Figure 1: a) 1000^3 voxel cube reconstructed from XRCT data and b) artificial counterpart **[2]**.

References

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4.9 Digital Material Laboratory

Holger Steeb[1], David Uribe[1]

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3-dim Image-based numerical modeling approaches have gain great interest during the last decade which could be mainly explained with the large progress in hardware developments of tomographic systems. We will mention just two examples: Fast X-ray Computed Tomographic investigations can be performed with sub-micrometer resolution and a temporal frequency up to 1 Hertz at various CT-beamlines of large-scale Synchrotron facilities, **[1]**. Based on such facilities, even dynamic effects like Haines jumps (discrete pore-filling events in porous media filled with two immiscible fluids under low Capillary numbers) habe been studied in real-time. Further, high-resolution X-Ray scans with a spatial resolution up to 50 nanometer are possible even with benchtop devices (Carl Zeiss Xradia 810 Ultra) in specified university laboratories.

From a numerical modeling point of view, dynamic time series or high spatial resolution scans could be a challenging starting point for further e.g. numerical investigations. Besides the challenges of the "workflow", i.e. the advanced process from the reconstructed raw data to the segmented "binary" image, numerical modelling approaches of voxel based 3-dim scans have to fullfill certain requirements: First and probably most important, representative XRCT data sets are quite large. For heterogeneous microstructures of e.g. geological materials like sandstone or carbonate rocks, problem sizes of around 1000^3 voxels are necessary to obtain size-independent effective physical properties (like electric permitivity, hydraulic permeability and/or elastic wave speed, cf. discussion in e.g. Güven et al. **[2]**). But even 10000^3 voxel cube samples are now available and are "waiting" for further numerical analysis. It is obvious, that besides parallel computing, novel efficient numerical techniques have to be applied to handle such investigations in a reasonable time frame.

In the presentation, we discuss certain examples and related challenges especially from the field of fluid-saturated porous materials, cf. Figure 1.

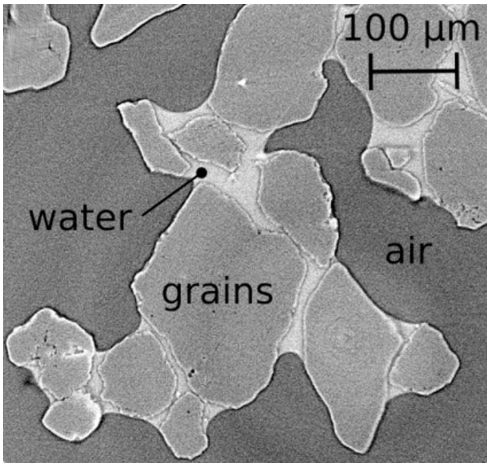

Figure 1: Reconstructed image of a partially saturated granular medium. Three phases can be observed: Water, air and solid grains.

References

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4.10 Pore-scale simulation of damage effects for porous rocks under external and pore pressure

H. Andrä[1], A. Fink[1], M. Kabel[1], M. Schneider[1], S. Staub[1]

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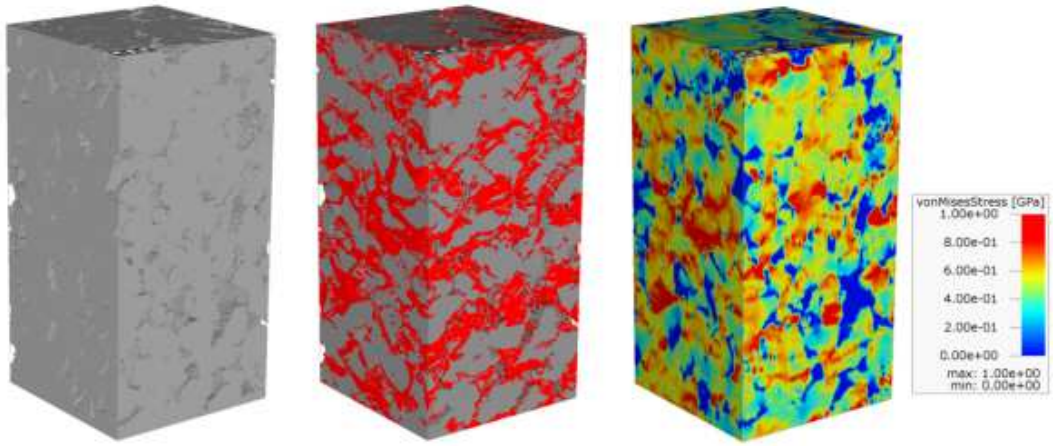

Figure 1: CT scan of Berea sandstone (left), damaged zones marked in red (middle), von Mises equivalent stress (right)

The microstructure of porous rock samples from drill cores can be characterized by μCT images of high resolution. In this paper such imaged rock samples are taken as computational domain to simulate the mechanical deformation due to both internal pore pressure and external compressive loads on the outer surface of the sample. The resulting local mechanical stresses may lead to the growth of microcracks which are approximated effectively by a continuum damage model [1]. The considered periodic boundary value problem in nonlinear elasticity is discretized on a regular grid (voxel grid) and solved by using a FFT-based iterative scheme. The parallelization and numerical effort for problem sizes of about 200 million unknowns are discussed. Furthermore, a numerical test is presented to demonstrate the change of the effective macroscopic permeability after release of the compressive load.

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[2] http://www.geodict.de

4.11 Patient–specific simulations of tibial fractures

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Two patient–specific models of tibial fractures, one treated with an intramedullary nail and one with an implant are generated from tomograms using the fully automated workflow presented in **[1]**. Therefore, the routinely acquired tomographic data is segmented semi–automatically followed by an adaptive mesh generation step based on the concept of hanging nodes. For the assignment of the material parameters with respect to the image information given in Hounsfield units, different mappings are implemented and analysed.

In the simulations, the stresses and strains arising in the osteosynthesis treatments as well as the movement in the fracture area are computed. To achieve realistic boundary conditions for the finite element simulations, a new fully integrated sensor insole is used to get the patient–specific ground reaction forces during gait. Then in a second step, the ground reaction forces are integrated in the OpenSim environment to receive the knee forces and the knee moments of the patient during gait. The results of the OpenSim simulations combined with the ground reaction forces achieved from the insole allow the computation of the stresses and strains in the cortical and the trabecullar bone as well as in the different implants during a step forward of a patient. These results are compared with simulations based on the OrthoLoad database providing in vivo measurements of orthopedic implants in different gait analysis settings. In a third step, the results of these simulations are analysed with respect to the influence of different mappings of the Hounsfield units to material properties.

These considerations provide the orthopaedic trauma surgeons with more information about the biomechanical behaviour of patient–specific bone–implant–systems and can be used to support the surgeons in the selection and the planning of implants. The results of these simulations can also be used as starting point for several optimization processes, e.g. the fusion in the case of a non–union tibia fracture, **[2]** and **[3]**. In addition, the simulations allow a comparision of the stresses and strains results with their critical values.

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4.12 FE2TI - An approach for tuning FE^2 toward extreme scale computing

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Advanced High Strength Steels (AHSS) provide a good combination of both strength and formability and are therefore applied extensively in the automotive industry, especially in the crash relevant parts of the vehicle. Dual-phase (DP) steel is an example for such AHSS which is widely employed. The excellent macroscopic behavior of this steel is a result of the inherent micro-heterogeneity and complex interactions between the ferritic and martensitic phases in the microstructure. Thus, considering the microscale is indispensable for realistic simulations.

In order to bring large micro-macro simulations to modern supercomputers, we combine the well-known FE^2 scale bridging approach with a highly scalable implementation of the FETI-DP domain decomposition method (Finite Element Tearing and Interconnecting - Dual Primal), which is used as a solver on the microscale. This results in our highly-scalable software FE2TI. In FE^2, in each Gauss integration point of the macroscopic problem, a microscopic problem is solved on a representative volume element (RVE). The incorporation of the microscale replaces a phenomenological material law on the macroscale. The FE2TI approach has been used in the project "EXASTEEL - Bridging scales for multi-phase steels" within the first funding period of the DFG priority program SPP 1648 "Software for Exascale Computing" (SPPEXA). It is further developed in the second funding period of SPPEXA within the project "EXASTEEL-2: Dual-Phase Steels - From Micro to Macro Properties". EXASTEEL is a joint effort from computational mathematics (PIs A. Klawonn, O. Rheinbach), material science (PIs J. Schröder, D. Balzani), and computer science/performance engineering (PI G. Wellein), and, in the second period EXASTEEL-2, computer science/sparse direct solvers (PI O. Schenk). The MPI-parallel C/C++ implementation uses PETSc, and efficient solver packages such as BoomerAMG, MUMPS, and UMFPACK are interfaced.

The different RVEs are independent of each other, coupled only through the macroscopic problem and thus can be solved in parallel. In our approach, each RVE is assigned to its own MPI communicator and solved using an inexact-reduced FETI-DP variant. In these highly scalable FETI-DP variants (up to 786K BG/Q cores on Mira, Argonne National Laboratory, USA) the FETI-DP coarse problem is solved inexactly using an AMG (algebraic multigrid) method.

Weak scalability results for different three-dimensional nonlinear, micro-heterogeneous hyperelasticity problems are presented, scaling up to the complete JUQUEEN (458,752 BG/Q cores) at FZ Jülich and the complete Mira ((786,432 BG/Q cores) at Argonne National Laboratory, USA.

4.13 Database enhanced acceleration method based on multivariate simplicial interpolation for material-dominated calculations

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Concurrent multiscale computing is intended to achieve a high fidelity in the description of material behavior as soon as the material behavior becomes complex or even uncertain and cannot accurately described via phenomenological models directly. The material-point calculations often define the largest portion of the total computational costs of concurrent multiscale simulations, in particular if the global time step has to be very small as for explicit solvers. This leads to the goal to develop a generic and simple method which can be applied to general multiscale problems to accelerate the material-point calculations.

In this context, in **[1]** a general adaptive method for material-dominated calculations is developed which is based on phase-space simplicial interpolation of the material-response function. The actual acceleration of the developed scheme strongly depends on the dimensionality, the loading rate and complexity of the deformation, the macroscopic time-step size as well as the fineness of the phase-space interpolation which in turn defined the accuracy of the interpolation. Piecewise-quadratic interpolation in phase space is applied to a number of multidimensional elastodynamic simulations. The numerical results confirm the developed analytical estimate which allows to estimate the benefit of the application of the method in advance.

An improvement of the method is obtained via a database enhancement. In this database, the calculated information from each passed simplex, which involved material-point calculations, are added 'on the fly'. These information are subsequently used again, as soon as any material-point of the whole model will traverse the same simplex again. As soon as several material-points of the model undergo the same loading path, this leads to an increase of the acceleration ratio by several magnitudes. In particular for large computational models and costly material-point calculations, the benefit of the method outweigh the cost of the overhead of the method itself.

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4.14 A Fourier-accelerated nodal solution scheme for homogenization problems

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The finite element (FE) method is a powerful solution technique for many solid mechanics problems, including computational homogenization of artificial microstructures. However, it is computationally inefficient for highly resolved voxel discretizations of real microstructures. For such problems, solution schemes based on the fast Fourier transform (FFT) are more appropriate.

The FFT-based homogenization scheme proposed in the seminal work **[1]** makes use of the closed-form Green operator for strains given in Fourier space. This approach is related to a discretization using trigonometrical polynomials and leads to unfavorable spurious oscillations, especially in cases with high phase contrast. Many proposals have been made to avoid these artifacts, e.g., by using a centered differences scheme on a rotated grid **[2]** or based on pixel-wise constant polarization fields **[3]**. Both approaches result in a modified Green operator, which in the latter case has to be pre-computed numerically.

The idea to replace the Green operator by a numerically derived fundamental solution is also found in the space Lippmann–Schwinger (SLS) scheme **[4]**. We show that with some modifications, the SLS can be transferred to a nodal solution scheme, which employs a FE discretization on a (regular) Cartesian grid. The resultant Fourier-accelerated nodal solution (FANS) method can be implemented using a fixed point scheme or for the preconditioning of a conjugate gradient solver. Although developed independently from the FFT-based homogenization using hexahedral elements proposed in **[5]**, many similarities between both methods can be identified, which will be discussed.

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4.15 Data-driven homogenization of hyper-elastic materials using interpolation functions and reduced order modeling

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[1]: EMMA – Efficient Methods for Mechanical Analysis, Institute of Applied Mechanics (CE), University of Stuttgart, Germany The response of hyper-elastic microstructured materials is studied using a staggered approach. First, a finite element model of the heterogeneous material is generated. Using sensibly chosen loading directions in terms of near homogeneously distributed directions $\boldsymbol{N}^{(i)}$ on the unit ball in $\mathbb{R}^6$, finite element simulations are performed.

The outputs of these simulations are processed in order to build a reduced order model (ROM). In short, the hyper-elasticity problem is tackled by minimizing the strain energy $\bar{\psi}$ of the microstructured solid in a low-dimensional space by using a reduced basis for the strain field $\boldsymbol{\varepsilon}(\boldsymbol{x})$. The RB approach is similar to the pRBMOR for dissipative solids **[1]**, **[2]** .

Using again cleverly chosen directions (but more than before) in the ROM, a collection of data points of the strain energy $\bar{\psi}_{j,k}$ is created, where the j denotes the strain direction and k is the strain amplitude $r_k^{(j)}$. This sampling procedure can help to capture the anisotropy of the effective material in a sound way. Due to the use of the ROM the computing time can be significantly reduced during data acquisition.

In the third stage, a specific interpolation function I is defined by the gathered data. It determines the effective strain energy $\bar{\psi}$, the effective stress $\bar{\boldsymbol{\sigma}}$ and the effective tangent stiffness operator $\bar{\mathbb{C}}$ via

$$\bar{\psi} \approx I(\bar{\boldsymbol{\varepsilon}}), \qquad \bar{\boldsymbol{\sigma}} \approx \nabla I(\bar{\boldsymbol{\varepsilon}}), \qquad \bar{\mathbb{C}} \approx \nabla^2 I(\bar{\boldsymbol{\varepsilon}}).$$

The interpolation function I is based on a kernel method exploiting a direction-radius split. Thereby, the particular data structure of the preceding stages is considered and the physics of the problem are exploited.

The presented approach has favorable algorithmic properties. The provided approximations of the overall constitutive response are computationally efficient yet accurate. Examples showcase the capabilities of the approach which are realized using a simple C program that will be freely available for download under the GNU GPL license, soon.

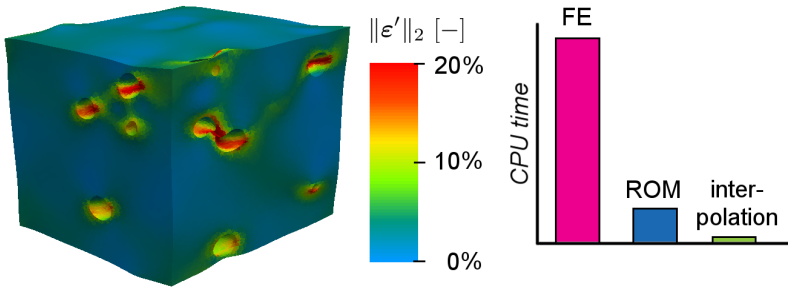

Figure 1: porous solid *(left)* and schematic comparison of the computational effort for the homogenized material response *(right)*

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