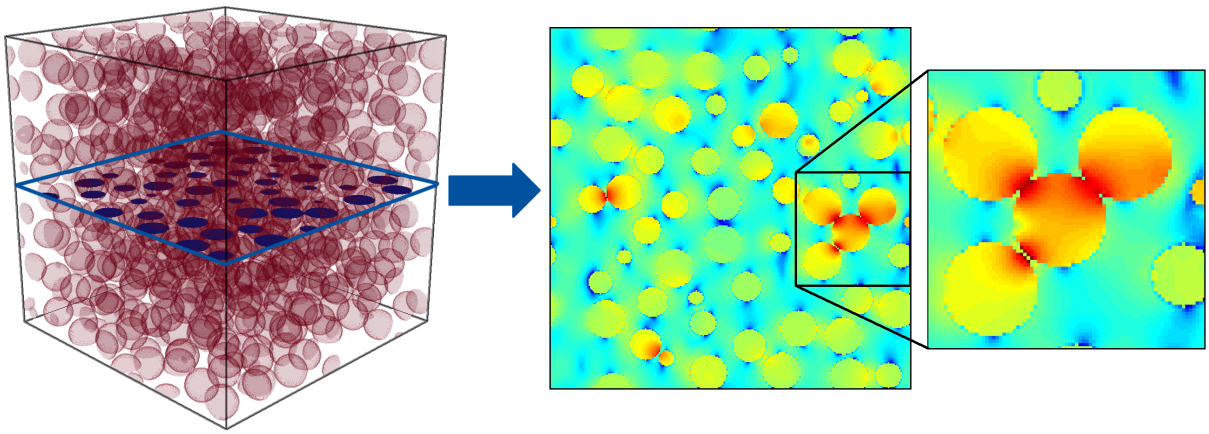
December 6-7, 2017

Thematic Workshop

Computational challenges for mechanical simulations based on digital image data



Institute of Engineering Mechanics
Chair for Continuum Mechanics

In collaboration with

GAMM AG DATA

University of Stuttgart
Germany

EMMA – Efficient Methods for Mechanical Analysis

1 Scope

The simulation of microstructured solids in the context of mechanical multiscale problems remains a challenging field with many questions being unanswered. Particularly, the reduction of the computational cost (cpu time and memory) while limiting numerical artifacts induced by the employed discretization methods is still sought after. The thematic workshop aims at developing discussions and interactions within a familiar atmosphere. Therefore, a scientific program including not only presentations but also dedicated time slots for small group discussions is proposed.

1.1 Workshop topics

Workshop topics include but are not limited to

- FFT-based numerical methods
- microstructure generation
- microstructure characterization
- coupled problems

A special session entitled **Challenges and Perspectives** is included which is intended to initiate discussions about open questions and possible research directions.

1.2 Link to GAMM AG Data

One focus of the GAMM activity group Data-driven modeling and numerical simulation of microstructured materials is the simulation and characterization of materials based on digital image data. The thematic workshop intends to provide a forum for discussions focussed on this specific topic.

1.3 Workshop fees

In line with the scope of this workshop, we wish to keep the workshop as simple as possible (but not simpler). No workshop fees are raised, and the overhead is kept at a bare minimum. In particular, if you wish to join us for lunch at the KIT mensa, you will have to pay yourself.
Fortunately, we were able to fund a workshop dinner without any extravagances (including one meal and one beverage, further details below).

2 Organizers

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Institute of Engineering Mechanics
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4 Support

This workshop is made possible through financial support by

DFG International Research Training Group GRK2078 “Integrated engineering of continuous-discontinuous long fiber reinforced polymer structures”

EMMA - Efficient Methods for Mechanical Analysis (DFG-FR2702/6)

5 Timetable

Dec. 6	11:30-12:00	Informal meeting	KIT ITM
Dec. 6	12:00-13:00	Lunch	KIT mensa
Dec. 6	13:15-15:15	Session Innovative Simulation Methods	“Tangentialraum”
Dec. 6	15:15-15:45	Coffee break	“Tangentialraum”
Dec. 6	15:45-17:45	Session Challenges and perspectives	“Tangentialraum”
Dec. 6	18:30- . . .	Workshop Dinner	Hoepfner Burghof
Dec. 7	09:00-10:00	Session Microstructure characterization and generation	“Tangentialraum”
Dec. 7	10:00-10:30	Coffee break	“Tangentialraum”
Dec. 7	10:30-11:30	Session (ctd.) Microstructure characterization and generation	“Tangentialraum”
Dec. 7	11:30-12:00	Final discussion	“Tangentialraum”
Dec. 7	12:00-13:00	Lunch	KIT mensa

6 Locations

6.1 Getting to KIT Campus Süd

In front of the main exit of Karlsruhe Central Station, all trams passing by KIT leave in rightwards direction. Direct connections are offered by tram 2 (“Wolfartsweier”) or S4 (“Bretten/Gölshausen” or “Heilbronn”). Get off at the tram stations “Kronenplatz” or “Durlacher Tor/KIT Campus-Süd”.

6.2 KIT ITM

The Institute of Engineering Mechanics (ITM) is located on the third floor, building 10.23, see Fig. 1 or online.

6.3 KIT mensa

Lunch on Dec. 6 and Dec. 7 takes place at the KIT mensa, see Fig. 1. We have reserved a few tables in the large dining hall (at “Linie 5”), close to the windows.
At “Linie 6”, the “Update”, you can pay cash. For the other options, you need a KIT student or employee card (or someone to carry you along).

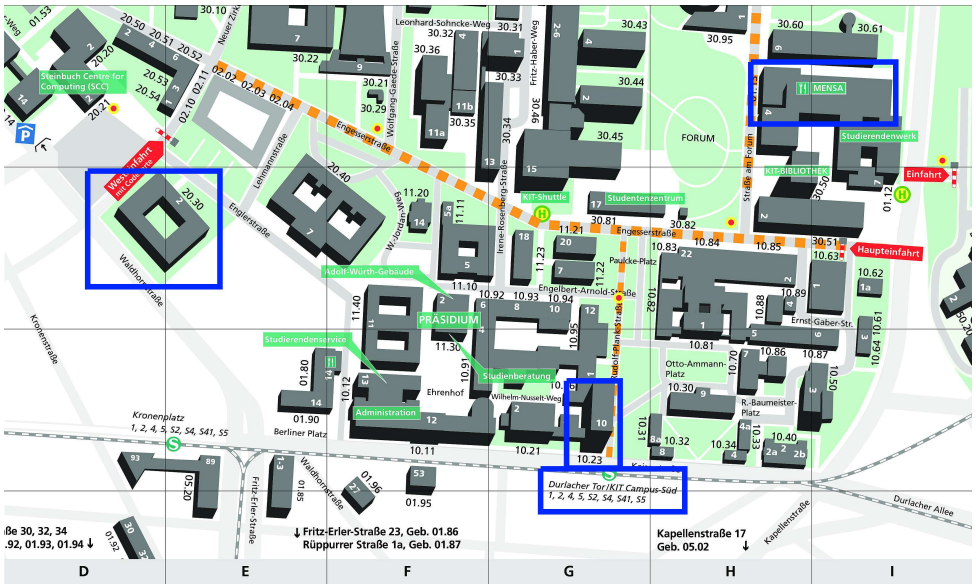

Figure 1: Map of the KIT Campus Süd. The tram/train station, the mensa as well as the buildings 10.23 (KIT ITM) and 20.30 (Seminar room) are marked in blue.

6.4 Seminar room “Tangentialraum”

The workshop venue, the seminar room SR 1.067 (“Tangentialraum”) is located on the first floor in the building 20.30.

6.5 Hoepfner Burghof

The conference dinner will take place at the “Hoepfner Burghof”, Haid-und-Neu-Straße 18, 76131 Karlsruhe, starting from 18:30h on Dec. 6, 2017. According to google maps it takes about 20 minutes to reach the restaurant from the seminar room “Tangentialraum”. Alternatively, you could use tram number 4 up to Karl-Wilhelm-Platz or Hauptfriedhof.

7 Schedule for the sessions

7.1 Session – Innovative Simulation Methods

This session takes place on Dec. 6, 2017, 13:15-15:15h with the following presentations:

13:15-13:45	F. S. Göküzüm, L. T. K. Nguyen and M.-A. Keip *Consistent FFT-based homogenization of electromechanically coupled materials*
13:45-14:15	T. Hofmann, H. Andrä, R. Müller and J. Zausch *Stress simulation in lithium-ion batteries*
14:15-14:45	M. Osorno, M. Schirwon, N. Falkner, R. Sivanesapillai, H. Steeb and D. Göddeke *Large scale SPH simulation of single phase flow through porous media: Scalability study*
14:45-15:15	J. Kochmann *Two-scale FE-FFT-based finite strain crystal plasticity simulations of polycrystalline materials*

7.2 Session – Challenges and perspectives

This session takes place on Dec. 6, 2017, 15:45-17:45h and contains three presentations. These are particularly intended to foster discussions.

F. Welschinger	*Computational multi-scale methods for polymers in an industrial environment*
V. Schmidt	*Stochastic modeling of the 3D microstructure of hierarchical composite materials*
F. Fritzen	*How much data is actually needed?*

7.3 Session – Microstructure characterization and generation

This session takes place on Dec. 7, 2017, 9:00-11:30h with the following presentations:

09:00-9:30	M. Schneider, T. Hofmann, H. Andrä, P. Lechner F. Ettemeyer, W. Volk and H. Steeb *Modelling the microstructure and computing effective elastic properties of sand core materials*
09:30-10:00	D. Westhoff *Structural Segmentation of Defective Particle Systems*
10:00-10:30	Coffee Break
10:30-11:00	M. Neumann *On microstructure-property relationships derived by virtual materials testing with an application to Fickian diffusion in silica monoliths*
11:00-12:00	Discussion and Closing

Consistent FFT-based homogenization of electromechanically coupled materials

Felix Selim Göküzüm[1], Lu Trong Khiem Nguyen[1] and Marc-André Keip[1]

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Future challenges of engineering such as medical applications, robotics or space exploration demand for materials, which are tailor-made and adaptive. In this context, the group of electroactive polymers has recently attracted attention **[1]**. The behaviour of these materials is often implied by their specific microstructure. The prediction of the material's macroscopic behaviour based on microstructure information is of special interest for research and industry. In 1994 Moulinec & Suquet **[2]**, suggested an FFT-based iterative scheme for predicting the mechanical response of heterogeneous materials. The present work extends the framework to electromechanically coupled materials, where the focus of the work lies on the formulation of a most general form of the preconditioned Lippmann-Schwinger equation. The role of the coupled reference medium on the convergence behaviour is investigated numerically. Additionally, we extend the consistent macroscopic tangent operator introduced in an earlier work to coupled problems. In this context, a fully coupled, a reduced non-coupled and a finite-difference based approach are compared to each other. The framework is formulated in a large-strain setting **[3]**. Finally, the model is tested in a FE-FFT multiscale simulation **[4]**.

References

[1] Y. Bar-Cohen: Electroactive polymers as artificial muscles: Capabilities, potentials and challenges, Robotics, 188–196 (2000).

[2] H. Moulinec, P. Suquet: A fast numerical method for computing the linear and nonlinear mechanical properties of composites, Académie des Sciences, 2, 1417–1423 (1994).

[3] M. Kabel, T. Böhlke, M. Schneider: Efficient fixed point and Newton-Krylov solvers for FFT-based homogenization of elasticity at large strains, Computational Mechanics, 54, 1497–1514 (2014).

[4] J. Spahn, H. Andrä, M. Kabel, R. Müller: A multiscale approach for modeling progressive damage of composite materials using fast Fourier transforms, Computer Methods in Applied Mechanics and Engineering, 268, 871–883 (2014).

Stress simulation in lithium-ion batteries

Tobias Hofmann[1], Heiko Andrä[1], Ralf Müller[2] and Jochen Zausch[1]

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Phase separation during the intercalation of lithium ions can lead to degradation effects in some cathode materials. A model describing lithium ion diffusion, electric potentials and small deformations is introduced on the microscale. The Cahn-Hilliard equation is used in an electrochemical model coupled to linear elasticity of small strains in the electrode material. An immersed boundary method is used with adaptive time steps. The charging of porous microstructures is numerically simulated.

Large scale SPH simulation of single phase flow through porous media: Scalability study

M. Osorno[1,3], M. Schirwon[2,3], N. Falkner[1,3], R. Sivanesapillai[1,3], H. Steeb[1,3] and D. Göddeke[2,3]

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Direct Numerical Simulation of fluid flow in high-resolution imaged geometries of real porous materials is highly relevant in several fields, such as, carbon dioxide sequestration, geothermal energy generation and groundwater contamination remediation.
One method commonly applied for DNS in these settings is the quasi-incompressible Smoothed Particle Hydrodynamics (SPH). SPH is a meshless Lagrangian method, highly suitable for modeling complex geometries and flow at high Reynolds numbers. However, SPH requires high computational resources, especially in the simulation of large domains.
To overcome these difficulties, we have implemented the SPH method in the highly optimized software HOOMD-blue, for both CPUs and GPUs. To overcome these difficulties, we have extended the highly optimized HOOMD-blue molecular dynamics software to support the SPH method. Our implementation targets both CPUs and GPUs.
We present initial scalability studies of the SPH module for a variety of representative test cases, with the long-term goal to extend the simulations to large-scale high-resolution imaged porous media. The simulations are performed on the supercomputers Hazel Hen (HLRS – Germany) and Piz Daint (CSCS – Switzerland) for the CPU and GPU parallelization respectively.

Two-scale FE-FFT-based finite strain crystal plasticity simulations of polycrystalline materials

Julian Kochmann[1]

[1]: Institute of Applied Mechanics, RWTH Aachen, Germany

Recently two-scale FE-FFT-based methods have been proposed to predict the local and effective mechanical behavior of composite **[1]** and polycrystalline materials **[2]**,**[3]** at small strains. More recently, Göküzüm and Keip **[4]** proposed a finite strain extension for composite materials. This work deals with finite strain crystal plasticity simulations of polycrystalline aggregates and the development of an efficient and numerically robust solution scheme for two-scale full-field problem settings.

References

[1] J. Spahn, H. Andrä, M. Kabel, R. Müller: A multiscale approach for modeling progressive damage of composite materials using fast Fourier transforms, Computer Methods in Applied Mechanics and Engineering, 268, 871–883 (2014).

[2] J. Kochmann, J. R. Mianroodi, S. Wulfinghoff, S. Reese, B. Svendsen; Two-scale FE-FFT and phase-field-based computational modeling of bulk microstructural evolution and macroscopic material behavior; Computer Methods in Applied Mechanics and Engineering; Elsevier; 2016; Vol. 305, 89-110

[3] J. Kochmann, S. Wulfinghoff, S. Reese, B. Svendsen, L. Ehle, J. Mayer; Efficient and accurate two-scale FE-FFT-based prediction of the effective material behavior of elasto-viscoplastic polycrystals; Computational Mechanics; Springer; 2017

[4] F. Göküzüm and M.-A. Keip: An algorithmically consistent macroscopic tangent operator for FFT-based computational homogenization. International Journal for Numerical Methods in Engineering (accepted) (2017)

Modelling the microstructure and computing effective elastic properties of sand core materials

Matti Schneider[1], Tobias Hofmann[2], Heiko Andrä[2], Philipp Lechner[3], Florian Ettemeyer[4], Wolfram Volk[3,4] and Holger Steeb[5]

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In this work we model sand core materials on the micro-meter scale, resolving individual sand grains and binding bridges, to obtain effective elastic moduli of the composite by computational homogenization, laying the foundations for investigating the strength properties of core blown parts with foundry applications.
We analyze sand core materials on the basis of X-ray micro-computed tomography (μXRCT) images and extract a couple of sand grains from this volume image. These grains enter a packing algorithm which can generate granular packs with high packing fraction and incorporate sand grains with high complexity. Furnished with binder the resulting microstructures are investigated, deriving their effective elastic properties and studying the sensitivity w.r.t. the entering parameters. If a realistic range of elastic parameters of both sand grains and binder are plugged into the simulation, the agreement with experimentally obtained P-wave moduli is excellent.

Structural Segmentation of Defective Particle Systems

Daniel Westhoff[1]

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A common approach for segmenting particle systems, as they are for example observed in lithium-ion battery electrodes, is using watershed techniques, see, e.g., **[1]**. Based on the corresponding distance map, particles are identified using a flooding starting from the local maxima. However, this approach does often not work for defective particle systems, i.e., if particles have cracks, holes or breakages. This is due to the fact that the defects influence the distance map and there is not exactly one local maximum for each particle anymore. Therefore, the algorithm developed in **[2]** is presented, which is able to first identify defects in the particle system and then segment the system into individual particles. For validation, we apply the algorithm to simulated data using a stochastic 3D model as described in **[3]**. By artificially inserting defects, we can quantify the accordance of the algorithm. Finally, the algorithm is applied to tomographic image data from a battery anode and cathode. In batteries, such defects can occur during thermal runaway, see, e.g., **[4]**. A segmentation of such a data set is possible using the presented algorithm, see Figure 2 for an example.

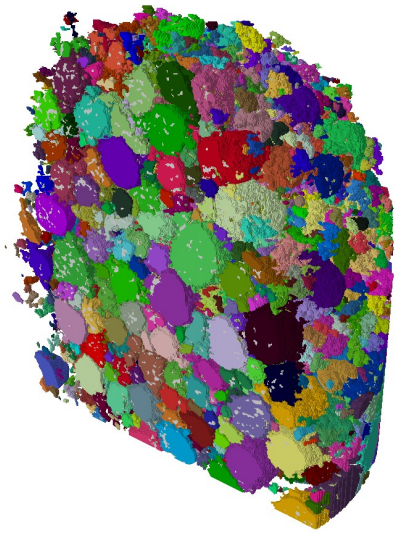

Figure 2: Segmentation of a particle system into individual particles (different colors) with defects highlighted using grey color.

References

[1] Roerdink JBTM, Meijster A (2001): The watershed transform: Definitions, algorithms and parallelization strategies. Fundamenta Informaticae, 41:187-228.

[2] Westhoff, D, Finegan, DP, Shearing, PR and Schmidt, V (2017): Algorithmic structural segmentation of defective particle systems: A lithium-ion battery study. Journal of Microscopy (in print), doi: 10.1111/jmi.12653

[3] Westhoff D, Feinauer J, Kuchler K, Mitsch T, Manke I, Latz A, Schmidt V (2017): Parametric stochastic 3D model for the microstructure of anodes in lithium-ion power cells. Computational Materials Science, 126:435–467.

[4] Finegan DP, Scheel M, Robinson JB, Tjaden B, Di Michiel M, Hinds G, Brett DJL, Shearing PR (2016): Investigating lithium-ion battery materials during overcharge-induced thermal runaway: an operando and multi-scale X-ray CT study. Physical Chemistry Chemical Physics, 18:30912–30919.

On microstructure-property relationships derived by virtual materials testing with an application to Fickian diffusion in silica monoliths

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Based on virtual materials testing, which combines image analysis, stochastic microstructure modeling and numerical simulations, quantitative relationships between microstructure characteristics and effective conductivity can be derived. The idea of virtual materials testing is to generate a large variety of stochastically simulated microstructures in short time. These virtual, but realistic microstructures are used as input for numerical transport simulations. Finally, a large data basis is available to study microstructure-property relationships quantitatively by classical regression analysis and tools from statistical learning. The quantitative relationship,

$$\sigma_{\text{eff}} = \sigma_0 \varepsilon^{1.15} \beta^{0.37} / \tau^{4.39} \tag{7.1}$$

between effective conductivity and the microstructure characteristics, which are relevant for transport (i.e. connected phase volume fraction ε, its mean geodesic tortuosity τ and constrictivity β) has been derived in **[1]**. Here σ_0 denotes the intrinsic conductivity of the material.
An extension of this simulation study has been performed in **[2]** where 8119 virtual microstructures have been generated. Using methods from statistical learning as neural networks and random forest it can be shown that that it is possible to predict effective conductivity more accurately. Due to the mathematical analogy, the obtained results can be transferred from conduction processes to Fickian diffusion in order to predict the effective diffusivity in porous microstructures. This is exemplarily demonstrated based on 3D image data of two different microstructures from silica monoliths **[3]**, where effective diffusivity is simulated by a random-walk particle-tracking algorithm **[4]**,**[5]**. In general, the proposed concept of virtual materials testing leads to a better understanding of microstructure-property relationships and thus, it has the potential to generate recommendations for new, more efficient microstructures.

References

[1] O. Stenzel, O. M. Pecho, M. Neumann, V. Schmidt, and L. Holzer. Predicting effective conductivities based on geometric microstructure characteristics. AIChE Journal, 62:1834 - 1843, 2016.

[2] O. Stenzel, M. Neumann, O. M. Pecho, L. Holzer, and V. Schmidt. Big data for microstructure-property relationships: A case study of predicting effective conductivities. AIChE Journal, 63:4224 - 4232, 2017.

[3] M. Neumann, O. Furat, D. Hlushkou, U. Tallarek, L. Holzer, V. Schmidt. On microstructure property-relationships obtained by virtual materials testing with an emphasis on effective conductivity. Communications in Computer and Information Science, Springer, submitted.

[4] D. Hlushkou, K. Hormann, A. Höltzel, S. Khirevich, A. Seidel-Morgenstern, U. Tallarek. Comparison of first and second generation analytical silica monoliths by pore-scale simulations of eddy dispersion in the bulk region. Journal of Chromatography A, 1303:28 - 38, 2013

[5] H. Liasneuski, D. Hlushkou, S. Khirevich, A. Höltzel, A., U. Tallarek, S. Torquato. Impact of microstructure on the effective diffusivity in random packings of hard spheres. Journal of Applied Physics, 116: 034904, 2014.

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