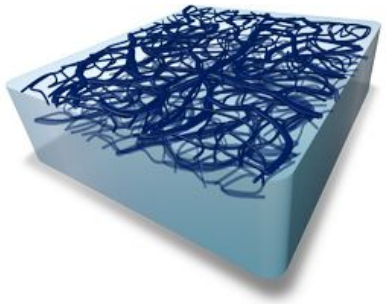
International Symposium on

Multiscale Computational Analysis of Complex Materials



August 29-31, 2017 Copenhagen, Denmark

Organized in the framework of Stanford-Columbia-DTU network "Multiscale multiphysics computational mechanics of advanced materials" supported by Danish Agency for Science, Technology and Innovation

Program

Overview and Objectives

Complex materials play an essential role in many applications, ranging from turbine blades, car chassis, computer and cell phone cases, battery systems, stretchable and wearable electronics, to biomedical applications. Those materials often operate and must maintain their high performance in harsh environments. The advancement of computationalmethods at multiple scales opens new possibilities for the design of such complex materials and the optimization of their intrinsic properties under extreme events. The bridging of different length and time scales though still represents an area of active research with many unresolved challenges. For example, material degradation is considered as a typical multiscale process, controlled by nanoscale defects, highly affecting the macroscopic material response.

This Symposium will bring together experts in the areas of multiscale computational modeling of complex, hierarchical, nanostructured materials. The symposium is organized in the framework of the Stanford- Columbia-DTU project “Multiscale multiphysics computational mechanics of advanced materials” supported by Danish Agency for Science, Technology and Innovation.

Symposium Topics

- Multiscale modeling of materials
- Multiphysics modeling of materials
- Computational materials science
- Micromechanics of materials
- Scale bridging and homogenization
- Materials under extreme environments
- Hierarchical materials
- Nanomaterials
- Biological and natural materials
- Geomaterials

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Program – August 29, 2017

9:00- 9:30 ***Registration***[1]

OPENING SESSION

9:30- 10:00 Opening, Leon Mishnaevsky Jr. (DTU, Denmark)
Christian Linder (Stanford) and Steve Sun (Columbia)
Welcome, Bent F. Sørensen (DTU, Denmark)

SESSION: MULTISCALING METHODOLOGY

10:00-10:30 Jacob Fish (Columbia U) Computational continua multiscale framework

10:30-11:00 Ole Sigmund (DTU) Multiscale approaches for topology optimization

11:00-11:20 ***Coffee***

11:20-11:50 John Hutchinson (Harvard) Bifurcation, localization, energy barriers and hysteresis in elastic structures and materials

11:50-12:20 Siegfried Schmauder (U Stuttgart) Multiscale materials modelling of fatigue

12:20-13:40 ***Lunch***

SESSION: MULTISCALE COMPOSITES

13:40-14:10 Bent F. Sørensen (DTU) Wind turbines blade structures and composite materials: Multiscale top-down approach to damage and fracture

14:10-14:40 Jiun-Shyan (JS) Chen (UC San Diego) Fracture to damage multiscale mechanics and meshfree modeling of concrete materials under extreme loadings

14:40-15:00 Lars P. Mikkelsen (DTU) Fatigue damage evolution in quasi-unidirectional non-crimp fabric based composite materials for wind turbine blades

15:10-15:40 Andrey V. Solov'yov (MBN Research Center) Exploration of thermo-mechanical properties of composites and interfaces with classical force fields and multiscale MD-MC approach

15:40-16:00 ***Coffee***

SESSION: POROUS AND GEOLOGICAL MATERIALS

16:00-16:30 Jose E. Andrade (Caltech) The new frontier of granular mechanics computation and experimentation

16:30-16:50 Christian Linder (Stanford) Inf-sup stable computational methods for strongly coupled

[1] Keynote and invited presentations last 25 minutes plus 5 minutes questions. Regular presentations last 15 minutes plus 5 minute questions.

	porous media at finite deformations
16:50-17:10	Norbert Huber (Helmholtz-Zentrum Geesthacht) A finite element modelling approach of mimicking the morphological characteristics of nanoporous metals with the aim of a detailed understanding towards their deformation mechanisms
17:10-17:30	WaiChing Sun (Columbia) A data-driven triple-scale discrete-continuum coupling method for fractured porous media
17:30-18:00	Ronaldo I. Borja (Stanford) Multiscale poromechanics: Fluid flow, solid deformation, and anisotropic thermoplasticity

18:30-22:30 ***Reception***

August 30, 2017

SESSION: DAMAGE AND INSTABILITIES

9:00-9:30	Alexander Hartmaier (Ruhr U Bochum) Atomistically informed continuum models of deformation and failure
9:30-9:50	Leon Mishnaevsky (DTU) Hierarchical composites with nanoengineered interfaces: Computational modelling
9:50-10:10	Rolf Mahnken (U Paderborn) A phase-field model for upper and lower bainite formation
10:10-10:40	Adnan Ibrahimbegovic (U Technologie Compiegne) Multiscale analysis of failure mechanics, stochastic upscaling and probability-based explanation of size effect

10:40-11:00 ***Coffee***

SESSION: COMPUTATIONAL TECHNIQUES

11:00-11:30	Stefanie Reese (RWTH Aachen) A multiscale FE-FFT- and phase-field-based computational approach to predict the mechanical response of polycrystalline materials
11:30-11:50	Michael Hauck (Fraunhofer ITWM,) Homogenization and design optimization for a periodic heterogeneous plate with frame structure under a given constraint.
11:50-12:10	Peter Lenz (Paderborn U) Derivation of (n)- and (n+1)-layered composite sphere models for thermos-chemo-mechanical volumetric and deviatoric effective properties
12:10- 12:30	Konstantinos Poulios (DTU) A large deformations homogenization method for unidirectional composites including reinforcement damage and matrix plasticity

12:30-13:40 ***Lunch***

SESSION: CRYSTALLINE MATERIALS

13:40-14:10	Christian Frithiof Niordson (DTU) Effects of micron scale plasticity on metal fracture
14:10-14:30	Ricardo Lebensohn (Los Alamos) Multiscale modelling with experimental integration of plastically-deforming polycrystalline materials

14:30-14:50	Wolfgang Pantleon (DTU) Dislocation-based constitutive laws and multiscale structural gradients
14:50-15:20	Grethe Winther (DTU) Hierarchical microstructures in metals due to dislocation-mediated plasticity
15:20-15:50	William Curtin (EPF Lausanne) X-Mechanics for Predictive Metallurgy

15:50-16:20 ***Coffee***

SESSION: STRUCTURED MATERIALS

16:20-16:50	Patrizia Trovalusci (Sapienza U. Roma) Multifield/non--local continuum modelling of materials with microstructure: a multiscale approach
16:50-17:10	Jandro L. Abot (Catholic U America) Piezoresistive response of carbon nanotube yarns: determining their hierarchical phenomenology towards modeling effort
17:10-17:30	Benjamin Klusemann (Leuphana U Lüneburg) Multiscale modeling of laser shock peening process involving laser induced plasma shock wave simulation

18:30-23:00 ***Dinner. Scandic Eremitage Hotel***

August 31, 2017

SESSION: SEMICONDUCTORS AND COUPLED PROBLEMS

09:00-9:30	Jörg Schröder (U Duisburg-Essen) Multiscale characterization of product properties of magneto-electric-mechanically coupling composites
09:30-10:00	Kurt Stokbro (QuantumWise A/S) Simulation of semiconductor devices with the Atomistix ToolKit
10:00-10:20	Krzysztof Grabowski (AGH Krakow) Multiscale modelling of sensors based on CNT/polymer for Structural Health Monitoring
10:20-10:40	Matthias Rambausek (U Stuttgart) Multiscale modeling of soft-matter magneto-electro-active composites
10:40-10:50	Mads Peter Sørensen (DTU) Multiscale modelling in superconducters and nanomechanical sensors

10:50-11:10 ***Coffee***

SESSION: BIOMATERIALS AND COMPOSITES

11:10-11:40	Ellen Kuhl (Stanford) Multiscale computational analysis of the brain
11:40-12:00	Immanuel Schäfer (U Stuttgart) Cellular solids in sea urchin spines: Abstraction of principles

and possible use cases in architecture

12:00-12:20 Adam Sciegaj (Chalmers U Technology) Two-scale finite element modelling of reinforced concrete based on first-order computational homogenization

12:20-12:40 David Neusiu (Fraunhofer ITWM) Computational truss model for large knitted structures of hyperelastic strings with Coulomb friction and adhesion

12:40-14:00 Lunch

SESSION: COMPUTATIONAL TECHNIQUES

14:00-14:30 Somnath Ghosh (Johns Hopkins) Wavelet transformation based multi-time scaling (WATMUS) for fatigue and coupled multi-physics problems

14:30-14:50 Varvara Kouznetsova (Eindhoven U Technology) Multi-scale transient computational homogenization for linear and non-linear materials local resonant metamaterials

14:50-15:10 Emilio Martínez-Pañeda (DTU) Modelling metal plasticity at the micron scale

15:10-15:30 Xiaozhe Ju (U Paderborn) Error-controlled homogenization for functionally graded composite materials

15:30-15:50 Saba Saeb (U Erlangen-Nuremberg) Computational homogenization accounting for size effects via interface elasticity

15:50-16:00 **Closing Remarks.** Leon Mishnaevsky Jr (DTU, Denmark), Christian Linder (Stanford) and Steve Sun (Columbia)

ABSTRACTS:

Piezoresistive Response of Carbon Nanotube Yarns: Determining their Hierarchical Phenomenology Towards Modeling Effort

Jandro L. Abot* and Jude C. Anike
Department of Mechanical Engineering, The Catholic University of America, Washington, DC 20064, USA

Carbon nanotube (CNT) yarns are continuous fiber-like structures composed of several thousand CNTs [1] that exhibit piezoresistivity, which could be tapped for sensing purposes. CNT yarns could be integrated in polymeric or composite structures and measure strain or monitor damage based on their piezoresistive response [2–3]. Recent experimental results reveal that the piezoresistive response is more complex than in most fibers and strongly dependent on the strain rate and other geometrical and mechanical parameters [4–8]. If the CNT yarns are integrated in a medium, the effect of its lateral constraint plays also a very significant role in the piezoresistive response by significantly increasing their sensitivity or gauge factors [7]. Based on the experimental observations, hypotheses are being drawn about the physical phenomena that govern the piezoresistive response of the CNT yarns. Two main mechanisms appear to control this response during the loading and unloading phases and they vary according to the strain rate. High strain rates lead to increased tensile strength and a positive piezoresistivity while low strain rates favor higher strain-to-failure and a negative piezoresistivity [8]. Future studies will include multiscale modeling of the observed effects to grasp fully the interplay of nano- and microstructure, load distribution and failure modes with the piezoresistive, mechanical and electrical response

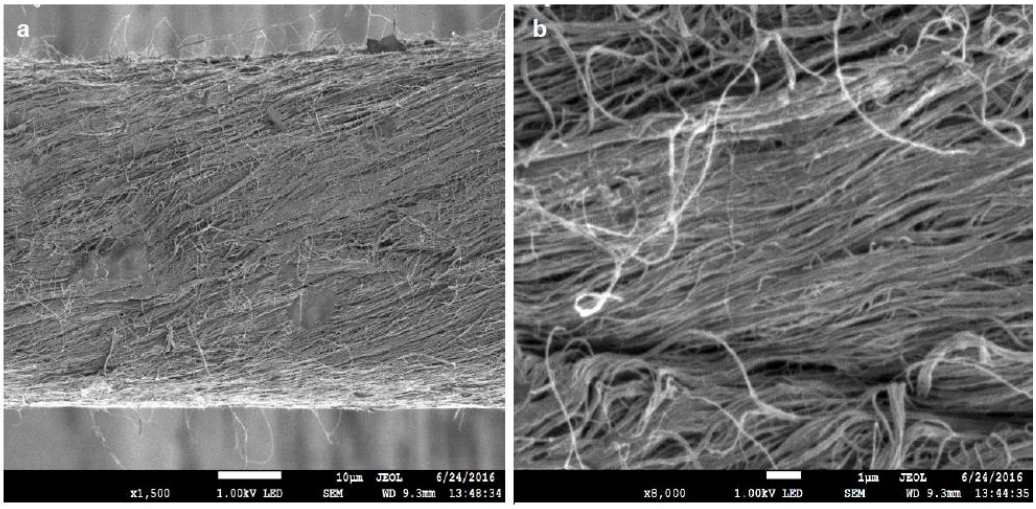

Figure 1. SEM images of CNT yarn: (a) Magnification of 1,500. (b) Magnification of 8,000. *Images taken with JEOL JSM-7100FA FE SEM.*

References

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The new frontier of granular mechanics computation and experimentation

Jose E. Andrade
California Institute of Technology , USA

In this talk, we will present new results on discrete element simulations compared with high-resolution experiments at a level of quantitative agreement never seen before. We have constructed an identical Avatar or digital twin of the experimental specimen, and have replicated the boundary conditions for triaxial loading. The results show remarkable agreement between the simulation and experiment—multiscale agreement ranging from grain rotations to the thickness and location of the shear band to the macroscopic load-displacement curve.
These advances have been possible due to the development of new technologies: X-ray computed tomography for experiments, and level set-based discrete element methods for computation. This new level of accuracy and resolution opens the door to better understand the complex behavior of granular materials under shear and could change the way we model the material behavior across scales.

Multiscale poromechanics: Fluid flow, solid deformation, and anisotropic thermoplasticity

Ronaldo I. Borja
Stanford University

Natural geomaterials often exhibit pore size distributions with two dominant porosity scales. Examples include fractured rocks where the dominant porosities are those of the fractures and rock matrix, and aggregated soils where the dominant porosities are those of the micropores and macropores. I will present a framework for this type of materials that covers both steady-state and transient fluid flow responses. The framework relies on a thermodynamically consistent effective stress previously developed for porous media with two dominant porosity scales. I will show that this effective stress is equivalent to the weighted sum of the individual effective stresses in the micropores and macropores, with the weighting done according to the pore fractions. Apart from this feature, some geomaterials such as shale exhibit pronounced anisotropy in their hydromechanical behavior due to the presence of distinct bedding planes. In this talk I will also present a thermo-plastic framework for transversely isotropic materials incorporating anisotropy and thermal effects in both elastic and plastic responses. Computational stress-point simulations under isothermal and adiabatic conditions reveal the importance of anisotropy and thermal effects on the inception of a deformation band. I will show that anisotropy promotes the formation of dilation band across a wide range of bedding plane orientations relative to the direction of loading.

Fracture to damage multiscale mechanics and meshfree modeling of concrete materials under extreme loadings

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M. Hillman, G. Zhou
Department of Civil and Environmental Engineering, The Pennsylvania State University, Pennsylvania, USA
M. J. Roth, J. Sherburn
US Army Engineer Research and Development Center, Vicksburg, Mississippi, USA

The failure processes in the materials exhibit distinct characteristics depending on the material ductility, the loading rate, and the environmental conditions. The mathematical models and the associated numerical methods for describing the material failure processes can be classified as the discrete description based on fracture mechanics and the continuum phenomenological description based on damage mechanics. This work first discusses how damage mechanics based models can be formulated by the homogenization of fracture models. The challenges in the numerical approximation and discretization of failure modeling based on fracture mechanics and damage mechanics will then be addressed. The mesh dependent issue in the micro-crack informed damage model remedied by the implicit gradient regularization or scaling laws under the Reproducing Kernel Particle Method (RKPM) will be introduced, and stability and convergence of the proposed numerical methods will be discussed. This includes the variationally consistent stabilized nodal integration and quasi-linear reproducing kernel approximation, among others. Finally, the numerical simulations of various damage processes in extreme events will be given.

X-Mechanics for Predictive Metallurgy

W. A. Curtin
Laboratory for Multiscale Mechanics Modeling
Institute of Mechanical Engineering, EPFL, Lausanne, Switzerland

X-Mechanics is a philosophy of using all the different mechanics tools (X=quantum, statistical, atomistic, mesoscale, continuum) as needed to solve complex problems related to the mechanical behavior of materials. Here, we outline the X-Mechanics philosophy and then provide one nice example that uses all of these tools to generate predictive understanding of the origins of low ductility in Al-5xxx (Al-Mg) alloys. The low ductility in Al-5xxx is a major barrier to their replacement of steels in automotive and other applications where failure by localization limits component design. Low ductility in Al-xxx alloys has long been associated with Dynamic Strain Aging– the material is stronger at lower strain rates, which encourages localization and instabilities – but no quantitative or predictive models exist. Here, we present a hierarchical, mechanistic, multiscale model that quantitatively predicts the ductility and enables the design of new higher-ductility alloys. The components of the model, all new to the metallurgy field, are:
(1) atomic-scale “cross-core diffusion” mechanism of aging;
(2) effects of cross-core diffusion on two mechanisms of dislocation strengthening;
(3) full thermo-kinetic constitutive model for thermally-activated plastic flow;
(4) implementation within an FEM model to predict coupon-scale response;
creation of predictive theory for solute strengthening;
first-principles solute/dislocation interaction energies for arbitrary solutes in Al;
computationally-guided design of new higher-ductility alloys.

The model quantitatively predicts the entire scope of steady-state flow behavior as a function of strain-rate, plastic strain, temperature, and alloy composition in Al-Mg alloys, with all key inputs coming from quantum, atomistic, or dislocation-level computations. In particular, the predicted reduction in ductility of Al-Mg 5182 alloys at room temperature and strain rate of 10-3/s is predicted in good agreement with experiments, tying the ductility loss directly to atomistic-scale phenomena. The model is then used to design new Al alloy compositions that have higher ductility at room temperature while maintaining the same yield and hardening behavior of the commercial alloys.

Computational continua multiscale framework

Jacob Fish
Columbia University, New York, USA

The talk presents a new multiscale framework, termed computational continua (C2) that is both computationally efficient and scale-separation-free. The multiscale software based on the stochastic C2 formulation has been successfully deployed in the aerospace industry (Lockheed-Martin, Northrop-Grumman, Boeing, Rolls-Royce, General Electric) for fatigue life prediction and environmental degradation of high temperature CMC and PMC components as well as in the automotive industry (General Motors, Automotive Composites Consortium) for crash prediction of composite cars. The C2 formulation is endowed with fine-scale details, introduces no scale separation, makes no assumption about infinitesimality of the fine-scale features, requires no higher order continuity, introduces no new degrees-of-freedom, is free of higher order boundary conditions and employs model hierarchy that permits reliance on limited experimental database. The computational efficiency of the C2 formulation stems from the residual-free formulation that eliminates the bottleneck of satisfying fine-scale equilibrium equations and hybrid impotent-incompatible eigenstrain formulation that alleviates locking arising from a lower order approximation of eigenstrains. The talk includes theory and applications in aerospace and automotive industry as well as in fracture prediction of femur.

Wavelet Transformation based Multi-Time Scaling (WATMUS) for fatigue and coupled multi-physics problems

Somnath Ghosh
Michael G. Callas Professor
Departments of Civil Engineering, Mechanical Engineering, Materials Science & Engineering
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Cyclic crystal plasticity finite element (CPFE) simulations of complex materials, e.g. polycrystalline metals, are widely used to study fatigue failure due to plasticity and damage. Typically, this requires the simulation of a large number of cycles to failure for accurate determination of evolving deformation variables. Modeling cyclic deformation using conventional methods of time integration in semi-discretization techniques can however be computationally challenging. Single time-scale integration methods typically follow the high frequency characteristics and discretize each cycle into a number of time steps over which integration is performed. To overcome this computational challenge, the wavelet transformation-based multi-time scaling (WATMUS) method is proposed for accelerated for CPFE modeling of polycrystalline alloys. WATMUS has adaptive capabilities to optimally construct the wavelet basis functions and determine coarse-scale cycle steps. Accuracy and efficiency of the WATMUS methodology is demonstrated by comparing with cyclic single-time scale crystal plasticity finite element simulations on image-based microstructure of alloys.

The WATMUS method is also applied for simulating coupled transient electromagnetic and dynamic mechanical problems with fields that differ widely in the frequency ranges. A WATMUS framework for coupling the fields to predict the evolution of electric and magnetic fields in a vibrating substrate will be presented.

Multiscale modelling of sensors based on CNT/polymer for Structural Health Monitoring

Krzysztof Grabowski, Tadeusz Uhl, Pawel Packo
Faculty of Mechanical Engineering and Robotics, AGH University of Science and Technology, Krakow, Poland

Carbon nanotubes (CNT's) due to their extraordinary properties have gained much interest in scientific communities. One of possible uses is as sensing mechanism for Structural Health Monitoring (SHM). However, due to the scale of CNT's it is rather hard to model sensors parameters *a priori*, which would allow to calibrate such sensors.
This paper presents the development of a numerical framework for modelling of composite materials based on carbon nanotubes that are used as strain sensors. The proposed model allows for multiscale analysis of electro-mechanical properties of such systems. Model is based on two scales namely meso and macro and utilizes RVE approach. Mesoscale (microscale) investigates electro-mechanical behavior of the CNT/polymer composite. Then, stresses and conductivity from the mesoscale are passed to the macroscale using the Hill-Mandel principle. Numerical framework is then validated and compared to experimental results. Moreover, discussion on uncertainties between numerical and experimental results is presented, concluding with proposal of inverse approach for modelling of CNT/polymer composites.

Atomistically informed continuum models of deformation and failure

Alexander Hartmaier
Interdisciplinary Center for Advanced Materials Simulation (ICAMS)
Ruhr-Universität Bochum, Germany

In order to understand the mechanical performance of multiphase materials, which possess a heterogeneous microstructure, we need to describe the elastic-plastic deformation of all individual phases and their interfaces. It is clear that such description must involve several length and time scales. One possible approach is the bottom-up scalebridging method, in which information is gained on the most fundamental level and then this information is systematically coarse grained. In our work, we follow a complementary top-down approach in which we start from a macroscopic model that is based on physical laws in which material parameters and scaling relations obtained from atomistic simulations are incorporated. This is accomplished by introducing representative volume elements (RVE) of rather complex microstructures. This RVE-based microstructural model is then subjected to different mechanical loads and the resulting mechanical problem is solved by the Finite Element Method (FEM). In the framework, crystal plasticity models are applied to describe plastic flow on the level of individual grains. Interface properties are model by the cohesive zone method. Furthermore, damage models are applied to describe ductile failure and fatigue crack initiation. It will be demonstrated how such RVE-based micromechanical simulations can be applied to make predictions on macroscopic mechanical behavior of multiphase materials, such as plastic flow, fatigue and hydrogen embrittlement.

Homogenization and Design optimization for a periodic heterogeneous plate with frame structure under a given constraint

Michael Hauck, Julia Orlik
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The design optimization problems for heterogeneous elastic plates with frame structure arise in many different applications, for instance in filters under local bending or analysis of textiles. We consider a plate with an in-plane periodic structure under a local point-bending moment or force. We employ basic homogenization techniques for linear periodic heterogeneous plates and pass to the anisotropic Kirchhoff-Love plate in the limit, where the effective bending coefficients were obtained from the auxiliary bending unit experiments on the periodicity cell by averaging of the local moments of outer-plane stresses. Since the plate structure is made of beam, we use the beam-FE method for solving the cell-problems. We homogenize the plate and then find an analytic solution under the local bending perturbation. Our further aim is to minimize the deflection caused by a localized load in the effective anisotropic plate. For that case we need to define a design space, which takes into account the constraint of anisotropy. We provide a particular example, where we can show how the design parameters influence the maximal plate deflection.

Bifurcation, localization, energy barriers and hysteresis in elastic structures and materials

John W. Hutchinson
School of Engineering and Applied Sciences, Harvard University

Examples drawn from experiments and analysis of shell structures and soft material systems are used to illustrate a sequence of instability phenomena comprising localization of the bifurcation mode accompanied by loss of quasi-static stability with dynamic snapping to a large amplitude localized deflection. Under cyclic loading which pushes into the large amplitude regime in each cycle, hysteretic behavior occurs even when the material response is strictly elastic. The transition to the large amplitude deflection is characterized by an energy barrier which serves to measure the tolerance to both unexpected disturbances and deliberate probing of the structure or material. Recent theoretical and experimental efforts to exploit a force probe to assess the degree of stability of loaded structures will be discussed.

Multiscale analysis of failure mechanics, stochastic upscaling and probability-based explanation of size effect

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In this work, we discuss the role of probability in providing the most appropriate multiscale based uncertainty quantification for the inelastic nonlinear response of heterogeneous materials undergoing localized failure. Two alternative approaches are discussed: i) the uncertainty quantification in terms of constructing the localized failure models with random field as parameters

of failure criterion, ii) the uncertainty quantification in terms of the corresponding Bayesian updates of the corresponding evolution equation.
The detailed developments are presented for the model problem of cement-based composites, with a two-phase meso-scale representation of material microstructure, where the uncertainty stems from the random geometric arrangement of each phase. Several main ingredients of the proposed approaches are discussed in detail, including microstructure approximation with a structured mesh, random field KLE representation, and Bayesian update construction. We show that the first approach is more suitable for the general case where the loading program is not known and the best one could do is to quantify the randomness of the general failure criteria, whereas the second approach is more suitable for the case where the loading program is prescribed and one can quantify the corresponding deviations. More importantly, we also show that models of this kind can provide a more realistic prediction of localized failure phenomena including the probability based interpretation of the size effect, with failure states placed anywhere in-between the two classical bounds defined by continuum damage mechanics and linear fracture mechanics.

A finite element modelling approach of mimicking the morphological characteristics of nanoporous metals with the aim of a detailed understanding towards their deformation mechanisms

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[1]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Germany
[2]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany

The current work presents a numerical modelling approach for investigating the effect of ligament shape, disorder and connecting nodal mass on the macroscopic mechanical response of nanoporous gold (NPG). The approach starts from a 'single ligament' analysis with respect to three fundamental deformation modes, bending, torsion, and compression, that depend on the ligament shape. It can be shown that the predictive capability of the highly computationally efficient beam model is sufficient for a large variation in ligament shapes. Using a representative volume element (RVE) composed of such ligaments, different degrees of disorder are included. From the comparison of the RVE elastic response with the single ligament results and the further analysis of statistical information from the elements in the RVE, it is found that bending is the major deformation mode for perfectly ordered RVEs, whereas torsion gains importance for increasing RVE disorder. This explains the reduced lateral expansion during compression deformation of NPG. Moreover, it was also found that the nodal mass contributes significantly on the stiffening and strengthening of NPG, a nodal corrected modelling concept has been proposed and integrated to beam RVEs, which offers realistic mechanical responses with respect to elasticity and plasticity, and this is validated with several solid element RVEs.

Error-controlled homogenization for functionally graded composite materials

Xiaozhe Ju and Rolf Mahnken
Chair of Engineering Mechanics (LTM), Paderborn University
Paderborn, Germany

The research field of model adaptivity has been well established, aiming at adaptive selection of mathematical models from a well-defined class of models (model hierarchy) to achieve a preset

level of accuracy (see e.g. [1,2,3]). The present contribution addresses its application to a class of linear elastic composite problems. We will show that the classical bounding theories according to [4,5] can provide a model hierarchy in a natural and theoretically consistent manner, without combination of different methods using a priori knowledge. To arrive at easily computable higher order bounds, the classical singular approximation following [6] is made. As a new finding, this may, under certain circumstances, give rise to an overlap effect. To overcome this, a correction is proposed. Additionally, the model adaptivity is coupled to the well-established adaptive finite element method (FEM), such that both macro model and macro discretization errors are controlled. The proposed adaptive procedure is driven by a goal-oriented a posteriori error estimator based on duality techniques. For efficient computation of the dual solution, a patch-based recovery technique is proposed, where a comparison with other existing methods is also given. For a numerical example, we consider a functionally graded composite.

References

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Multiscale Modeling of Laser Shock Peening Process involving Laser Induced Plasma Shock Wave Simulation

Benjamin Klusemann[1,2], Sören Keller[2], Vasiliy Pozdnyakov[2], Sergey Chupakhin[2], Jens Oberrath[1], Nikolai Kashaev[2]

[1]Institute of Product and Process Innovation, Leuphana University of Lüneburg, Germany

[2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Germany

Laser shock peening is a surface modification technique which improves the fatigue performance of metallic structures by inducing compressive residual stresses for mitigation of crack growth. A pulsed laser vaporizes the first layer of the component and turns the solid material into plasma. Thermal expansion of the plasma in the confining medium initiates high pressure shock waves propagating into the material. Residual stresses are the result of local plastic deformations caused by the pressure waves. The process is highly nonlinear and difficult to optimize based on experiments alone due to the high number of process parameters, short time events and extreme values of physical quantities which are hard to measure (e.g. shock wave propagation, plasma forming). Aiming at deeper understanding of the process and an optimized residual stress profile, a multiscale approach is proposed. Starting with a laser induced plasma shock wave simulation, a global model for determining the shock pressure depending on the laser parameters is implemented. The results of the shock pressure distribution over time are used in a subsequent finite element model, to predict the resulting residual stress profile within the material. Afterwards the numerical

results are compared and validated on basis of the experimental results for different aluminum alloys.

Multi-scale transient computational homogenization for linear and non-linear materials local resonant metamaterials

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Locally resonant metamaterials are a relatively new class of metamaterials exhibiting acoustic band gaps at subwavelength frequencies, originating from complex interaction between the micro-inertia of the local resonators and the macroscopic transient phenomena. Pushing the material behavior into a non-linear regime opens even more possible applications, e.g. tunable waveguides, adaptive passive vibration control, superdamping, acoustic diodes, cloaking, noise insulation and (vibro-acoustic) energy harvesting.
The development and design of such materials and devices made thereof, requires advanced modelling techniques, capable, on one hand, to deal with complex geometries, boundary conditions and excitations, and on the other computationally more efficient than direct numerical simulations.
In this work, a novel computational homogenization approach is presented for multi-scale modelling of locally resonant materials. The point of departure is the computational homogenization technique, well established for quasi-static problems and recently extended to transient problems. For linear problems, the static-dynamic decomposition of Craig-Bampton type can be used to derive the closed form homogenized equations representing an enriched continuum, in which additional kinematic degrees of freedom emerge to account for micro-inertia effects. In non-linear case, fully coupled two scale transient computational homogenization is used to study the wave dispersion in finite size macroscopic structures.
Acknowledgements: The research leading to these results has received funding from the European Research Council under the European Union's Seventh Framework Programme (FP7/2007-2013) / ERC grant agreement n°[339392]. The support from 4TU Research Center High Tech Materials (4TU.HTM) is also gratefully acknowledged.

Multiscale computational analysis of the brain

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Axonal damage is a critical indicator for traumatic effects of physical impact to the brain. However, the precise mechanisms of axonal damage are still unclear. Here we establish a mechanistic and highly dynamic model of the axon to explore the evolution of damage in response to physical forces [1]. Our axon model consists of a bundle of dynamically polymerizing and depolymerizing microtubules connected by dynamically detaching and reattaching crosslinks [2]. While the probability of crosslink attachment depends exclusively on thermal fluctuations, the probability of detachment increases in the presence of physical forces [3]. We systematically probe the landscape of axonal stretch and stretch rate and characterize the overall axonal force, stiffness, and damage as a direct result of the interplay between microtubule and crosslink dynamics. Our simulations reveal that slow loading is dominated by crosslink dynamics, a net reduction of crosslinks, and a gradual accumulation of damage, while fast loading is dominated by crosslink deformations, an rapid

increase in stretch, and an immediate risk of rupture. Microtubule polymerization and depolymerization decrease the overall axonal stiffness, but do not affect the evolution of damage at time scales relevant to axonal failure. Our study explains different failure mechanisms in the axon as emergent properties of microtubule polymerization, crosslink dynamics, and physical forces. We anticipate that our model will provide insight into causal relations by which molecular mechanisms determine the timeline and severity of axon damage after a physical impact to the brain.

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Multiscale modelling with experimental integration of plastically-deforming polycrystalline materials

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Multiscale models based on crystal plasticity are increasingly used in engineering applications to obtain microstructure-sensitive mechanical response of polycrystals. Three key elements of these models to capture the complexity of this ubiquitous class of materials are a proper consideration of the single crystal plastic deformation mechanisms, a representative description of the microstructure, and an appropriate scheme to connect the microstates with the macro response. The latter can be based on homogenization (e.g. self-consistent methods [1]), which relies on a statistical description of the microstructure, or be full-field solutions, which requires a spatial description of the microstructure (e.g. spectral methods [2]). Full-field models are computationally very intensive, preventing their direct embedding in multiscale calculations. On the other hand, they can be used to generate reference solutions for assessment of approaches based on homogenization or semi-analytical theories [3]. In this talk we will review our recent efforts to develop material models based on polycrystal plasticity, emphasizing the integration of experimental data for input and validation of the models, and the different strategies adopted to embed these models in Finite Elements [4,5], to solve problems involving complex geometries and boundary conditions with microstructure-sensitive material response.

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Derivation of (n)- and (n+1)-layered composite sphere models for thermos-chemo-mechanical volumetric and deviatoric effective properties

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Our work presents extensions of multi layered composite sphere models known from the literature [1, 2, 3] to temperature-dependent elastic effects accompanied by curing. Volumetric and deviatoric effective properties in dependence on the degree of cure are obtained by homogenization for a representative unit cell (micro-RVE) on the heterogeneous microscale. To this end, analytical solutions for (n)- and (n + 1)-layered composite sphere models, [3, 4], are derived, in addition to Voigt and Reuss bounds resulting from the assumption of a homogeneous mixture. The deviatoric effective properties are derived in the context of both, a shear stress approach and a shear deformation approach, this results into an overdetermined system of equations which solved with the least squares method. For simplification, we restrict the material behavior of the micro-RVE to thermo-chemo-mechanical coupling with linear elasticity. As a further result the equivalence of the volumetric effective properties of the (n)- and (n + 1)-layered composite sphere model is shown. In a numerical study it is demonstrated that the effective elastic and thermal properties lie within bounds, whilst for the chemical part of the model, an analogous result is obtained for the effective strains. Furthermore, a convincing agreement with experimental data for glass microspheres embedded in a polyester matrix is demonstrated.

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Inf-sup stable computational methods for strongly coupled porous media at finite deformations

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The modeling of the interaction between the solid skeleton and an inter-penetrating fluid in porous materials has been a highly active field of research since the early defining works by Biot. In the context of the finite element method it has been recognized early that in highly coupled situations the satisfaction of the well-known inf-sup condition is mandatory for mixed formulations and that the same interpolation schemes that guarantee stability in cases such as Stokes flow or

incompressible elasticity provide stable results in poroelasticity as well. A rigorous mathematical proof of certain elements is however unfeasible in many cases and numerical tests have been proposed to judge whether a proposed interpolation scheme is reliable [1]. While this test has been successfully evaluated for standard cases such as Stokes flow, an evaluation for poroelastic problems remains unsatisfactory [2].
This contribution presents ideas how a numerical test can be evaluated successfully in the case of poroelasticity to judge whether a novel interpolation scheme is reliable and hence guaranties uniqueness and necessary stability estimates. Based on these observations we evaluate a number of recent schemes that have recently been proposed in our research group. We present a novel low-order mixed finite element formulation based on an incompatible strain enhancement that provides inf-sup stability while preventing well-known hourglass modes in the limit of large deformations [3]. In addition, in the context of isogeometric analysis we prove the stability of a variety of interpolation schemes based on degree-elevated methods and subdivision-based methods in numerical tests to provide alternatives to classical schemes that, while stable in classical finite element schemes, can fail to provide inf-sup stability. The capability of the proposed schemes is underlined in exemplifying numerical examples including the consolidation of saturated soil under footings and swelling tests of polymeric gels.

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A phase-field model for upper and lower bainite formation

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Upper and lower bainitic transformations are complex transformations in steel. In particular, the transformation from austenite to bainitic ferrite is assumed to be displacive [1] in contrast to the perlitic growth which is highly dependent on the carbon movement. However regarding the whole microstructure named bainite, consisting of bainitic ferrite, carbides and (residual) austenite, the movement of the carbon is of great importance. In upper bainite the carbon starts to diffuse across the phase interface from the supersaturated bainitic ferrite into the austenite phase. If the carbon concentration becomes high enough at the interface, carbides will precipitate. In lower bainite the carbon within the ferrite separates [1] and precipitates as carbides within the bainitic ferrite phase. Furthermore some carbon atoms succeed in leaving the ferrite to enrich the surrounding austenite.

In our work we present a phase-field model to simulate the phase transformations from austenite to bainitic ferrite and the precipitation of carbides [2]. The model is coupled to a diffusion equation governing the carbon concentration. The underlying system of partial differential equations is based on a thermodynamic framework of generalized stresses as introduced by Gurtin and Fried [4, 5] for a two phase Ginzburg-Landau system and a Cahn-Hilliard equation. We extend our framework for
multiphase-field models coupled to a viscous Cahn-Hilliard equation [3] as it is required for the lower bainitic transformation. The key aspects of the thermodynamic framework are generalized stresses and microforces which perform work in conjunction with derivatives of the phase-field variables and the carbon concentration. The numerical examples demonstrate the qualitativ mechanism of the lower and upper bainitic transformation as described in [1].

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Modelling metal plasticity at the micron scale

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Experiments have consistently shown that metallic materials display strong size effects at the micron scale, with smaller being harder. As a result, a significant body of research has been devoted to model this size dependent plastic phenomenon (see [1] and references therein). At the continuum level, phenomenological strain gradient plasticity (SGP) formulations have been developed to extend plasticity theory to small scales. Grounded on the physical notion of geometrically necessary dislocations (GNDs, associated with non-uniform plastic deformation), SGP theories relate the plastic work to both strains and strain gradients, introducing a length scale in the constitutive equations. The numerical implementation of SGP formulations is however not free from challenges and numerical complexities have long hindered a comprehensive embrace of gradient plasticity models.
In this talk several ad hoc numerical basis for the main SGP formulations will be presented. Both lower and higher order gradient plasticity models will be considered and standard and enriched numerical solutions proposed. The robustness and efficiency of the numerical framework presented will be demonstrated by addressing engineering problems beyond micron-scale applications; namely, crack initiation and subsequent growth. GNDs are likely to impact fracture mechanics as,

independently of the size of the specimen, the plastic zone adjacent to the crack is physically small and contains strong spatial gradients of deformation. The influence of GNDs will be then examined in a wide range of areas where they are expected to play a major role: crack tip fields characterization [2], cohesive zone modeling of crack propagation, hydrogen diffusion towards the fracture process zone [3] or environmentally assisted cracking [4].

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Fatigue damage evolution in quasi-unidirectional non-crimp fabric based composite materials for wind turbine blades

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The fatigue failure of wind turbine blades is controlled by failure mechanisms on multiple scales spanning single fiber fatigue failure at the sub-micron scale, over the fiber bundle structure on the millimeter scale to the quasi-unidirectional non-crimp fabric on the meter scale. At the smaller scales, the 3D x-ray computer tomography technique is used non-destructive to observe the fatigue damage evolution on the fiber and bundle scale. Those observations are then linked to the larger scales through mechanical testing of representative volumes of the non-crimp fabric bundle structure. Numerically, those non-crimp fabric bundle structures extracted from the 3D x-ray scans can be used in a multi-scale based finite element models used for understanding the parameters controlling the fatigue damage evolutions. During tension-tension fatigue testing, the damage mechanism is shown to be controlled by local architecture of the so-called backing bundle structure present in the non-crimp fabric. This mechanism is demonstrated to be highly dependent on the presence of curing induced residual stresses. Residual stresses which for an epoxy matrix system can be controlled by the chosen cure profile and thereby the mold time during wind turbine blade manufacture.

Hierarchical composites with nanoengineered interfaces: Computational modelling

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Mechanical properties and strength of materials can be enhanced by modifying the structures of the materials at micro- and nanoscales. One of the promising directions of the materials modification for the properties enhancement is based on the control and modification of interface properties.

Interfaces, phase and grain boundaries represent often relatively instable and deformable regions of materials. The introduction of geometrical structural inhomogeneities (e.g., defects or nanoparticles) into instable phases allows to control the local stress concentration and to channels the deformation energy into the lower scale level. Thus, nanomodification of weak regions and structural defects can be used to influence the damage evolution and improve the damage resistance of the material. A series of computational micromechanical studies of the effect of nanostructuring and nanoengineering of interfaces, phase and grain boundaries of materials on the mechanical properties and strength of composite materials was carried at the DTU Wind Energy. We considered several groups of materials (composites, nanocomposites, nanocrystalline metals, wood) and explored (using numerical experiments [1-4]) how the interface structures influences the properties of the materials. Figure 1 shows an example of hierarchical FE model of a composite with nanoreinforced interphase/interface layer [1-2]. In the simulations, it was demonstrated that the availability of special structures in grain boundaries/phase boundaries/interfaces represents an important and promising source of the enhancement of the materials strength.

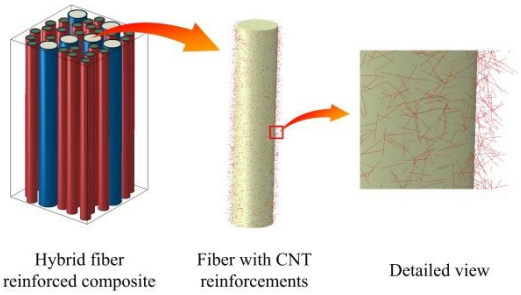

Figure 1. Schema of the multiscale modelling of CNT reinforced hybrid composites

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Computational truss model for large knitted structures of hyperelastic strings with Coulomb friction and adhesion

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We consider a truss model for simulation of textiles with frictional contact between threads and no bending resistance. In the model, 1D hyperelasticity and the Capstan equation are combined and an additional adhesion between yarns is modelled. The 1D hyperelasticity model is reformulation for arbitrary force-stretch curves, which are more relevant for yarns and fibers. The measured curves are interpolated by splines and plugged into the numerical model. For the friction model, the Capstan equation, or Euler-Eytelwein formula, are extended by an adhesional force and, then,

extended to the case of extensible threads. The whole model results in the nonlinear evolution equations. This mathematical model fits various models with rate-independent dissipation.
In the numerical algorithm, we apply classical regularization technique for the non-smooth frictional term and solve the resulting smooth problems with Newton-Raphson method, performed in two steps w.r.t. the elastic stretch-variable and the contact sliding.
We have developed a numerical algorithm and can provide numerical experiments along with comparisons of the results with real measurements.

Effects of micron scale plasticity on metal fracture

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Micron scale size-effects in metals showing the trend that "smaller is stronger" have been confirmed in numerous experiments. It is generally accepted that these size-effects relate to plastic incompatibility and associated geometrically necessary dislocations, which lead to additional hardening or so-called strengthening. Significant plastic incompatibility on small scales may arise due to inhomogeneous overall deformation within experiments such as torsion and indentation, but it can also arise under homogeneous deformation when boundaries are passivated, such that plastic deformation is hindered due to blockage of dislocations. Strain gradient plasticity theories that are able to capture these non-trivial size-effects, have undergone intense development in the past decades.
During fracture in metals, highly inhomogeneous plastic deformation takes place in the vicinity of a crack tip, and ensuing size-effects are of key importance to the failure process. In this presentation, the potential for enhancing modeling techniques for fracture based on modern strain gradient plasticity theories will be treated. This will include both ductile failure, where the void growth and coalescence mechanism is affected by size, as well as failure in aggressive environments, where fracture properties are affected by size-dependent plastic straining near the crack-tip due to hydrogen embrittlement.

Dislocation-based constitutive laws and multiscale structural gradients

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A constitutive law for the evolution of the flow stress with plastic strain is derived based on a quantitative description of the dislocation content. In this manner, the occurrence of different work-hardening stages can be accounted for and different dominating microstructural processes associated with the stages II to V. Such constitutive laws are usually formulated and applied solely in case of continued work-hardening, presuming that no work-softening by dislocations occurs during continuous deformation. Following changes in the deformation conditions, a structure alien to the new deformation conditions has to reorganize into a structure conform to them. In the course of this re-organization, work-softening by dislocations may indeed occur due to the microstructural evolution in accordance with the evolution of the dislocation density. For example, during rolling of electrodeposited nickel-iron the dislocation density is continuously decreasing and a proper description of the work-softening is achieved with well-established constitutive equations. In

structures with purposely introduced property and structural gradients, an even more complex scenario arises as the same evolution equation leads to increasing dislocation densities in some, but decreasing dislocation densities in other regions; a proper description of such gradient structures is nevertheless achieved by applying an appropriate constitutive law.

A large deformations homogenization method for unidirectional composites including reinforcement damage and matrix plasticity.

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This work concerns a homogenized model of unidirectional composite materials under plane strain conditions, including strong kinematic and material nonlinearities. The reinforcing layers are treated as quasi-brittle with Lemaitre type damage behavior, while the binding matrix material is represented in the framework of hyperelastoplasticity with a standard isotropic J2 yield surface. The proposed homogenization approach relies on an enhanced kinematic description of the composite unit-cell, similar to that of generalized continua. Based on this kinematic description and an integration of the virtual work expression of the non-homogenized solid through the microstructure unit-cell, a finite-element model is obtained which relies directly on the constitutive laws of the two phases. The obtained finite-element is valid for large deformations both at the macro-scale and the micro-scale. The accuracy of the homogenized model in representing the underlying micro-mechanics is demonstrated through comparisons with a reference model with explicitly discretized fibers.

Multiscale modeling of soft-matter magneto-electro-active composites

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Magneto-electrically (ME) coupling materials are employed in innovative fields of application. They are used for the design of, e.g., ME random access memories and electrical magnetic-field sensors. Since, all known single phase materials exhibit extremely weak coupling, ME composites become relevant. Classical approaches for this kind of composites are based on ceramic materials [1, 2]. In the present contribution, however, we discuss a new realization of ME coupling based on soft-matter composites [3]. These soft composites are less fragile than their ceramic counterparts. Additionally, their constituent phases are cheap and their manufacturing is straight-forward.
In this talk, we present several studies on the performance of prototypical electrical magnetic-field sensors based on soft ME composites. Thereby, we focus on the question which material properties have the greatest influence on the device performance. For this purpose, we employ a multiscale (FE^2) framework based on an energy formulation, which allows us to investigate the influence of both effective local coupling properties of the composite and equally important non-local device-level coupling effects [4, 5].

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Multiscale FE-FFT- and FE-POD-based approaches to predict the mechanical response of polycrystalline and biological materials. Multiscale modeling using finite elements, fast Fourier transforms and proper orthogonal decomposition in production and medical technology

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The necessity to provide physically reasonable and mathematically sound descriptions of mechanical behaviour at different scales is without discussion. Nevertheless, for engineering design quick estimations of important quantities such as stresses and strain are needed. At a larger scale, information about the overall behaviour of complex systems has to be supplied.
For this reason, we need to develop computational methods which on the one hand enable a detailed material description, on the other hand allow the bridging to coarser scales without losing too much information. In the present contribution, various methods concerning applications in production technology (process signature) and medical technology (tissue-engineered heart valves) are discussed. The scale bridging is achieved by coupling finite element modeling on the macro scale with (1) fast Fourier transforms discretization using the phase field method (see e.g. [1,2]) or (2) proper orthogonal decomposition (see e.g. [3]) on the micro scale. Another possibility is standard up-scaling using differently detailed finite element models [4].

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Computational homogenization accounting for size effects via interface elasticity

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The objective of this presentation is to establish a computational homogenization framework to model the behavior of heterogeneous materials in which the influence of interfaces at the micro-scale is taken into account. The term "interface" refers to a zero-thickness model that represents the finite thickness "interphase" between the different constituents of a micro-structure. Therefore, the interface is essentially a two-dimensional manifold embedded in a three-dimensional space. The interface model presented here does not allow for a displacement jump across the interface and thus captures only coherent interfaces. However, a traction jump associated with interface elasticity is captured.

The interface effect is of particular importance for multiphase materials at the nano-scale due to the increasing area-to-volume ratio at smaller scales. Classical computational homogenization lacks a physical length-scale and thus fails to account for a size effect in the material response. We show that including interfaces at the micro-scale introduces a length-scale into first-order computational homogenization. Furthermore, size effects due to interfaces are physically interpretable and agree well with atomistic simulations.

Central to computational homogenization is the Hill-Mandel condition which ensures the incremental energy equivalence between the scales. An extended form of the standard Hill-Mandel condition is proposed that accounts for the presence of interfaces at the micro-scale. Accordingly, suitable boundary conditions to satisfy the Hill-Mandel condition are derived. In this presentation, we focus on strain-driven computational homogenization at finite deformations. That is, the macroscopic deformation gradient is the input of the micro-problem and the macroscopic stress is sought. In doing so, we employ extended average theorems such as the average stress theorem to relate the macroscopic quantities to their microscopic counterparts.

Computational aspects of the finite element formulation of the presented framework are elaborated. The influence of different boundary conditions on the overall response of different micro-samples under different conditions is studied through presenting several numerical examples. Moreover, we investigate microstructures with periodically and randomly arranged particles within the matrix. Our numerical results confirm that, when energetic interfaces are present, the overall response of random microstructures mostly overestimate the overall response of periodic microstructures which is in contrast to what is commonly observed in classical computational homogenization.

Cellular solids in sea urchin spines: Abstraction of principles and possible use cases in architecture

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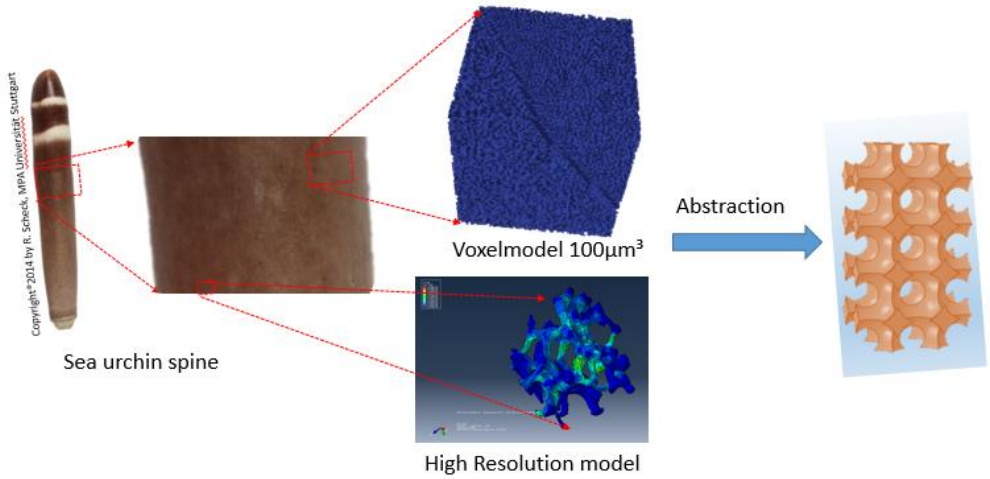
The sea urchin species Heterocentrotus Mamillatus, the slate pencil urchin, can grow up to 12 cm long and 1 cm thick spines which consist of highly porous Mg-enriched calcium carbonate. Interestingly the spines show a very complex hierarchical and lightweight structure and can resist high mechanical loads. When getting compressed, they show a graceful failure behaviour (Presser et al. 2009).
The analysis starts with a step of image processing methods to generate a model of a part of the sea urchin spine. Basis for that are computer tomography (CT-) images. The results needs to be analysed in a way to show the influence of different microstructures or gradients of the porosity found at different places in the sea urchin spine through e.g. statistical methods like the Weibull distribution. Through a correlation of microstructure and resulting mechanical response, principles can be extracted and transferred into new materials for the use not only in architecture which will be produced later on. The abstracted and simplified cellular structures are also under investigation. In the ongoing research, not only the mechanical properties are of interest, but also the possibilities to use the same or an adapted microstructure to transfer e.g. heat, or even water for the use in buildings.



Modelling approach of cellular solids of a sea urchin spine

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Multiscale Materials Modelling of Fatigue

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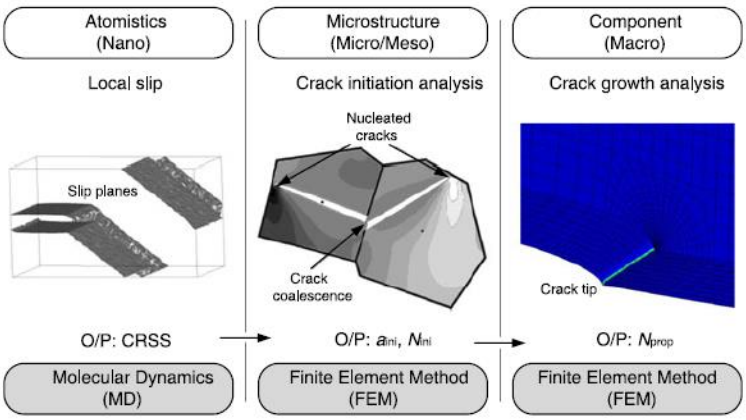
Considerable efforts have been made recently in developing numerical models for predicting fatigue lifetime of specimens and components. At the atomistic level Molecular Dynamics (MD) is able to derive the Critical Resolved Shear Stress (CRSS), on the microstructural level, the Tanaka-Mura model proves to be one of the most promising models to estimate the number of cycles for a fatigue crack to be initiated. Concerning the macro level and long crack growth predictions, there are numerous established models that produce more than acceptable results; among those is the well-known Paris law. The aim of this work is to numerically reiterate the experimental results obtained under fatigue loading by means of coupling those two levels, i.e. to simulate the complete fatigue lifetime of a flat steel specimen and further of a component under fatigue loading. Experimental input data include the material properties as well as microstructural features. Very good agreement with experiment is found for S-N-curves as well as Paris parameters.



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Two-scale finite element modelling of reinforced concrete based on first-order computational homogenization

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Crack growth in reinforced concrete is of practical importance since it directly influences the durability of the structure. Crack widths are consequently limited in design codes (e.g. [1]), and finite element modelling is a powerful tool when predicting them. However, not only the cracking of concrete must be modelled, but also the bond between the reinforcement bars and the concrete must be considered to describe crack growth correctly, cf. [2]. Multi-scale modelling may be used to alleviate the computational cost of full resolution models.
In this work, a two-scale model based on first-order computational homogenization (cf. [3, 4]) is established, where the steel reinforcement, concrete and bond between them are studied in detail. The pertinent "effective'' large-scale problem is defined, and suitable boundary conditions are outlined for the subscale problem. A nested finite element procedure, in which the large-scale solution is obtained via computational homogenization on the representative volume elements (RVEs) located at the quadrature points, is outlined. A numerical study of a reinforced concrete deep beam subjected to four point bending was carried out. RVEs with different sizes and boundary conditions (Dirichlet-Dirichlet and Dirichlet-Neumann prescribed on concrete/steel respectively) were used, and the results were compared with a fully-resolved solution.

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Multiscale approaches for topology optimization

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Topology optimization is a numerical tool for finding optimal material distributions for mechanical structures, fluids, electromagnetics, optics and many other engineering disciplines. The method consists in repeated FE simulations, adjoint sensitivity analyses and gradient-based design updates. Using element-based design variables, the approach has ultimate design freedom and is by now extensively being used in industry to save weight and/or improve dynamical response.

Fired by recent progresses in additive manufacturing techniques, multiscale topology optimization approaches have recently received intense interest and many efficient and interesting approaches have been presented.
Common challenges of multiscale schemes include lack of separation of scales, tiling of locally optimized microstructures and manufacturability.
In one approach we revisit the original homogenization-based topology optimization schemes and suggest a simple graphical projection scheme that realizes fine-grained optimal structures from coarse scale homogenization solutions.
In another approach we introduce a local volume constraint to provide porous and optimized infill structures for closed-walled 2d and 3d structures realized by additive manufacturing technologies. By adding advanced projection schemes we allow variable outer shape to be included in the design process as well. The structures provide two-scale designs without the requirement of separation of scales.

Exploration of thermo-mechanical properties of composites and interfaces with classical force fields and multiscale MD-MC approach

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MBN Explorer [1] is a multi-purpose software package designed by MBN Research Center team to study structure and dynamics of molecular systems of various degree of complexity. A broad variety of interatomic potentials implemented in the MBN Explorer allows to simulate the structure and dynamics of different molecular systems, such as atomic clusters, fullerenes, nanotubes, metallic nanomaterials, proteins and DNA, crystals, composite bio-nano systems and material intefaces, see [2] and references therein. A distinct feature of the package, which makes it significantly different from other codes, is in its universality and implemented multiscale features that make it applicable to the description of many very different Meso-Bio-Nano (MBN) systems.

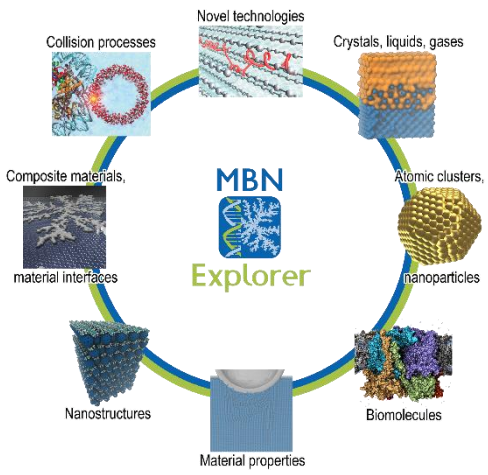

Fig. 1 Illustrative examples of MesoBioNano systems structure and dynamics of which were unravelled with MBN Explorer [1].

The talk will give an overview of the main features of the package and will highlight a number of recent case studies of composite materials and material interfaces investigated by means of MBN Explorer and a special multi-task software toolkit MBN Studio [3]. Particular attention will devoted to the modelling of thermo-mechanical properties of composites, material interfaces, phase and morphological transitions studied by means of atomistic Molecular Dynamics (MD) simulations [4], irradiation driven MD [5] and multiscale simulation techniques bases on the combined use of MD and MC (Monte Carlo) approaches [6].

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Wind turbines blade structures and composite materials: Multiscale top-down approach to damage and fracture

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Large wind turbine rotor blades are light-weight structures made of composite materials. While the elastic behavior (deflection, Eigen frequency, buckling) of rotor blades can be adequately described by beam-type models, the analysis of damage and fracture is much more challenging and requires models at various length scales. Typically, damage starts from microcracks at the fibre/matrix scale to macrocracks that can propagate along weak interfaces (delamination). The failure evolution is thus quite complex and can involve large-scale bridging, cracks shifting plane (from one interface to another) and additional cracks can develop along near-by planes.
Starting from a few cases of representative failure modes observed in blades, this presentation will identify the key damage types by going from a full scale blade to macroscale and microscale. Examples are cracking of ply-drops, (without and with fibre bridging) tunneling crack in laminates and bondlines. Analysis of these requires models and experiments at component level, macro level and microscale and the coupling between them. The role of material properties (e.g. brittle fracture versus interfaces with fibre bridging) on the growth of damages will be discussed.

Multiscale modelling of superconducters in wind turbine generators

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In [1] we have investigated the feasibility of using high temperature superconducting electromagnets in generators for wind turbines. The main goal is to increase the magnetic field substantially in order to obtain a considerably higher power output without increasing the weight of the wind turbine generator. Simulating superconducting generators is a truly multiscale problem. The action of the current is taken place at the scale of micrometers resulting in electromagnetic fields with a spatial extend of the scale of meters.

Two issues are presented in this work. First, a method to simulate the electromagnetic properties of superconductors with high aspect ratio such as the commercially available second generation superconducting YBCO tapes [2]. In a finite element implementation we have achieved accurate simulation results two orders of magnitude faster than traditional approaches by means of structured (mapped) meshes. Secondly, we have used a homogenization method to model a stack of second generation high temperature superconducting tapes under AC applied transport current. The homogenization method further improves the speedup of the simulations by two orders of magnitude [3].

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Simulation of semiconductor devices using the Atomistix ToolKit (ATK)

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Semiconductor devices are reaching a scale where single atoms begin to affect the device performance, for instance due to a small number of dopant atoms, atomic-scale defects, quantum confinement, quantum tunneling, etc. To gain insight into these phenomena atomic-scale based modelling tools are important [1]. However, still the entire device region is large on an atomic-scale and there is a need for a multi-scale approach where atomic-scale modelling is combined with traditional TCAD tools operating at the continuum length scale.

In this presentation, I will present the ATK atomic-scale simulation tool [2] and its application for device and process modelling of semiconductor devices. I will briefly describe the theoretical background of the methods and their application range. I will present different application examples of atomic-scale modelling for semiconductor devices and the integration with TCAD simulation tools.

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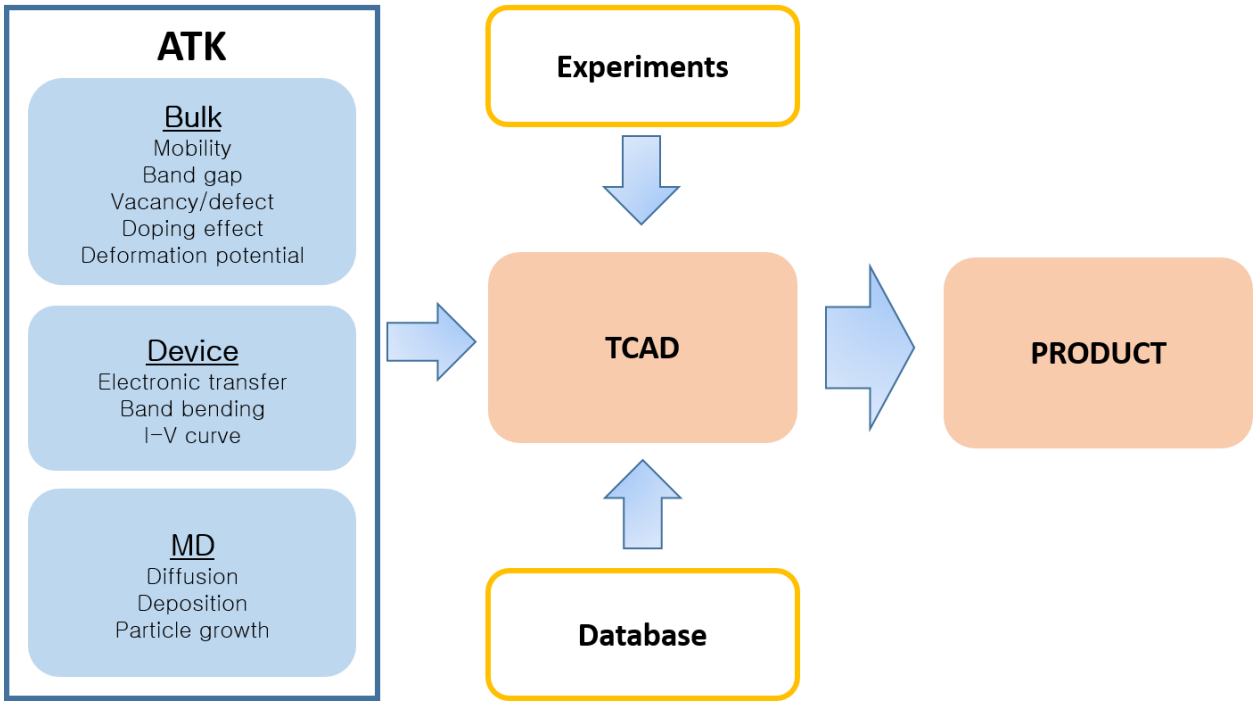

A data-driven triple-scale discrete-continuum coupling method for fractured porous media

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Many geological materials, such as shale, mudstone, carbonate rocks, limestone and rock salt are porous media in which pores of different scales may co-exist in the host matrix. When fractures initiate and propagate, the void created by the crack propagation may induce significant increase the magnitude of the permeability tensor and rotate the principal direction. At the meso-scale level, the pore-fluid inside the cracks and the pores of host matrix may interact and exchange mass, but the difference in hydraulic properties of these pores often means that a single homogenized effective permeability tensor field is insufficient to characterize the evolving hydraulic properties of these materials at smaller time scale. Furthermore, the complexity of the hydro-mechanical coupling process and the induced mechanical and hydraulic anisotropy originated from the micro-fracture and plasticity at grain scale also makes it difficult to propose separated macroscopic constitutive laws for multiphysical simulations. This article presents a data-driven technique designed to capture the multiscale hydro-mechanical coupling effect of porous media with pores of various different sizes. At each scale, data-driven models generated from supervised machine learning are hybridized with classical constitutive laws in a directed graph that represents the numerical models. By fusing experimental data with sub-scale simulations, an offline homogenization procedure is used to replace the upscaling procedure to generate cohesive laws for localized physical discontinuities at both grain and specimen scales. Through a proper homogenization procedure that preserves spatial length scales, the proposed method enables field-scale simulations to gather insights from meso-scale and grain-scale micro-structural attributes. This method is proven to be much more computational efficient than the classical DEM-FEM or

FEM2 approach while at the same time more robust and flexible than the classical surrogate modeling approach. Due to the usage of bridging-scale technique, the proposed model may provide multiple opportunities to incorporates different types of simulations and experimental data across different length scales for machine learning. Numerical issues will also be discussed.

Multifield/non--local continuum modelling of materials with microstructure: a multiscale approach

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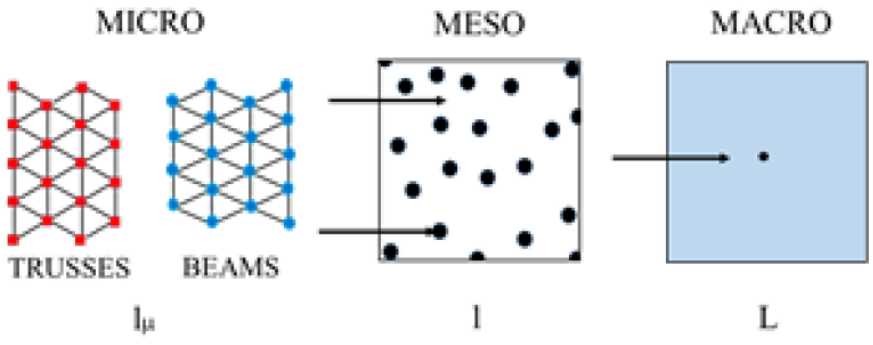
A two–steps multi-scale procedure for the study of hierarchically structured particle composites is presented. In order to provide continuous field formulations, able to properly preserve memory of the discrete and heterogeneous nature of the materials, non-classical and non-local theories are adopted and discussed. Among non-local theories, the so-called 'implicit' or 'weak' non-locality, concerning continua with extra degrees of freedom (multifield), is here accounted for.
The complex material is investigated at three scales of interest. At the finer level of description (micro), characterized by non-dilute concentration of particles, the deterministic texture of the material is considered. At the intermediate level (meso), characterized by dilute concentration of particles, the random spatial distribution is taken into account. At the macroscopic level the material is perceived as anisotropic homogeneous continuum. Consequently, two different strategies are used for the scale transitions: i) (micro/meso) a coarse-graining discrete-continuum procedure based on a generalized Cauchy–Born (Voigt-Poincaré) correspondence map and energy equivalence; ii) (meso/macro) a statistically–based homogenization procedure which exploits hierarchies of boundary value problems solution. The resulting macroscopic continuum is a micropolar continuum with internal lengths, able to account for size effects and un-symmetric stress and strain behavior.
Some applications of the mentioned approach to periodic as well as to random particle composite materials, by varying the material contrast between matrix and inclusions, will be reported and commented.



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Hierarchical microstructures in metals due to dislocation-mediated plasticity

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Dislocations are highly beneficial line defecs in the crystallographic lattice of metals. They are the carriers of plasticity and their motion is strongly linked to crystallography. During deformation, the dislocation density increases, leading to hardening but also evolution of the microstructure in the metal.
Industrial metals have a hierarchical microstructure. They are polycrystals composed of numerous grains with typical diameters of tens of micrometres. Each grain is characterised by the orientation of its crystal lattice. Initially each grain is a homogenous entity with a single orientation. As deformation proceeds by dislocation motion, each grain develops significant orientation spreads due to the interaction between the grains; the lattice of initially similarly oriented grains rotate differently (leading to intergranular orientation differences) and intragranular orientation spread also develops.
The dislocations self-assemble in dislocation boundaries inside each grain with a spacing of a few micrometres. Characteristic patterns of boundaries, typically parallel planar boundaries, form. This pattern varies substantially between grains, leading to different local properties. Finally, a boundary consists of a network of dislocations with a spacing of a few nanometers. An overview of the evolution of the hierarchical microstructure is presented with emphasis on our understanding of the underlying mechanisms.