ECCOMAS Thematic Conference

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UK Association for Computational Mechanics

University of Glasgow

FAU FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

TU/e Technische Universiteit Eindhoven University of Technology

UPEM UNIVERSITÉ PARIS-EST MARNE-LA-VALLÉE

GC GC

Welcome to Glasgow for the international ECCOMAS Thematic Conference on Computational Modeling of Complex Materials across the Scales (CMCS 2019)

About

The objective of CMCS is to elucidate cutting-edge developments in multi-scale computational modelling of complex materials, possessing distinct fine-scale structure and/or exhibiting coupled phenomena. Particular emphasis is on emergent coarse-scale behaviour due to the underlying fine-scale structure. CMCS thus focuses on both the (experimentally informed) modelling of complex fine-scale structural phenomena, and on their upscaling to coarser scales. CMCS will gather scientists from different disciplines working on scale-bridging challenges in complex materials to advance the field significantly. CMCS will foster inspiring and rewarding discussion and will serve as a platform for establishing and nurturing links between researchers.

Organisation

Paul Steinmann (University of Glasgow, UK / University of Erlangen-Nuremberg, Germany)
Andrew McBride (University of Glasgow, UK)
Marc Geers (Eindhoven University of Technology, The Netherlands)
Julien Yvonnet (Université Paris-Est, France)

General Information

Lunch options

There are numerous lunch options in the vicinity of the conference venues. These include options at the University (One A The Square), sandwich shops, and restaurants. Lunch will only be provided on Tuesday.

Tuesday 1st October

The conference will start at 08:15 with registration from 08:00. All sessions on Tuesday will take place in the Senate Room https://goo.gl/maps/h2cxbGnugb9Ku5rbA .

Lunch will be provided on Tuesday only.

The conference reception (drinks and canapés will be served) and poster session will take place from 19:00 at Òran Mór (a 10-minute walk from the Senate Room) https://goo.gl/maps/EH6B5Kapm5cv8YHv6 .

We ask that all poster presenters arrive at Òran Mór by 18:30 to mount their posters.

Wednesday 2nd October

The morning sessions will take place in the Senate Room. The afternoon sessions will take place in Òran Mór.

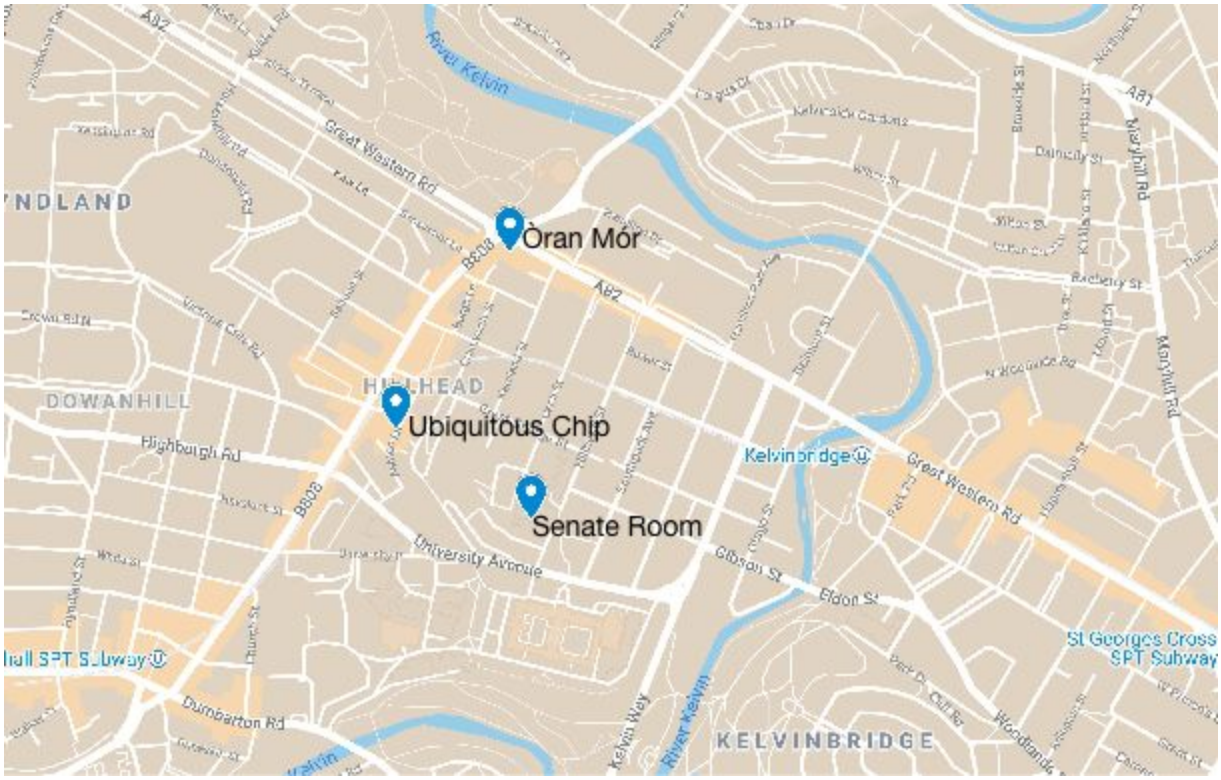
Thursday 3rd October

All sessions will take place in the Senate Room.

The conference dinner will take place at the Ubiquitous Chip (a 5-minute walk from the Senate Room) in the lively Ashton Lane – a hidden gem filled with pubs and restaurants, and well worth exploring before and after the dinner - https://goo.gl/maps/NUiAV14EfhqBB6MW8 .

Friday 4th October

All sessions will take place in the Senate Room. The conference will close at 12:30.



Programme

		1 October **Tue**	2 October **Wed**	3 October **Thurs**	4 October **Fri**
8:00	8:30	**Registration**	**Registration**		
8:15	8:30	**Opening**			
8:30	9:00	Tue-I (4)	Wed-I (4)	Thurs-I (4)	Fri-I (4)
9:00	9:30				
9:30	10:00				
10:00	10:30				
10:30	11:00	**Tea / Cofee**			
11:00	11:30	Tue-II (4)	Wed-II (2)	Thurs-II (3)	Fri-II (3)
11:30	12:00				
12:00	12:30		**Lunch**	**Lunch**	
12:30	13:00				
13:00	13:30	**Lunch**			
13:30	14:00		Wed-III (4)		
14:00	14:30	Tue-III (4)		Thurs-III (4)	
14:30	15:00				
15:00	15:30				
15:30	16:00		**Tea / Cofee**		
16:00	16:30	**Tea / Cofee**	Wed-IV (3)	**Tea / Cofee**	
16:30	17:00	Tue-IV (3)		Thurs-IV (3)	
17:00	17:30				
17:30	18:00				
19:00		**Reception**		**Dinner**	

		1 October **Tue**	2 October **Wed**	3 October **Thurs**	4 October **Fri**
8:00	8:30	**Registration**	**Registration**		
8:15	8:30	**Opening**			
8:30	9:00	Pearce	Bargmann	Llorca	Limbert
9:00	9:30	Deshpande	Poh	Sigmund	Linder
9:30	10:00	Sab	Peerlings	Allaire	Stupkiewicz
10:00	10:30	Wieners	Kouznetsova	Terada	Heltai
10:30	11:00	**Tea / Cofee**			
11:00	11:30	Cho	Oliver	Basoalto	Reese
11:30	12:00	Oterkus	Simone	Böhlke	Bangerth
12:00	12:30	Javili		Zeman	Garikipati
12:30	13:00	Holzapfel	**Lunch**		
13:00	13:30	**Lunch**		**Lunch**	
13:30	14:00		Fritzen		
14:00	14:30	Stainier	Gudmundson	Larsson	
14:30	15:00	Kiefer	Hackl	Jänicke	
15:00	15:30	Klusemann	Niordson	Cottereau	
15:30	16:00	Svendsen	**Tea / Cofee**	Ibrahimbegovic	
16:00	16:30	**Tea / Cofee**	Dunne	**Tea / Cofee**	
16:30	17:00	Gil	Menzel	Pandolfi	
17:00	17:30	Keip	Steeb	Noels	
17:30	18:00	Jabareen		Korelc	
19:00		**Reception**		**Dinner**	

Notes:

The sessions Wed-III and Wed-IV and the reception will take place at Oran Mor

Lunch will be provided on Tues 1 Otober

Tuesday - I

Pearce - *Configurational mechanics for modelling continuous crack propagation in heterogeneous materials*
Deshpande - *Hydrogen induced fast-fracture*
Sab - *Atomistic processes of brittle failure initiation*
Wieners - *A mesoscale continuum approach of dislocation dynamics and the approximation by a Runge-Kutta discontinuous Galerkin method*

Tuesday - II

Cho - *Bridging Scale between CG MD and Continuum FEM in Photo-Responsive Polymer: Smectic, Nematic, and Isotropic phases*
Oterkus - *Recent Advances in Peridynamics Research*
Javili - *Continuum-kinematics-inspired peridynamics*
Holzapfel - *Advances in the Modeling of Fiber-reinforced Solids: Application to Fibrous Tissues*

Tuesday - III

Stainier - *Effective transient behaviour of heterogeneous media in diffusion problems*
Kiefer - *Computational Approaches to the Modeling of Multiferroic Solids with Evolving Microstructure*
Klusemann - *Combined experimental-numerical study along process-structure-property-performance chain*
Svendsen - *Geometrically exact phase field chemomechanics for multiphase, multicomponent defective solids*

Tuesday - IV

Gil - *Large strain electro-mechanics based on convex multi-variable strain energies and application to composite materials*
Keip - *Pattern transformations of soft solids: from magneto-electro-active elastomers to hydrogels*
Jabareen - *Computational multiphysics model for electro-active polymers*

Wednesday - I

Bargmann - *Tailoring lightweight materials: on tunable auxeticity and elastomechanical symmetry*
Poh - *A micromorphic computational homogenization framework for tetra-chiral auxetics*
Peerlings - *A micromorphic homogenization strategy for mechanical metamaterials*
Kouznetsova - *Multi-scale modelling of emergent dynamic behaviour of metamaterials*

Wednesday - II

Oliver - *Fighting the “tyranny of scales” in hierarchical non-linear multi-scale modeling of materials: the HR-FE2 technique*
Simone - *Accelerating finite element simulations of history-dependent materials by means of model order reduction and artificial neural networks*

Wednesday - III

Fritzen - *Adaptive data-driven surrogate models for FE Square Reduced simulations*
Gudmundson - *Strain gradient plasticity model based on dislocation mechanics*
Hackl - *A relaxation-based approach to damage modeling*
Niordson - *Modeling size-effects in void growth to coalescence*

Wednesday - IV

Dunne - *Micromechanics and mechanistic modelling of fatigue crack growth*
Menzel - *Modelling of curvature effects in fibre-reinforced composites*
Steeb / Schmidt -

Thursday - I

LLorca - *A roadmap for multiscale modelling of precipitation and precipitation hardening in metallic alloys from first principles simulations*
Sigmund - *On optimal design and structural performance of multiscale structures*
Allaire - *Optimal design of modulated and oriented lattice materials by the homogenization method*
Terada - *PCA-based computational homogenization for nonlinear elasticity*

Thursday - II

Basoalto -
Böhlke - *Texture-based Modeling of Phase-specific Residual Stresses in Duplex Steels*
Zeman - *Wang tilings for computational micromechanics*

Thursday - III

Larsson - *On Error-Controlled Numerical Model Reduction for Computational Homogenization*
Jänicke - *Homogenization and numerical model reduction of fine-scale poroelasticity towards a poro-viscoelastic macro-scale model*
Cottereau - *Improving the convergence rate of a non-intrusive stochastic coupling scheme*
Ibrahimbegovic - *Coupled mechanics-probability multiscale computational framework for massive composite structures safety*

Thursday - IV

Pandolfi - *A microstructured brittle damage model for the simulation of laboratory tests*
Noels - *An inverse Mean-Field-Homogenization-based micro-mechanical model for stochastic multiscale simulations of unidirectional composites*
Korelc -*Sensitivity analysis based multi-scale methods of coupled path-dependent problems*

Friday - I

Limbert - *A computational approach to unravel the interplay of structural and material properties of skin*
Linder - *A micro-macro approach to study the effect of strain induced crystallization on the fracture onset of rubber-like materials*
Stupkiewicz - *Diffuse-interface modelling of transformation patterns in shape-memory alloys at micro- and macro-scale*
Heltai - *Multiscale modeling of vascularized and fiber reinforced tissues via non-matching immersed methods*

Friday - II

Reese - *Data-driven mechanics, model order reduction, and hierarchical tensor approximation – suitable methods to cross the scales?*
Bangerth - *Supporting complex simulations with open source finite element software*
Garikipati - *A graph theoretic framework for representation, exploration and analysis on computed states of physical systems*

Poster Presentations by Young Researchers

Ankush Aggarwal - *GCEC, University of Glasgow*

Madie Victoria Allen - *National Structural Integrity Research Centre (NSIRC), Brunel University*

Ignatios Athanasiadis - *GCEC, University of Glasgow*

Christophe Chalons - *GCEC, University of Glasgow*

Anna Magdalena de Villiers - *Stellenbosch University*

Heleen Fehervary - *GCEC, University of Glasgow*

Sebastian Gajek - *Karlsruhe Institute of Technology - Institute of Engineering Mechanics - Chair for Continuum Mechanics*

Philipp Gebhart - *Institute of Solid Mechanics, Technische Universität Dresden*

Ludwig Herrnböck - *LTM, Friedrich-Alexander Universität Erlangen-Nürnberg*

Dominik Horny - *Karlsruhe Institute of Technology, Institute for Applied Materials - Computational Materials Science*

Chun Hean Lee - *GCEC, University of Glasgow*

Karol Lewandowski - *GCEC, University of Glasgow*

Zhaowei Liu - *University of Glasgow*

Hoang Nguyen - *GCEC, University of Glasgow*

Son Pham-Ba - *École polytechnique fédérale de Lausanne*

Marion Picquart - CentraleSupelec & ArianeGroup

Maximilian Ries - *LTM, Friedrich-Alexander Universität Erlangen-Nürnberg*

Callum Runcie - *GCEC, University of Glasgow*

Prashant Saxena - *GCEC, University of Glasgow*

Tom Shire - *GCEC, University of Glasgow*

Andrei Shvarts - *GCEC, University of Glasgow*

Chris Triantafyllou - *Materials and Manufacturing Research Group, University of Glasgow*

Luan Trinh - *Bernal Institute, University of Limerick*

Mebratu Fenta Wakeni - *GCEC, University of Glasgow*

Xiong Wan - *Tsinghua University*

Maxence Wangemez - *LMT-Cachan/ENS-Cachan/CNRS/Université Paris-Saclay*

Ross Williams - *Materials and Manufacturing Research Group, University of Glasgow*

Abstracts - Invited Oral Presentations

Tuesday - I

Pearce - *Configurational mechanics for modelling continuous crack propagation in heterogeneous materials*

Deshpande - *Hydrogen induced fast-fracture*

Sab - *Atomistic processes of brittle failure initiation*

Wieners - *A mesoscale continuum approach of dislocation dynamics and the approximation by a Runge-Kutta discontinuous Galerkin method*

Configurational mechanics for modelling continuous crack propagation in heterogeneous materials

Chris J. Pearce
H. Nguyen, K. Lewandowski, A. Shvarts, I. Athanasiadis and Ł. Kaczmarczyk
Glasgow Computational Engineering Centre, University of Glasgow

Configurational mechanics (CM) provides the theoretical basis for modelling crack propagation in brittle materials. The local form of the first law of thermodynamics provides an equilibrium condition for the crack front, expressed in terms of the configurational forces and material resistance. Applying the principle of maximal energy dissipation, the direction of crack propagation is given by the direction of the configurational forces. An implicit crack propagation formulation has subsequently been developed that exploits the crack front equilibrium condition to continuously update the position of the evolving crack front.

In classical fracture mechanics, well-established stress intensity factors are not, in general, applicable in the case of heterogeneous materials, since an analytical solution for the stress field in the vicinity of the crack front does not exist. In the current work, the authors' previous formulation [1] has been extended to incorporate the influence of heterogeneous materials in the form of spatially varying material stiffness. The result is an additional force that drives the crack front from stiff to less stiff material. In the case of homogeneous materials, with uniform stiffness distribution, this additional force is zero.

A monolithic solution strategy is adopted, solving simultaneously for both the material displacements (i.e. crack extension) and the spatial displacements. The resulting crack path is resolved as a discrete displacement discontinuity, where the material displacements of the nodes on the crack front change continuously, without the need for significant refinement of mesh around the crack front or the use of enrichment techniques. In order to trace the dissipative loading path, an arc-length procedure is adopted that controls the incremental crack area growth. In order to maintain mesh quality, smoothing of the mesh is undertaken as a continuous process. Hierarchical basis functions of arbitrary polynomial order are adopted to (a) increase the order of approximation without the need to change the finite element mesh and (b) to aid the use of mult-grid solvers. Performance of the formulation is demonstrated by means of several representative numerical simulations, demonstrating both accuracy and robustness.

[1] Ł. Kaczmarczyk, Z. Ullah, C. J. Pearce, Energy consistent framework for continuously evolving 3D crack propagation, Computer Methods in Applied Mechanics and Engineering 324 (2017) 54–73.

Hydrogen induced fast-fracture

S. S. Shishvan, G. Csányi and V.S. Deshpande
Department of Engineering, University of Cambridge, Cambridge CB2 1PZ, UK

One of the recurring anomalies in the hydrogen induced fracture of high strength steels is the apparent disconnect between the toughness and the tensile strength of un-notched bars. Here we propose, supported by detailed atomistic and continuum calculations, that unlike macroscopic toughness, hydrogen-mediated tensile failure is a result of a fast-fracture mechanism. Specifically, we show that failure originates from the fast propagation of cleavage cracks that initiate from cavities that form around inclusions such as carbide particles. The failure process occurs in two stages. In stage-A, hydrides rapidly form around the roots of stressed notches on the cavity surfaces with hydrogen fed from the hydrogen gas within the cavity. These hydrides promote cleavage fracture with the cracks propagating at >100 m/s until the hydrogen gas in the cavity is exhausted. Predictions of this hydrogen-assisted crack growth mechanism are supported by atomistic calculations of binding energies, mobility barriers and molecular dynamics calculations of the fracture process.

Typically, cracks grow by less than 1 μm via this hydrogen-assisted mechanism and thus insufficient to cause macroscopic fracture of the specimen. However, this stage is then followed by a stage-B process where these fast propagating cracks can continue to grow, now in the absence of hydrogen supply, given an appropriate level of remote tensile stress. This is surprising because the fracture energy is now that of Fe in the absence of H and cleavage fracture requires opening tractions on the order of 15 GPa to be generated. Thus, fracture is usually precluded due to plasticity around the crack-tip. However, we show via macroscopic continuum crack growth calculations in a rate dependent elastic-plastic solid with fracture modelled using a cohesive zone that cleavage is possible if the crack propagates fast enough. This is because strain-rates at the tips of fast propagating cracks are sufficiently high for the drag on the motion of dislocations resulting from phonon scattering to limit plasticity.

This combined atomistic/continuum model is used to explain a host of well-established experimental observations including (but not limited to): (i) insensitivity of the strength to the concentration of trapped hydrogen; (ii) the extensive microcracking in addition to the final cleavage fracture event and (iii) the higher susceptibility of high strength steels to hydrogen embrittlement.

Atomistic processes of brittle failure initiation

S. Souguir, L. Brochard and K. Sab
Laboratoire Navier (ENPC, IFSTTAR, CNRS UMR 8205)

Brittle failure is ubiquitous in civil engineering materials from concrete to rocks and faults. And yet, how brittle failure initiates is still debated. While the failure of pre-cracked bodies is predicted by an energy criterion (fracture mechanics), that of flawless materials is usually given by a stress criterion, and no clear scientific consensus exists about intermediate cases [1,2].

In this work, we use atomistic simulation techniques to investigate the elementary mechanisms behind brittle failure. We study graphene, which is one of the few materials with a sufficiently small process zone size to be addressed by molecular simulations. In a preliminary study, we found that the failure behavior of graphene can overcome both strength and toughness in situations of very high or low stress concentrations, respectively; which is consistent with one particular theory, namely finite fracture mechanics which considers crack initiation as the unstable nucleation of a crack over a finite length [3].

To further investigate the atomic processes of failure, we consider the athermal limit (0K). Since atomic interactions are conservatives, failure can be viewed as an instability arising when one of the eigenvalues of the hessian matrix becomes negative. And the associated eigenvector provides a description of the elementary mechanism of failure (mode of failure) [4]. The mode of failure in absence of stress concentration exhibits collective movements of the atoms, separating infinite failure bands. In contrast, the mode of failure in presence of stress concentrations is highly localized in a domain corresponding to the process zone. Another key change with stress concentration is the degeneracy of the mode of failure. The smallest eigenvalue is highly degenerated in absence of stress concentration, but little or not degenerated for high stress concentrations. Degeneracy becomes important at non-zero temperature, since it explains the difference of scaling of strength and toughness with respect to system size. Indeed, degeneracy quantifies the number of transition states to failure. Through an extensive study over many time and length scales, we identify a temperature-time-size equivalence that can be formalized by a universal scaling law of strength and toughness, extending Zhurkov's theory to size effects [5]. Interestingly, the scalings of strength and toughness differ only regarding the scaling in size, which can be formally related to the degeneracy of the negative eigenvalues in the athermal limit.

[1] Romani et al. (2015). Eur. J. Mech. A-Solid, 51, 172–182
[2] Nguyen et al. (2016) Int. J. Fracture, 197(2), 213–226
[3] Brochard et al. (2016) JMPS, 95, 632–646
[4] Souguir et al. (2019) Atomistic processes of brittle failure initiation in the athermal limit, in preparation

A mesoscale continuum approach of dislocation dynamics and the approximation by a Runge-Kutta discontinuous Galerkin method

Christian Wieners, Lydia Wagner and Katrin Schulz
Institute for Applied and Numerical Mathematics, KIT
Institute for Applied and Numerical Mathematics, KIT
Institute for Applied Materials - Computational Materials Science, KIT

We consider a mesoscale continuum model for the evolution of dislocation density in small-strain crystal plasticity. The model is based on the continuum dislocation dynamics theory and extended by a formulation for impenetrable grain boundaries. We introduce a fully coupled numerical method combining a conforming finite element approximation of elasto-plasticity with an implicit Runge-Kutta discontinuous Galerkin discretization of the dislocation microstructure which allows for 3d~computations including multiple slip systems and dislocation interaction.

In our scheme, we use an explicit coupling scheme by alternately incrementing the dislocations solving the CDD system, and then updating the plastic strain by a flow rule depending on the dislocations and the stress which results from the equilibrium equation for the displacement. In our numerical model we consider the 3d dislocation density evolution for face-centered cubic (fcc) crystals with 12 slip systems. Similar to DDD, grain boundaries are modeled as impenetrable obstacles retaining dislocations in the respective grain. By this means, a continuum plasticity model is accomplished including a physically based representation of grain boundaries. The theory is validated considering a fcc tricrystal under tensile loading showing that dislocation density gradients close to the boundary can be reproduced dependent on the grain orientations without additional fitting parameters. The numerical results are compared with DDD simulations derived in the literature.

Tuesday - II

Cho - *Bridging Scale between CG MD and Continuum FEM in Photo-Responsive Polymer: Smectic, Nematic, and Isotropic phases*

Oterkus - *Recent Advances in Peridynamics Research*

Javili - *Continuum-kinematics-inspired peridynamics*

Holzapfel - *Advances in the Modeling of Fiber-reinforced Solids: Application to Fibrous Tissues*

Bridging Scale between CG MD and Continuum FEM in Photo-Responsive Polymer: Smectic, Nematic, and Isotropic phases

Maenghyo Cho, Junghwan Moon and Hayoung Chung
Department of Mechanical and Aerospace Engineering, Seoul National University, Seoul, Korea
Department of Mechanical and Aerospace Engineering, Seoul National University, Seoul, Korea
Department of Structural Engineering, University of California, San Diego, USA

Liquid crystalline polymer (LCP) networks containing azobenzene molecules are complex and novel materials which can exhibit large and reversible deformations in response to the light energy. These photo-responsive polymers (PRPs) have been promising materials for soft photo-actuators. The difficulty in design and prediction of the macroscopic photo-deformations originates from the multiscale nature of phenomenon.

We have developed a multiscale analysis framework which combines the density functional theory (DFT), all-atom molecular dynamics (AA MD), and finite element method (FEM). However, the AA MD, an intermediate molecular scale simulation, has limitations of massive computational costs for describing diverse mesoscale morphologies, such as liquid crystalline (LC) phase, the spacer length, and crosslinking density of the polymer. Therefore, we utilized the coarse-grained molecular dynamics (CG MD) simulations to effectively reduce the number of degrees of freedom. The mesoscale photo-isomerization interaction potential is constructed by using the iterative Boltzmann inversion (IBI) method, which targets the structural changes induced by the photo-isomerization. Then, the light-induced LC phase transition (smectic A (Sm A) – nematic (N) – isotropic (I)) is successfully realized, which cannot be captured by conventional MD simulations. The light-induced microscopic deformation and mechanical softening parameters obtained by the CG MD is upscaled to the continuum scale governing equations. Finally, the continuum FEM is utilized to predict the variation in temporal photo-deformation path in terms of the micro-morphology of the PRP.

We expect our scale-bridging framework can expand the capability of computational mechanics in the research field of photo-responsive smart materials.

Acknowledgements
This work was supported by a grant from the National Research Foundation of Korea (NRF) funded by the Korea government (MSIP) (Grant No. 2012R1A3A20488 41).

Recent Advances in Peridynamics Research

Erkan Oterkus
University of Strathclyde, Glasgow, UK

Peridynamics is a new continuum mechanics formulation. Although it was originally introduced for structural analysis mainly to predict failure in structures, it has been extended to many different fields including heat transfer, diffusion modelling, porous flow, etc. which makes it a powerful tool for multiphysics analysis with damage prediction capability. Moreover, due to the non-local aspect of the formulation, it has a potential to be used for non- local modelling and it is a suitable candidate for multiscale analysis. During the recent years, there is a significant interest on peridynamics at different parts of the world. In parallel, the peridynamic community is expanding and there is a rapid progress in peridynamic research. Several novel methods were recently introduced including peridynamic differential operator and dual-horizon concept. Moreover, several efficient numerical solution techniques for the solution of peridynamic equations have been recently proposed. In addition, peridynamics has been applied for the analysis of complex materials including composite materials, ice, etc. Hence, in this presentation, some recent advances in peridynamics research will be highlighted.

Continuum-kinematics-inspired peridynamics

Ali Javili, Andrew McBride and Paul Steinmann
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Glasgow Computational Engineering Centre, School of Engineering, University of Glasgow, Glasgow G12 8QQ, United Kingdom
Chair of Applied Mechanics, University of Erlangen-Nuremberg, Egerland Str. 5, 91058 Erlangen, Germany / Glasgow Computational Engineering Centre, School of Engineering, University of Glasgow, Glasgow G12 8QQ, United Kingdom

The main objective of this presentation is to develop a novel continuum-kinematics-inspired approach for peridynamics (PD), and to revisit PD's thermodynamic foundations. We distinguish between three types of interactions, namely, one-neighbour interactions, two-neighbour interactions and three-neighbour interactions. While one-neighbour interactions are equivalent to the bond-based interactions of the original PD formalism, two- and three-neighbour interactions are fundamentally different to state-based interactions in that the basic elements of continuum kinematics are preserved exactly. In addition, we propose that an externally prescribed traction on the boundary of the continuum body emerges naturally and need not vanish. This is in contrast to, but does not necessarily violate, standard PD.

We investigate the consequences of the angular momentum balance and provide a set of appropriate arguments for the interactions accordingly. Furthermore, we elaborate on thermodynamic restrictions on the interaction energies and derive thermodynamically-consistent constitutive laws through a Coleman-Noll-like procedure. Notably, we show that various choices for temperature or coldness satisfy the dissipation inequality and provide meaningful temperature or coldness evolution equations together with Fourier-like conduction equations.

Advances in the Modeling of Fiber-reinforced Solids: Application to Fibrous Tissues

Gerhard A. Holzapfel, Kewei Li and Ray W. Ogden
Institute of Biomechanics, Graz University of Technology, Austria
Department of Structural Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway
School of Mathematics and Statistics, University of Glasgow, Glasgow, Scotland, UK

Fiber-reinforced solids are composed of a matrix material, which is reinforced by fibers of one or more families or by distributions of fibers with different orientations. In fibrous tissues such fibers are collagen, and typically the matrix material consists of elastic fibers. For example, for arterial walls the matrix can be considered as an isotropic (neo-Hookean) material, while the collagen fibers, which are in general not perfectly aligned but are arranged in a rather dispersed structure, generate anisotropy (for a review see, e.g., [1]). It is important to note that the collagen fabric can be damaged/disrupted by various diseases.

A method of choice is to base constitutive models on a multiscale approach in which it is important to integrate simulations and experiments in order to achieve a detailed understanding of the influences of the various constituents. After reviewing structural aspects of fibrous tissues, we present a recently documented multiscale model of fiber recruitment and damage with a discrete fiber dispersion method [2]. The model is based on the triangular discretization of a unit sphere with a finite number of elementary areas. Over each elementary area we define a representative fiber direction and an elementary fiber density based on the fiber dispersion. In brief, summation of the fiber contributions from all the elementary areas yields the resultant fiber strain energy, which can easily accommodate the exclusion of compressed fibers. Fiber recruitment, softening and damage are considered. The model framework was implemented into FEAP and illustrated with representative examples.

[1] G.A. Holzapfel and R.W. Ogden. Biomechanical relevance of the microstructure in artery walls with a focus on passive and active components. Am. J. Physiol. Heart Circ. Physiol., 315:H540-H549, 2018.
[2] K. Li and G.A. Holzapfel. Multiscale modeling of fiber recruitment and damage with a discrete fiber dispersion method. J. Mech. Phys. Solids, 126:226-244, 2019.

Tuesday - III

Stainier - *Effective transient behaviour of heterogeneous media in diffusion problems*

Kiefer - *Computational Approaches to the Modeling of Multiferroic Solids with Evolving Microstructure*

Klusemann - *Combined experimental-numerical study along process-structure-property-performance chain*

Svendsen - *Geometrically exact phase field chemomechanics for multiphase, multicomponent defective solids*

Effective transient behaviour of heterogeneous media in diffusion problems

Laurence Brassart and Laurent Stainier
Department of Materials Science and Engineering, Monash University, Australia
Institut de Recherche en Génie Civil et Mécanique (GeM, UMR 6183 CNRS/ECN/UN) École Centrale Nantes, France

We are interested in describing the effective transient diffusion behaviour in heterogeneous media in which there is a large contrast between the phase diffusivities. In this case mobile species can diffuse over long distances through the fast phase in the time scale of diffusion in the slow phase. At macroscopic scale, contrasted phase diffusivities lead to a memory effect that cannot be properly described by classical Fick's second law. Here we obtain effective governing equations through a two-scale approach for composite materials consisting of a fast matrix and slow inclusions. The micro-macro transition is similar to first-order computational homogenisation, and involves the solution of a transient diffusion boundary-value problem in a Representative Volume Element of the microstructure.

Different from computational homogenisation, we propose a semi-analytical mean-field estimate of the composite response based on the exact solution for a single inclusion. A key outcome of the model is that the macroscopic concentration is not one-to-one related to the macroscopic chemical potential, but obeys a local kinetic equation associated with diffusion in the slow phase. The history-dependent macroscopic response admits a representation based on internal variables, enabling efficient time integration. We show that the local chemical kinetics can result in non-Fickian behaviour in macroscale boundary-value problems. The model is based on analytical solutions of transient diffusion in inclusions, which are limited to the linear case. The presentation will end with a discussion on perspectives for handling the non-linear case, through computational homogenization and data-driven approaches.

Computational Approaches to the Modeling of Multiferroic Solids with Evolving Microstructure

Bjoern Kiefer
TU Bergakademie Freiberg

The term multiferroic classfies materials that exhibit combinations of ferroelastic (spontaneous straining), ferroelectric (spontaneous polarization), or ferromagnetic (spontaneous magnetization) properties, which occur in the context of solid-solid phase transitions. The complex effective behavior of such materials is usually directly correlated to the formation of microstructures (crystallographic patterns, domains), and their dissipative, i.e.~loading history dependent, evolution.

This contribution discusses constitutive modeling approaches that effectively account for microstructure evolution in ferroic materials and build on local and global variational principles, where a special focus is placed on their numerical treatment. Ferromagnetic materials are particularly challenging in this context, since they are known to form domain patterns in a manner that minimizes the energy stored in the entire demagnetization field. While this effect is naturally incorporated in micromagnetic approaches, macroscopic models seldomly explicitly account for it. Macroscopic phenomenological approaches are, in fact, typically local in nature, which from a numerical standpoint means that updates of the dependent state variables (stress, magnetic induction) can be computed at the material point level. This is no longer possible, if the magnetostatic energy in the whole domain must be known to propagate the constitutive quantities, such as the magnetization field, in time.

To address this, a finite element framework is proposed that incorporates variables parameterizing the microstructure as nodal degrees of freedom, whose evolution is governed by a global stationarity problem. A particular challenge in such an approach is that inequality constraints (optimality conditions, range limitations) must be enforced on the finite element level. We present the successful implementation of a complementarity function based scheme, that converts the problem into a dual unconstrained setting and introduces the associated Lagrange multipliers as additional nodal quantities. As a particular application of this general methodology, a recently established energy-relaxation based model for magnetic shape memory behavior was implemented and tested. Numerical examples are provided to demonstrate the predictive capabilities of the suggested framework in the context of simulating single-crystalline MSMA responses under complex loading conditions and strong dependence on sample geometry.

Combined experimental-numerical study along process-structure-property-performance chain

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The understanding of the process-(micro)structure-property-performance relation is crucial for the application of complex processes for high performance materials. To interpret and model the behavior of the material or structure across different length scales, enables to choose suitable process parameters or to design optimal structural properties. However, this requires analyzing and understanding the interactions of different, even competing mechanisms at different scales, which in turn are depending on a number of factors such as chemical composition, initial microstructures or loading conditions. To address these challenges, a multidisciplinary approach is needed where experiments and numerical models are linked strongly. In this regard, the talk will provide examples of combined experimental-numerical studies at different scales connected to technological processes such as forming, welding or local modification techniques. A successful example along the process-structure-property-performance chain, starting with the process parameters and finally predicting the fatigue behavior based on a multi-step simulation strategy, will be given.

Geometrically exact phase field chemomechanics for multiphase, multicomponent defective solids

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The School of Materials, University of Manchester, U.K.
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In this work, a continuum framework is developed for the chemomechanical modeling of defective solids containing multiple chemical components diffusing among multiple solid phases (Svendsen et al., J. Mech. Phys. Sols., 112, 619, 2018). In particular, solid phase modeling is based on a chemomechanical free energy and stress relaxation via the evolution of phase-specific concentration fields, order-parameter fields, and internal variables. At the mixture level, differences or contrasts in phase composition and phase local deformation in phase interface regions are treated as mixture internal variables whose evolution toward equilibrium is relaxational. In this context, three different interface models are considered. Besides a simple "thick" or "bulk" interface case, these include two models for "thin" interfaces. In the equilibrium limit, the corresponding "relaxed" values of phase contrasts in composition and local deformation in the interface region are determined via (bulk) energy minimization.

On the chemical side, the equilibrium limit of the current model formulation reduces to a multiple component, multiple phase generalization of the two-phase binary alloy interface equilibrium conditions of Kim et al. (Phys. Rev. E 60, 7186, 1999). On the mechanical side, the equilibrium limit of the bulk interface model represents a multiple-component, multiple-phase generalization of Reuss-Sachs conditions from mechanical homogenization theory (i.e., equal phase stresses: e.g., Steinbach and Apel, Physica D, 153, 2006). Analogously, those of the "thin" interface models represent multiple-component, multiple-phase generalizations of interface equilibrium conditions consistent with interface kinematic compatibility and mechanical equilibrium (e.g., Mosler et al., J. Mech.~Phys. Sols.~68, 251, 2014; Durga et al., Comp. Mat.~Sci. 99, 81, 2015, Schneider et al., Comp. Mec.~60, 203, 2017, Kiefer et al., Int. J. Numer. Meth. Engng., 112, 1097, 2017). A number of examples will be given.

Tuesday - IV

Gil - *Large strain electro-mechanics based on convex multi-variable strain energies and application to composite materials*

Keip - *Pattern transformations of soft solids: from magneto-electro-active elastomers to hydrogels*

Jabareen - *Computational multiphysics model for electro-active polymers*

Large strain electro-mechanics based on convex multi-variable strain energies and application to composite materials

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Dielectric Elastomers (DE) are a class of Electro Active Polymers with outstanding actuation properties. Voltage induced area expansions of 1980% on a DE membrane have been recently reported. In this case, the electromechanical instability is harnessed as a means for obtaining these electrically induced massive deformations with potential applications in soft robots. Computational simulation in this context becomes extremely challenging [2] and must be addressed ab initio by the definition of well-posed constitutive models. For instance, the authors postulated a new Convex Multi-Variable (CMV) definition of the electromechanical internal energy for single-phase dielectric elastomers. Crucially, this definition guarantees material stability or, equivalently, the ellipticity condition for the entire range of deformations and electric fields.

It has also been reported that the performance of dielectric elastomers can be dramatically improved when they are designed and arranged in composite configurations. This presentation focuses on the general description of a new computational framework for CMV-based constitutive models and its initial extension to the case of composite multi-layered dielectric elastomers.

A series of highly demanding numerical examples (i.e. including onset and propagation of wrinkles) will be presented in order to demonstrate the performance of the new computational framework.

Pattern transformations of soft solids: from magneto-electro-active elastomers to hydrogels

Marc-Andre Keip and Elten Polukhov

University of Stuttgart, Department of Civil and Environmental Engineering, Institute of Applied Mechanics

We discuss instability phenomena of soft solids with periodic microstructures. Depending on the material, instabilities can be triggered by different means. In a first part of the talk, we analyse elecrically and magnetically induced pattern transformations of heterogeneous microstructures containing particles and voids. As example materials we consider electroactive polymers and magnetorheological elastomers. In a second part, we discuss pattern transformations of periodic hydrogels in the realm of transient dissipative processes. Both parts rely on numerical implementations of Bloch-Floquet wave analysis into a finite-element setting.

[1] G. Geymonat, S. Müller and N. Triantafyllidis. Homogenization of nonlinearly elastic materials, microscopic bifurcation and macroscopic loss of rank-one convexity. Archive for Rational Mechanics and Analysis 122:231-290 (1993)
[2] K. Bertoldi, M. Boyce, S. Deschanel, S. Prange and T. Mullin. Mechanics of deformation-triggered pattern transformations and superelastic behavior in periodic elastomeric structures. Journal of the Mechanics and Physics of Solids 56:2642-2668 (2008)
[3] C. Tipton, E. Han and T. Mullin. Magneto-elastic buckling of a soft cellular solid. Soft Matter 8:6880-6883 (2012)
[4] Wu, G., Xia, Y., Yang, S. Buckling, symmetry breaking, and cavitation in periodically micro-structured hydrogel membranes. Soft Matter 10:1392-1399 (2014)
[5] Polukhov, E., Vallicotti, D., Keip, M.-A. Computational stability analysis of periodic electroactive polymer composites across scales. Computer Methods in Applied Mechanics and Engineering 337:165-197 (2018)

Computational multiphysics model for electro-active polymers

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Faculty of Civil and Environmental Engineering Technion - Israel Institute of Technology

Electro-active polymers (EAPs) are an emerging class of soft active materials, which may experience large deformations when they are subjected to an external electric field. EAPs are inexpensive light-weight polymeric materials, therefore, they are considered ideal candidates for high performance and low-cost engineering applications. A typical actuator of EAPs consist of a thin film, which is sandwiched between two flexible electrodes coating its major surfaces. Applying an electric potential difference through the thickness, causes thinning of the film and lateral expansion. These changes occur due to Coulomb forces between the opposite charges that accumulate on the major surfaces when an external field is applied. VHB is one of the most promising dielectric elastomers, which has a great potential for being incorporated in EAP based actuators. Therefore, different experimental works (e.g. single step relaxation tests, multi-step relaxation tests and loading-unloading cyclic tests) were carried out in order to provide a comprehensive mechanical and electrical characterization of VHB. With regard to the computational aspect, one of the important features that should be taken into account while developing the finite element formulation is the near incompressibility of polymers. Considering the aforesaid, there is a need of a computationally efficient finite element, which is able to eliminate possible locking pathologies and account for the visco-elastic behavior of EAPs. In this work, a solid-shell formulation is developed adopting both the assumed natural inhomogeneous strain method ANIS and the enhanced assumed strain method EAS.

Wednesday - I

Bargmann - *Tailoring lightweight materials: on tunable auxeticity and elastomechanical symmetry*

Poh - *A micromorphic computational homogenization framework for tetra-chiral auxetics*

Peerlings - *A micromorphic homogenization strategy for mechanical metamaterials*

Kouznetsova - *Multi-scale modelling of emergent dynamic behaviour of metamaterials*

Tailoring lightweight materials: on tunable auxeticity and elastomechanical symmetry

Swantje Bargmann, Celal Soyarslan and Vincent Blümer
Chair of Solid Mechanics, University of Wuppertal

Thin-walled metamaterials based on triply periodic minimal surfaces are relatively simple, light-weight structures that, as shown in the following, possess extraordinary material properties. As opposed to their filled counterparts, these structures can be tuned to be isotropic and completely auxetic - the latter is the material property of extending in all directions under tensile loading in one direction. Our computational findings show that core-shell structures respond drastically differently not only in their stiffness but also for each of these observed properties compared to their counterparts with complete filling.

1. C. Soyarslan, V. Blümer, S. Bargmann Tunable auxeticity and elastomechanical symmetry in a class of very low density core-shell cubic crystals submitted, 2019
2. S. Bargmann, B. Klusemann, J. Markmann, J. Schnabel, K. Schneider, C. Soyarslan, J. Wilmers Generation of 3d representative volume elements for heterogeneous materials: a review Progress in Materials Science 96, 322-384, 2018

A micromorphic computational homogenization framework for tetra-chiral auxetics

Raja Biswas, Amit Shedbale and Leong Hien Poh
National University of Singapore

Tetra-chiral auxetic structures exhibit many unique and enhanced mechanical properties, which emerge from coupling of stretching and rotational mechanisms within the underlying unit cell. The standard first-order computational homogenization approach has been shown to be inadequate in capturing the influence of internal ring rotations, induced by the chirality effect under a generic loading condition. In this contribution, the micromorphic computational homogenization framework developed in Biswas and Poh (2017), is adopted to address these limitations. Together with the standard macro-distortion tensor, an additional kinematic variable is introduced to explicitly characterize the deformation and rotation of the central ring. These two kinematic fields, characterizing different aspects of the unit cell deformation, enable the micromorphic framework to adequately represent dominant deformation modes. The resulting micro-scale responses are homogenized to recover a micromorphic continuum at the macro-scale, without any a priori assumptions.

Considering an axial loading problem, it is shown that the proposed micromorphic framework accurately captures the coupling of internal ring rotation and stretching of the tangential ligaments. In contrast, the first-order computational homogenization approach provides a trivial solution. The superior predictive capability of the micromorphic approach is furthermore demonstrated with a flat punch indentation problem in the regime where a clear separation of the length scales is lacking. The first-order approach becomes inadequate at the onset of plasticity. The homogenized micromorphic model accurately predicts the overall force-displacement response, as well as the deformation mechanisms of the underlying unit cells.

A micromorphic homogenization strategy for mechanical metamaterials

Ron Peerlings, Maqsood Ameen, Ondrej Rokos and Marc Geers
Eindhoven University of Technology

Mechanical metamaterials generally attain their special properties as a result of intricate mechanistic deformation patterns which they exhibit upon loading. Where this pattern formation is restricted due to boundary conditions, boundary layers appear, which in turn cause a size effect – a dependence on the ratio of the macroscopic and microstructural dimensions of the problem. Conventional computational homogenization methods do not take into account the formation of patterns and as a consequence fail to capture the size effect due to boundary layers.

In this contribution we develop an extended computational homogenization approach which does take into account the possible emergence of patterns. It is based on an additive split of the deformation into a coarse-scale contribution, a quasi-periodic patterned contribution and a remaining microstructural fluctuation field. The coarse-scale part and the amplitude of the pattern are assumed to vary only at the macroscopic scale. Injecting this Ansatz into a variational formulation of the full-scale problem and performing an ensemble procedure results in governing equations for the macroscopic fields which have a micromorphic character, i.e. a set of coupled equilibrium equations in terms of multiple independent kinematic fields. In order to compute the stress quantities featuring in these equations, a microstructural periodic cell problem needs to be solved for each point of interest in the macro-structure – i.e. in each integration point of the macroscopic discretization.

The performance of the methodology in capturing patterning and size effects is illustrated for a couple of example problems, for which predictions made by it are compared against averaged full-scale solutions. An adequate, albeit not perfect, match is obtained for scale ratios as low as two. For larger scale ratios, the predictions are more accurate, and they converge to the conventional limit in the limit of infinite scale separation.

Multi-scale modelling of emergent dynamic behaviour of metamaterials

Varvara Kouznetsova, Ashwin Sridhar, Priscilla Brandão Silva, Lei Liu, Tim van Nuland and Marc Geers
Department of Mechanical Engineering, Eindhoven University of Technology, The Netherlands

Dynamic metamaterials are materials exhibiting emergent coarse scale wave dispersion behavior due to interactions between propagating mechanical waves and fine scale micro-inertia mechanisms, based on either localized resonance or Bragg scattering, or their combination. This opens new possibilities for advanced wave manipulation applications, e.g. tunable waveguides, adaptive passive vibration control, superdamping, acoustic diodes, cloaking and focusing, 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.

This talk will present several new multi-scale techniques towards efficient analysis of initial boundary value problems involving dynamic metamaterials. First, a technique specifically developed for locally resonant metamaterials will be discussed. Originating from the classical computational homogenization, well established for quasi-static problems, an extension to transient problems has recently been developed. For linear problems, the static-dynamic decomposition can be used to derive the closed form homogenized equations representing an enriched micromorphic continuum, in which additional kinematic degrees of freedom emerge to account for micro-inertia effects. The application of this approach to metamaterials with negative refraction index and attenuation of flexural vibration of metamaterial beams will be illustrated. In non-linear case, fully coupled two scale transient computational homogenization is used to study the wave dispersion in finite size macroscopic structures, demonstrating various phenomena emerging due to the presence of non-linearities, e.g. amplitude dependent attenuation response, higher-order harmonics generation and energy exchange.

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Wednesday - II

Oliver - *Fighting the “tyranny of scales” in hierarchical non-linear multi-scale modeling of materials: the HR-FE2 technique*

Simone - *Accelerating finite element simulations of history-dependent materials by means of model order reduction and artificial neural networks*

Fighting the “tyranny of scales” in hierarchical non-linear multi-scale modeling of materials: the HR-FE2 technique

J. Oliver, M. Raschi, O. Lloberas-Valls
International Center for Numerical Methods in Engineering (CIMNE) / Technical University of Catalonia (UPC/BarcelonaTech), Barcelona, Spain

A model order reduction (MOR) technique, termed Hyper-reduced FE2 method, and acronymized HR-FE2, is proposed for hierarchical multiscale modelling of non-linear materials, in order to overcome the well-known paradigm, known as "the tyranny of scales", that precludes the use of FE2 techniques in industrial highly non-linear and 3D real-life cases, due to their inherent enormous computational cost.

The proposed computational cost reduction techniques consist of the combination, at the RVE level, of standard POD-based Reduced Order Modelling (ROM) methods, and hyper-reduction order modelling (HROM) techniques based on reduced order cubature (ROC) methods. In order to assess the efficiency and generality of the proposed HR-FE2 techniques two specific challenging problems are considered as benchmarks: 1) “Non-smooth multiscale problems”, i.e. cracking in quasi brittle materials (concrete). This was considered, for years, an “irreducible” problem even for the ROM stage. The specific challenges of the problem, in terms of the model sampling for POD, the inherent discontinuity setting, and the application of the ROC techniques end-up in a HR-FE2 model that provides encouraging results, in terms of speed-up vs. error for a set of tested 2D problems of multi-scale fracture. 2) An actual 3D-material used in the industry, i.e.: laminate composites made, at the low scale, of plies constituted, in turn, by an epoxy matrix reinforced by glass fibers, and piled-up in different fiber directions. The composite material is endowed with a highly non-linear modelling capability by considering a set of well-known dominant non-linear effects: a) propagation of ductile damage/fracture through the matrix, b) inelastic behaviour of the embedded fiber, c) pull-out and decohesion of the fibers from the matrix and d) delamination of the plies along the contact interfaces.

All those effects are captured by simple phenomenological models with properties that are easily characterizable through physical experiments. Then, the HR-FE2 technique is applied to the computational cost reduction of the RVE for a set of morphological representations of the target laminate-composite material and their performance, in terms of speed-up vs error, is analyzed. Finally, further properties of the resulting HR-FE2 model are analyzed through selected structural multi-scale benchmarks.

Accelerating finite element simulations of history-dependent materials by means of model order reduction and artificial neural networks

Angelo Simone and Fariborz Ghavamian
University of Padova
Delft University of Technology Delft University of Technology

There are widely used procedures in computational mechanics, such as parameter sensitivity analyses or multiscale simulations, that remain computationally expensive despite constant advances in computing power. In this contribution we discuss some novel techniques, based on model order reduction and artificial neural networks, that can be employed to reduce the cost of typical FEM-based many-query applications. More specifically, we will discuss a particular model order reduction technique, known as discrete empirical interpolation method, that is capable of consistently addressing the construction of an efficient nonlinear reduced model for a strain-softening material. We will also show applications of two artificial neural networks. We first employ a recurrent neural network (RNN) surrogate for the history-dependent micro level response in FE2 multiscale simulations of history-dependent materials. We then discuss the application of a convolutional neural network (CNN) that serves as an efficient surrogate for the FEM analysis of electrochemical mechanical processes in a Li-ion battery.

Wednesday - III

Fritzen - *Adaptive data-driven surrogate models for FE Square Reduced simulations*

Gudmundson - *Strain gradient plasticity model based on dislocation mechanics*

Hackl - *A relaxation-based approach to damage modeling*

Niordson - *Modeling size-effects in void growth to coalescence*

Adaptive data-driven surrogate models for FE Square Reduced simulations

Felix Fritzen
Institute of Applied Mechanics, University of Stuttgart, Germany

The authors Concentric Interpolation (also: RNEXP) was previously used in order to boost multiscale simulations on workstation computers. In this talk the approach is extended to build a more flexible scheme: An adaptive model is derived from the basic Concentric Interpolation scheme which enables the consideration of additional data available, enabling model adjustments on demand. Further, the new model benefits from algorithmic refinements that render the overall compute complexity O(N) instead of O(N^2). The resulting Adaptive Concentric Interpolation scheme is deployed as a substitute model for the RVE problem in twoscale FE simulations. The accuracy is compared to Machine Learned surrogates relying on Artificial Neural Networks.

Strain gradient plasticity model based on dislocation mechanics

Peter Gudmundson and Carl Dahlberg
KTH Royal Institute of Technology

Many experimental studies have shown a plastic strengthening effect for structural length scales approaching microstructural dimensions. Over the last 30 years different strain gradient plasticity (SGP) theories have been developed in order to capture these length scale dependences. However, up to now no generally accepted theory has emerged.

In the present presentation, focus is directed into a dislocation mechanics based SGP model for initiation of plastic deformation and subsequent hardening. The plastic behavior is governed by a dissipative and an energetic part. It is shown that a model based on the self-energies of dislocations can be translated into an internal free energy that depends on the density of geometrically necessary dislocations (GND). The dissipative part of the model is based on the Taylor model, which also gives a direct connection to GNDs. Similar to previous research on SGP theories it is here assumed that the density of GNDs can be expressed in terms of an effective measure of plastic strain gradients and the Burgers vector. In this way, a physical connection is made between the SGP framework and dislocation mechanics. It is shown that the same microstructural length scale emerges for both the energetic and the dissipative part of the model. Apart from a non-dimensional factor of the order of unity, the length scale is defined by the Burgers vector divided by the strain for initiation of plastic deformation.

In the presentation focus is primarily directed on the effects of the free energy part of the SGP model and its consequences for initial yield strength and hardening. It is shown that this part of the model controls the increase in initial yield stress at decreasing structural dimensions. The free energy contribution also has an influence on the subsequent hardening, at least for moderate plastic strains. Different models for the dependence of dislocation density on free energy are investigated.

Simulations are presented for tensile loading with a passivation layer that prohibits plastic deformation on the surfaces as well as pure bending with free and fixed boundary conditions for plastic strain. Comparisons are made with experimental data. It is shown that the model in a good way can capture the length scale dependences when the structural length scale approaches the microstructural length scale.

A relaxation-based approach to damage modeling

Klaus Hackl, Philipp Junker and Stephan Schwarz
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Material models exhibiting softening effects due to damage or localization share the problem of leading to ill-posed boundary-value problems that lead to physically meaningless, mesh-dependent finite element results. It is thus necessary to apply regularization techniques that couple local behavior, described e.g. by internal variables, at a spatial level. The common way to do this is to take into account higher gradients of the field variables thus introducing an internal length scale.

In this presentation we suggest a different approach to regularization that does not make use of any nonlocal enhancement like the inclusion of higher gradients or integration over local subdomains nor of any classical viscous effects. Instead we perform an appropriate relaxation of the (condensed) free energy in a time-incremental setting which leads to a modified potential that is coercive and satisfies quasiconvexity in an approximate way. Thus, in every time-increment a regular boundary-value problem is solved. The proposed approach holds the same advantage as other methods, but with less numerical effort. We start with the theoretical derivation, discuss a rate-independent version of the proposed model and its relation to classical fracture mechanics and present details of the numerical treatment. Finally, we give finite element results that demonstrate the efficiency of this new approach.

Modeling size-effects in void growth to coalescence

C.F. Niordson, I. Holte, K. L. Nielsen and V. Tvergaard
Department of Mechanical Engineering, Technical University of Denmark

Ductile failure of metals takes place as a consequence of void nucleation, followed by void growth to coalescence. Typical void sizes span the micron scale, where non-trivial size-effects arise due to geometrically necessary dislocations associated with plastic strain gradients. Homogenized models such as the Gurson model and its extensions are often used as a basis for modeling the ductile failure process, in terms of a macroscopic yield surface together with evolution laws for micromechanical parameters such as the void volume fraction. However, most such models do not explicitly model the intrinsic size-effects associated with the size-scale of material porosities.

The aim of the present study is to investigate the void size effect and subsequently to propose a model for size-dependence, that may be applied as a simple generalization of existing porous metal plasticity models. To this end, finite element unit cell analyses of intrinsic size-effects related to void growth and coalescence, are based on a finite strain generalization of strain gradient plasticity theory. The suppression of void growth on the micron scale is quantified, and a simple modeling approach is proposed for homogenized porous metal models that are based on an explicit dependence of the yield function on the void volume fraction and the mean stress. It is proposed that the void size effect can be captured by conventional homogenized models by introducing two simple extensions: 1) An effective void volume fraction smaller than the physical one. 2) A reduced mean stress sensitivity. The proposal is verified for the Gurson-Tvergaard model, and the effects of void shape are discussed.

Wednesday - IV

Dunne - *Micromechanics and mechanistic modelling of fatigue crack growth*

Menzel - *Modelling of curvature effects in fibre-reinforced composites*

Steeb / Schmidt -

Micromechanics and mechanistic modelling of fatigue crack growth

Fionn Dunne, David Wilso,n Zebang Zheng and Bo Chen
Imperial College London

An integrated experimental, characterization and computational discrete and crystal plasticity study of microstructurally-sensitive fatigue crack growth is presented in order to assess mechanistic drivers. Discrete dislocation studies provide a quantitative measure of the dislocation structure and interaction configurational energy density (much of which is stored as GNDs) which is argued to be key to crack growth at the microstructural length scale. This quantity can be captured at the crystal plasticity level as a stored energy density [1].

Experimentally validated modelling provides knowledge of key microstructural quantities (accumulated slip, stress and GND density) at experimentally observed fatigue crack nucleation sites. The local (elastic) critical stored energy density, measured over a length scale determined by the density of GNDs, has been shown to predict crack nucleation sites in single, oligo- and polycrystal tests [2]. The dislocation configurational energy/stored energy density is investigated as a mechanistic driver of microstructurally-sensitive fatigue crack growth in ductile metals employing the eXtended Finite Element Method (XFEM) to represent the crack. Microstructural fatigue crack growth is studied in single crystals, bicrystals and in polycrystals of cubic (fcc, bcc) and hexagonal (hcp) structure. Along with the crystallographic slip, the stored energy density is shown to predict microstructurally-sensitive crack growth tortuosity, and to capture many features that have been observed experimentally, including crack deflection and retardation at the grain boundaries [3,4].

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[2] Bo Chen et al. Is Stored Energy Density the Primary Meso-scale Mechanistic Driver for Fatigue Crack Nucleation? Intl. Jnl.Plasticity. 101, 213-229, 2018.
[3] David Wilson et al. A mechanistic modelling methodology for microstructurally-sensitive fatigue crack growth. Jnl. Mech. Phys. Solids. 124, 827-848, 2019.
[4] David Wilson et al. Microstructurally-sensitive fatigue crack growth in HCP, BCC and FCC polycrystals. Jnl. Mech. Phys. Solids. 126, 204-225, 2019.

Modelling of curvature effects in fibre-reinforced composites

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In addition to information on the deformation state, classic modelling approaches for fibre-reinforced composites take into account information on the fibre direction field to account for the anisotropic properties induced by the fibres. From a modelling perspective this gives rise to the definition of structural tensors which resemble the respective material symmetry groups in the constitutive functions. However, for certain deformation modes and fibre orientation fields, the classic structural tensor approach is not sufficient to account for the action of the fibres.

Against this background, an extended modelling approach for fibre-reinforced composites is pursued in accordance with [1] which additionally takes into account information on the gradient of the spatial fibre direction field, in particular on the fibre curvature. The latter includes second-gradient contributions of the placement field and motivates the usage of an extended continuum approach which features a natural length scale and hence allows for the modelling of size effects as experimentally observed on the nanoscale.

The solution of the underlying coupled system of partial differential equations is approached by means of a mixed-type multi-field finite element formulation which is validated in a first step by a comparison with analytical solutions, [2]. Focussing on a specific form of the Helmholtz free energy density function in a second step, we show that fibre curvature measures may be extracted from the generalised list of invariants and give rise to physically well-interpretable contributions to the stress and couple stress tensor, [3]. Elaborating a specific model we analyse representative boundary value problems to study the influence of the fibre curvature-based energy contribution and the predicted size effect.

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Steeb

Thursday - I

LLorca - *A roadmap for multiscale modelling of precipitation and precipitation hardening in metallic alloys from first principles simulations*

Sigmund - *On optimal design and structural performance of multiscale structures*

Allaire - *Optimal design of modulated and oriented lattice materials by the homogenization method*

Terada - *PCA-based computational homogenization for nonlinear elasticity*

A roadmap for multiscale modelling of precipitation and precipitation hardening in metallic alloys from first principles simulations

Javier LLorca
IMDEA Materials Institute and Polytechnic University of Madrid

A multiscale modelling roadmap is presented to simulate precipitation and precipitation hardening in metallic alloys. The methodology us applied to Al-Cu alloys. In the first step, the homogeneous and heterogeneous nucleation and growth of precipitates during high temperature ageing in Al-Cu alloys is simulated using the standard nucleation theory in combination with the phase-field model. The parameters that determine the different energy contributions (chemical free energy, interfacial energy, lattice parameters, elastic constants) were obtained from either computational thermodynamics databases or from first-principles density functional theory. From the information, the evolution and equilibrium morphology of precipitates in 3D was obtained.

The model was able to reproduce the equilibrium shape of the different orientation variants theta' and theta'' precipitates during homogeneous nucleation as well as the heterogeneous nucleation of theta' precipitates on dislocations, leading to the formation of precipitate arrays. From this information, two different strategies were used to determine the strengthening provided by either Guinier-Preston (GP) zones or theta' precipitates. GP zones are formed by monolayers disks of Cu atoms of a few nm in diameter on {100} planes of the FCC Al lattice. The GP zones are sheared by dislocations through a thermally-activated process and the energy barrier was determined using transition state theory. Under these assumptions, the rate at which the dislocations overcome the GP zone is given by an Arrhenius equation with a pre-exponential factor and an activation energy, that can be obtained by means of molecular dynamics simulations.

In the case of theta' precipitates, the dislocations overcome the precipitates by the formation of an Orowan loop and precipitate strengthening was analyzed by means of discrete dislocation dynamics. In particular, the interaction of dislocations with precipitates were simulated using the Discrete Continuous Model coupled with the fast Fourier transform algorithm to solve the boundary value problem in a representative volume element of the microstructure. The simulations took into account the size, shape and spatial distribution of the precipitates, the effect of the elastic modulus mismatch and of the stress-free transformation strain around the precipitates, which were provided from the precipitation model above. Moreover, the dislocation properties (including dislocation mobility and cross-slip probability) were obtained from molecular dynamics simulations. The simulations results were validated against experimental data in Al-Cu alloys, showing the potential of the roadmap to predict precipitation and precipitation hardening in metallic alloys using multiscale modelling strategies based in first principles calculations.

On optimal design and structural performance of multiscale structures

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Recent progresses in additive manufacturing methods allow for realization of highly complex and optimized multiscale structures. Three decades ago, Bendsøe and Kikuchi founded the so-called homogenization approach to topology optimization. Based on mathematical insight and knowledge of optimal microstructures, this approach provided structures with ultimate stiffness using locally optimized, functionally-gradient microstructures assuming separation of scales. This approach was later abandoned in favour of simpler density-based approaches, due to complexity of both algorithms and resulting designs. However, recently, the approach has been revived, partly through introduction of so-called dehomogenization methods and partly due to the possibility of realizing complex structures by AM.

The talk will give an overview of recent progresses within 2d, 3d and multi-load dehomogenization approaches. Furthermore, it will discuss recent studies within optimal design at the micro and macro-level for combined stiffness and structural stability objectives. At little sacrifice in stiffness, microstructures can be designed for superior (periodic) buckling performance.

Optimal design of modulated and oriented lattice materials by the homogenization method

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Safran Tech and CMAP, Ecole Polytechnique
LJAD, Université Côte d'Azur

This talk will discuss the optimization of so-called lattice structures made of periodically perforated material, where the microscopic periodic cell can be macroscopically modulated and oriented. This is a three-step process. First, one compute the homogenized properties of a well-chosen family of parametrized periodicity cells. Second, one optimize the homogenized formulation of the macroscopic problem, which is an easy task of parametric optimization. Third, the optimal microstructure is projected on the macroscopic domain at a desired lengthscale, which is a delicate issue, albeit computationally cheap. The combination of these three steps is a topology optimization method for lattice structures.

The main novelty of our work is the third projection step which amounts to build a global orientation of the microstructures. It requires a regularization of the orientation and the construction of a diffeomorphism following this orientation. In 2-d, such a diffeomorphism is built thanks a conformal treatment of the optimal orientation, ensuring that, although the periodicity cell has varying parameters and orientation throughout the computational domain, the angles between its members or bars are preserved. In 3-d, conformality cannot be achieved and a different direction-by-direction reconstruction is proposed.

Several numerical examples are presented for compliance minimization in 2-d and 3-d. The issue of possible singularities in the orientation field will be briefly discussed.

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PCA-based computational homogenization for nonlinear elasticity

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The method of nonlinear multiscale analysis based on computational homogenization is classified into two classes. One is the coupling method, in which the behavior of microstructures is strongly coupled with the macroscopic material responses. The other class is the decoupling method, in which the homogenization process for microstructures are separated from the macroscopic analysis and appropriate macroscopic constitutive equations must be presumed. The former does not have need of macroscopic constitutive equations, but massively parallel computing is essential. On the other hand, the latter is capable of significantly reducing computational cost in comparison with the coupling method and amenable to practical situations using commercial software. However, there is no guarantee that adequate macroscopic constitutive equations can be found in accordance with the results of numerical analyses for homogenization, which is referred to as numerical material testing (NMT).

This study addresses the potential for the third class of two-scale analysis for nonlinear elasticity. The method is based on the PCA in the context of the machine learning technology and thus can be a member of data-driven multiscale computational homogenization. First, the stresses in a selected periodic microstructure (unit cell) are calculated by NMTs in response to various of macroscopic deformation patterns. Second, PCA is performed on the data to reduce the data size. Here, the PCA enables us to approximate the original NMT results with a smaller number of the basis vectors by analyzing a plenty of multidimensional data vectors. Since the number of PCA cases is the same as NMT cases, the set of the components of the reduced basis vectors also amount to the same number. Therefore, the third step is to approximate each of the components as a function of the macroscopic strains so that the microscopic stress distributions can be determined in response to an arbitrary pattern of macroscopic deformations. With this surrogate model of the components, two-scale analyses would be possible with neither appropriate macroscopic constitutive equations nor point-wise and step-wise calculations of microscopic stress distributions.

Several numerical examples are presented to demonstrate the performance of the proposed method.

Thursday - II

Basoalto -

Böhlke - *Texture-based Modeling of Phase-specific Residual Stresses in Duplex Steels*

Zeman - *Wang tilings for computational micromechanics*

Basoalto

Texture-based Modeling of Phase-specific Residual Stresses in Duplex Steels

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In the talk, the mechanism-based modelling of residual stresses of first and second kind in duplex steels is discussed. The modelling is realized by a two-scale approach based on a classical mean field homogenization [1] taking into account the phase-specific crystallographic texture determined by diffraction-based analysis. In comparison to full field approaches the computation time is reduced significantly. This allows for an application of the model approach at the integration point level of three-dimensional finite elements.

The mean field theory is used to derive a system of equations for the macroscopic residual stress of first kind and the microscopic residual stresses of second kind, i.e., the phase averages of the residual stresses on the microscopic scale. For this estimate, the macroscopic stress, strain and stiffness data are used. In order to allow for the simulation of geometrically large deformations present in, e.g., deep drawing, a rate formulation of the local constitutive equations using incrementally objective strain increments is used. Both the elastic and the plastic phase-specific anisotropy are modelled.

The mechanical behaviour of the phases is experimentally characterized by X-ray diffraction within a quasi in-situ tensile test. For pre-defined loading steps the tensile test is interrupted and phase specific stresses are determined. Additionally, phase specific residual stresses are analysed after unloading from each loading step. This allows for the determination of material parameters as an input for the simulation as well as the comparison of the simulation results with respect to the residual stresses of first and second kind. These methods are applied to the duplex steel X2CrNiN23-4 (1.4362), which consists of a ferritic phase and an austenitic phase of equal volume fraction. Due to the high amount of both phases and the good separability of the diffraction lines the material is excellently suited for the experimental analysis of phase-specific residual stresses. The predicted residual stresses are compared to experimental data from bending [2] and deep-drawing [3] experiments for which the phase-specific residual stresses have been determined by diffraction-based analysis (neutron diffraction and X-ray diffraction) over the thickness of the workpiece.

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Wang tilings for computational micromechanics

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Discovered originally as a visual alternative to proving theorems in mathematical logic [1], Wang tilings have found applications in computer graphics [2] and biological computing [3]. In this contribution, we discuss the use of Wang tilings in geometrical modeling, simulations, and the design of microstructured materials with non-periodic microstructure.

The talk is organized into four parts. After providing the essentials of the Wang tiling concept, we discuss the concept's potential for the modeling of random microstructures, trying to emphasize how the idea extends the established periodic unit cell representation. Three tile design strategies are outlined, covering the optimization [4], sample [5], and level-set [6] based approaches. We also comment on the concept's potential for data sharing and reproducible results in computational micromechanics. The third part addresses the development of dedicated simulation tools for heterogeneous materials with their microstructures modeled with Wang tilings. We highlight the connection between the Huet notion of apparent properties and Wang tilings, which can be conveniently used to determine representative volume through stochastic sampling and simulations [7]. Next, we discuss the difficulties faced when constructing reduced-order models built on partition-of-unity approaches. The talk concludes with the first proof-of-concept results on two-scale optimization of modular structures, with envisioned applications in the rational design of microstructured materials with non-uniform microstructures.

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Thursday - III

Larsson - *On Error-Controlled Numerical Model Reduction for Computational Homogenization*

Jänicke - *Homogenization and numerical model reduction of fine-scale poroelasticity towards a poro-viscoelastic macro-scale model*

Cottereau - *Improving the convergence rate of a non-intrusive stochastic coupling scheme*

Ibrahimbegovic - *Coupled mechanics-probability multiscale computational framework for massive composite structures safety*

On Error-Controlled Numerical Model Reduction for Computational Homogenization

Fredrik Ekre, Fredrik Larsson, Kenneth Runesson and Ralf Jänicke
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The "Finite Element squared" (FE2) technique is a popular multiscale method for analyzing problems on two distinct length scales, typically a macroscale where the overall response is sought and a microscale where fine-scale features are resolved. Each macroscale quadrature point is connected to a (discretized) boundary value problem on a Representative Volume Element (RVE). For linear static problems, effective macro-scale properties can be computed off-line, prior to the actual analysis. However, for nonlinear and/or time-dependent problems, such a priori upscaling is not feasible, and the nested problems must be solved concurrently. Although efficient compared to a single scale finite element analysis of a highly heterogeneous problem, the FE2 procedure is still computationally extremely demanding. The fact that many similar problems on RVEs are solved for with small number of input/output data makes the procedure well suited for reduction techniques applied to the discrete equations, here denoted Numerical Model Reduction. However, the richness of the reduced model will clearly affect the accuracy of the approximation. In order to obtain reliable approximations it is therefore of outmost importance to quantify, and control, this error.

In this contribution, we address applications of linear transient problems in the context of FE2-procedures with NMR. In particular, suitable error estimators are developed that (in the linear case) are guaranteed w.r.t. the full-fledged finite element solution. The key ingredients in the error estimator is the weak formulation of the RVE problem in space-time, construction of a suitable norm, and the definition of associated problem. The fact that the approximation is compared to the discrete finite element solution allows for explicit evaluation at low cost. Finally, the estimator is also extended to compute bounds on user-defined quantities of interest within the realm of goal-oriented error estimation.

The numerical efficiency and the robustness of the proposed procedure is investigated for micro-heterogeneous heat flow and poro-elasticity applications, where the micro-scale is resolved in three spatial dimensions. In particular, we investigate how selecting different reduced bases for the NMR affects the approximation and the sharpness of the error estimator.

Homogenization and numerical model reduction of fine-scale poroelasticity towards a poro-viscoelastic macro-scale model

Ralf Jänicke, Fredrik Larsson and Kenneth Runesson
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In poroelastic media, hydro-mechanical coupling between the solid matrix and the (compressible) pore fluid under mechanical loading induces fluid pressure gradients and, accordingly, redistribution of fluid in the pore space. In this work, the simple constitutive assumption of Darcy, that governs such redistribution, is adopted. This contribution deals with the efficient modeling and numerical treatment of pressure diffusion associated with fluid transport in a poroelastic medium that is strongly heterogeneous. Such heterogeneities might be constituted by, e.g., patches that are saturated with different pore fluids or varying elastic properties of the solid phase, whereas the intrinsic properties of the saturating fluid are unchanged. An extreme version of the latter scenario is a poroelastic medium with an embedded fluid-saturated fracture network. Exposed to a macroscopic loading, the heterogeneities cause local (i.e. on a scale much smaller than the scale of the observer) fluid pressure gradients to be equilibrated via pore pressure diffusion. Due to the locality of the process, the macroscopic observer is unable to measure the diffusion, associated with fluid transport, directly. However, the intrinsic attenuation of a material with apparent poro-viscoelastic properties can be sensed.

The aim of this contribution is to establish a method that enables us to identify the poro-viscoelastic properties of the macro-scale model by upscaling the sub-scale processes. Thereby, we exploit Variationally Consistent Homogenization and subsequently employ Numerical Model Reduction (NMR). We establish an NMR procedure based on Proper Orthogonal Decomposition (POD). The starting point is the additive decomposition of the pore fluid pressure into a stationary part (associated with the macroscopic poroelastic properties) and a transient fluctuation part (associated with the overall viscoelastic properties). The transient fluctuation part is represented by a reduced set of basis modes that may be identified using POD of snapshots stemming from "offline" training computations executed on Representative Volume Elements. We demonstrate how this data basis allows us to derive the poro-viscoelastic substitute model in terms of a highly efficient reduced finite element squared (FE2) procedure. The proposed method is validated with the aid of several numerical experiments.

Improving the convergence rate of a non-intrusive stochastic coupling scheme

Régis Cottereau
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This presentation will describe an overlapping coupling scheme between a stochastic model of a polycrystalline material and its homogenized counterpart. This coupling technique allows to model the influence of localized defects, such as for instance the influence of the heterogeneity at the tip of a fracture, which cannot be taken into account through classical homogenization. A fully scalable implementation will also be presented, where the solution of each model is approximated by its own dedicated software and the coupling is solved through an iterative scheme, itself approximated with a third dedicated software. A careful implementation allows to use different parallelization choices (memory-shared or memory-distributed for instance) for each of the model-dedicated software, and for the coupling step. The presentation will more particularly concentrate on the convergence rate of the global iterative scheme, comparing conditioning of the matrices corresponding to a single realization of the random medium and averages appearing naturally in the stochastic-deterministic coupling technique. Influence of the mesh on the convergence rate will be discussed, as well as potential strategies to devise adapted pre-conditioners for the coupling scheme.

Coupled mechanics-probability multiscale computational framework for massive composite structures safety

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In this work we address the challenge pertinent to guaranties of safety for massive engineering structures, both in terms of integrity to failure under extreme conditions and durability within their environment. Of particular interest are industrial domains of excellence in France, such as energy-production, and air- or land- transportation. The main obstacle to overcome pertains to our inability to certify the structural safety by performing with real-size and real-time experiments, either due to excessive structure size, to excessive cost due to irreplaceable structure component. We seek to propose the state-of-the-art advances in computational methods that can be brought to bear upon this class of problems, providing the full understanding of the potential failure modes of the given system, along with the very detailed simulation of extreme conditions brought by man-made and natural hazards. We seek further developments in recently proposed approach to coupled mechanics-probability computations that can be successfully used to provide a detailed interpretation of structure tests under heterogeneous stress field and to identify both model parameters and their probability distribution. Finally, we propose to use such a combined approach with probability computations for uncertainty propagation, which can offer a clear explanation of the size effect influence on dominant failure modes of massive composite structures.

Thursday - IV

Pandolfi - *A microstructured brittle damage model for the simulation of laboratory tests*

Noels - *An inverse Mean-Field-Homogenization-based micro-mechanical model for stochastic multiscale simulations of unidirectional composites*

Korelc - *Sensitivity analysis based multi-scale methods of coupled path-dependent problems*

A microstructured brittle damage model for the simulation of laboratory tests

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A multiscale brittle damage model is used to simulate the behavior of confined rock materials in laboratory tests. The material model is characterized by microstructures in the form of recursive equidistant parallel cohesive/frictional faults, and it is defined by a reduced number (seven) of material constants. Simulations show that the model is able to capture several important features observed in rocks, in particular the reduction of the overall stiffness for increasing deterioration of the material, fragile to ductile transition, strain localization, shear band formation, and more general size-effect. The model is applied to the simulation of the behavior of the rocks at the material point scale and at the laboratory scale as a boundary value problem. The model shows good predictive properties for a large number of geo-materials, in particular it is able to establish a correspondence between the actual microstructure and the macroscopic geometry of shear bands. Specifically, simulations at the full scale are able to model strain localization with the formation of single or multiple shear bands.

An inverse Mean-Field-Homogenization-based micro-mechanical model for stochastic multiscale simulations of unidirectional composites

Ling Wu and Ludovic Noels
University of Liege, Computational & Multiscale Mechanics of Materials

Homogenization approaches have been widely developed in order to account for micro-structural geometrical and material properties in the framework of multiscale analyses. Most of the approaches postulate the existence of a statistically Representative Volume Element (RVE). However, such representativity is not always ensured, in particular when studying the failure of composite materials, because of the existing micro-structural uncertainties.

In this work we develop a stochastic multi-scale approach for unidirectional composite materials in order to predict the scatter existing at the structural behaviour. Statistical characteristics of the micro-structure are first extracted from SEM images in order to build a Stochastic Volume Elements (SVE) [1] generator [2]. Probabilistic meso-scale stochastic behaviours are then extracted from direct numerical simulations of the generated SVEs. Finally, in order to provide an efficient way of exploiting the meso-scale random fields, while keeping information such as stress/strain history at the micro-scale during the resolution of macro-scale stochastic finite element, a probabilistic Mean-Field-Homogenization (MFH) method is developed [3,4]. To this end, the phase parameters of the MFH are defined as random fields, which are identified from the stochastic homogenized behaviours obtained through the stochastic direct simulations of the SVEs. As a result, non-deterministic macro-scale behaviours can be studied while having access to the micro-scale different phase stress-strain evolution, allowing to predict composite failure in a probabilistic way.

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Sensitivity analysis based multi-scale methods of coupled path-dependent problems

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A generalised essential boundary condition sensitivity analysis based implementation of FE^2 and mesh-in-element (MIEL) multi-scale methods is derived as an alternative to standard implementations of multi-scale analysis, where the calculation of Schur complement of the microscopic tangent matrix is needed for bridging the scales. The paper presents a unified approach to the development of an arbitrary MIEL or FE^2 computational scheme for an arbitrary path-dependent material model. Implementation is based on efficient first and second order analytical sensitivity analysis, for which automatic-differentiation-based formulation (ADB) of essential boundary condition sensitivity analysis is derived. A fully consistently linearized two-level path-following algorithm is introduced as a solution algorithm for the multi-scale modelling. Sensitivity analysis allows each macro step to be followed by an arbitrary number of micro sub-steps while retaining quadratic convergence of the overall solution algorithm.

Friday - I

Limbert - *A computational approach to unravel the interplay of structural and material properties of skin*

Linder - *A micro-macro approach to study the effect of strain induced crystallization on the fracture onset of rubber-like materials*

Stupkiewicz - *Diffuse-interface modelling of transformation patterns in shape-memory alloys at micro- and macro-scale*

Heltai - *Multiscale modeling of vascularized and fiber reinforced tissues via non-matching immersed methods*

A computational approach to unravel the interplay of structural and material properties of skin

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Considering the place of the skin in our life and its multiple physiological functions, understanding its complex physiology and biophysics in health, disease and ageing has become, particularly in the last two decades, a broad and very active multidisciplinary research arena. To unravel some of the secrets of such a complex organ new experimental, imaging and computational techniques are needed and novel mechanistic theories explaining particular mechanobiological processes need to be formulated and put to the test. Developing and exploiting such an integrated framework underpin many aspects of our research which aims to understand the interplay between the microstructural and material properties of the skin, particularly as they evolve over the life course. The skin microstructure can play a critical role in how macroscopic deformations are modulated at the microscopic level. These structural mechanisms are also at the heart of skin tribology by being part of, and conditioning mechanical load transmission and the nature of surface physics interactions. Skin biophysics is therefore fundamental to many industrial sectors from biomedical devices, personal care and cosmetic products to vehicle safety, sport equipment, wearable electronics and tactile surfaces.

In this talk, I will present some of the modelling approaches we have been developing to gain a mechanistic understanding of the interplay between material and structural properties of the skin, and ultimately, to exploit this knowledge for a variety of clinical and industrial applications. Examples will include computational contact homogenisation procedures to study skin friction, constitutive modelling of skin ageing and analysis of skin surface instabilities to understand mechanisms of wrinkle formation.

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A micro-macro approach to study the effect of strain induced crystallization on the fracture onset of rubber-like materials

Christian Linder, Prajwal Arunachala and Reza Rastak
Stanford University

The enhanced fracture resistance in rubber-like materials has often been attributed to the phenomenon of strain induced crystallization. For this study, a multi-scale polymer network model of the phenomenon is used to study its effect on the fracture onset. At the microscopic scale, a new polymer chain model accounting for the thermodynamics of the polymer chain and its crystallization under stretch is presented along with a rate-dependent evolution law. This evolution law is constructed such that it ensures that the second law of thermodynamics is satisfied. The contribution of the deformation of the molecular bonds to the internal energy is also accounted for in this non-Gaussian statistical mechanics model.

The recently developed maximal advanced path constraint [1] in addition to the principle of minimum free energy is utilized to connect the deformation in the microscale to the macroscale, thus resulting in a non-affine model. At the macroscale, a continuous crystallinity distribution is considered which describes the crystallization along all polymeric orientations with only a few parameters [2]. A chain scission criterion based on the internal energy contribution by the stretch of the atomic bonds is incorporated to study fracture initiation. The aspects of the model like stress response, crystallinity evolution and distribution, and fracture initiation and behavior have been validated by existing experimental results.

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Diffuse-interface modelling of transformation patterns in shape-memory alloys at micro- and macro-scale

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Functional properties of shape-memory alloys (SMAs), notably the shape-memory effect and pseudoelasticity, result from the reversible martensitic phase transformation which is the main mechanism of inelastic deformation in those materials. At the micro-scale, the transformation proceeds through formation and evolution of complex martensitic microstructures. At the macro-scale, the overall response of polycrystalline SMAs often exhibits softening, which leads to strain localization and inhomogeneous transformation in the form of Lüders-like bands or more complex transformation patterns, for instance, multi-prong interfaces observed in NiTi tubes under tension. Evolution of microstructure at the micro-scale and formation of transformation patterns at the macro-scale are both accompanied by nucleation, propagation and annihilation of interfaces. Spatially-resolved modelling of the corresponding phenomena can be efficiently carried out using the diffuse-interface approach.

In this talk, our recent related results will be summarized. The phase-field method has been applied to model the martensitic microstructures at the micro-scale with the focus on size effects, rate-independent dissipation, and microstructure evolution during nano-indentation. In order to model strain localization and transformation patterning in polycrystalline NiTi, a macroscopic model of SMA employing a gradient enhancement has been developed along with a micromorphic-like regularization that facilitates the finite-element implementation. Thermomechanical couplings have been introduced into the model in order to describe the loading-rate effects in a physically sound manner. Finite-element simulations of representative 3D problems illustrate that the model correctly represents the loading-rate effects in a NiTi dog-bone specimen under tension and complex transformation patterns in NiTi tube under tension.

Multiscale modeling of vascularized and fiber reinforced tissues via non-matching immersed methods

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We present a multiscale approach based on immersed methods for the efficient computational modeling of tissues composed of an elastic matrix (in two or three-dimensions) and networks of fibers and/or thin vascular structures (treated as a co-dimension two manifolds). We derive a variational formulation of the coupled problem, in which the effect of the fibers and of the vasculature are incorporated in the elasticity equations via singular or hyper-singular forcing terms. These terms only depend on information defined on co-dimension two manifolds (such as fiber center line, vessel center line, cross sectional area, and mean pressure over vessels cross section), drastically reducing the complexity of the computational model.

We perform several numerical tests, ranging from simple cases with known exact solutions to the modeling of materials with random distributions of vessels and fibers. In the latter case, we use our immersed method to perform an in silico characterization of the mechanical properties of the effective biphasic material tissue via statistical simulations.

Friday - II

Reese - *Data-driven mechanics, model order reduction, and hierarchical tensor approximation – suitable methods to cross the scales?*

Bangerth - *Supporting complex simulations with open source finite element software*

Garikipati - *A graph theoretic framework for representation, exploration and analysis on computed states of physical systems*

Data-driven mechanics, model order reduction, and hierarchical tensor approximation – suitable methods to cross the scales?

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Data analysis and data science have become fundamental domains in the past decade. Data science has not only a big impact on financial markets but also in engineering areas. Experimental measurements get increasingly reliable and data-rich. To find a description of the usually strongly non-linear material behaviour, complex constitutive laws have to be developed and fitted to the experimental measurements. An interesting alternative idea is the use of the data directly. In our work we intend to use data from experiments to extract pairs of stress and strain to execute computations by evaluating them without constitutive model. Hereby, we bypass any kind of modelling error as well as any problem concerning parameter fitting. Methods such as model order reduction in combination with hierarchical tensor approximation serve to create a functional representation of a highly-dimensional solution space. A long-term goal is to use the latter to model the behaviour of a RVE in a multi-scale analysis.

Supporting complex simulations with open source finite element software

Wolfgang Bangerth
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Many aspects of computational modeling of materials are well supported by commercial, closed-source software. On the other hand, there are often good reasons to develop finite element models of material behavior using software in which one has access to all parts of the source code. For example, this is clearly the case if the goal is the development of better numerical methods (discretizations, linear and nonlinear solvers, preconditioners). Another example is modeling of materials with non-standard behavior -- such as coupled bulk and surface processes, or coupling of material behavior to external electric or magnetic fields. Finally, most commercial software does not scale very well to very large simulations, whereas a number of open source finite element packages today can routinely solve problems with billions of unknowns on thousands or tens of thousands of processors.

In this talk, I will give an overview of the open source finite element software library deal.II (see https://www.dealii.org) that is widely used in situations such as those listed above. In particular, I will (i) discuss its features, (ii) illustrate its functionality with a number of applications, (iii) mention how most users get started with their projects, and (iv) outline its use in the education of the next generation of scientists and engineers.

[1] D. Arndt, W. Bangerth, T. C. Clevenger, D. Davydov, M. Fehling, D. Garcia-Sanchez, G. Harper, T. Heister, L. Heltai, M. Kronbichler, R. M. Kynch, M. Maier, J.-P. Pelteret, B. Turcksin, D. Wells: "The deal.II Library, Version 9.1". Accepted, Journal of Numerical Mathematics, 2019. DOI: 10.1515/jnma-2019-0064

[2] W. Bangerth, R. Hartmann and G. Kanschat: "deal.II — a general-purpose object-oriented finite element library". ACM Transactions on Mathematical Software, vol. 33, no. 4, article 24, 2007.

A graph theoretic framework for representation, exploration and analysis on computed states of physical systems

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A graph theoretic perspective is taken for a range of phenomena in continuum physics in order to develop representations for analysis of large scale, high-fidelity solutions to these problems. Of interest are phenomena described by partial differential equations, with solutions being obtained by computation. The motivation is to gain insight that may otherwise be difficult to attain because of the high dimensionality of computed solutions.

We consider graph theoretic representations that are made possible by low-dimensional states defined on the systems. These states are typically functionals of the high-dimensional solutions, and therefore retain important aspects of the high-fidelity information present in the original, computed solutions. Our approach is rooted in regarding each state as a vertex on a graph and identifying edges via processes that are induced either by numerical solution strategies, or by the physics. Correspondences are drawn between the sampling of stationary states, or the time evolution of dynamic phenomena, and the analytic machinery of graph theory.

A collection of computations is examined in this framework and new insights to them are presented through analysis of the corresponding graphs.