GRK 2423 Fracture across Scales
www.frascal.research.fau.eu

FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG

1st FRASCAL Virtual Colloquium

Recent Advances in Computational Modeling of Fracture at Various Length and Time Scales

Book of Abstracts

Thursdays, April 22nd - July 22nd, 2021

Zentralinstitut
SCIENTIFIC
COMPUTING

frascal.research.fau.eu/fvc

Research Training Group GRK2423
Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)
Martensstraße 5a, 91058 Erlangen, Germany
www.frascal.research.fau.eu
grk2423-contact@fau.de

Spokesperson: Prof. Dr.-Ing. habil. Paul Steinmann
Co-Spokesperson: Prof. Dr.-Ing. Erik Bitzek

Editors: Lucie Spannraft, Jonas Ritter, Wuyang Zhao
Cover: Tarakeshwar Lakshmipathy, Dr. rer. nat. Christian Wick

1^{st} FRASCAL Virtual Colloquium

An amalgamation of diverse disciplines of engineering and science, ranging from continuum mechanics at the macro-scale to quantum chemistry at the sub-atomic level, is essential for developing a comprehensive understanding of the fracture behavior of materials. In line with this principal theme, the 1^{st} FRASCAL Virtual Colloquium aims at providing a platform to discuss recent advances in the computational modeling of fracture, with an emphasis on approaches considering this problem at various length and time scales, and combinations thereof.

In the 1^{st} FRASCAL Virtual Colloquium, recent studies on fracture and failure of materials are presented including material instability, crack formation and transition, material adhesion and grain boundary evolution. A large variety of materials, from brittle to ductile and from crystalline to disordered, are investigated by different approaches such as Molecular Dynamics simulations, statistical mechanics and continuum mechanics. Specifically, the following methods spanning various scales are discussed: Atomic-scale and coarse-grained Molecular Dynamic simulations, line tension models, statistical-mechanics models, fiber bundle models, cohesive zone models, phase-field methods, eigenerosion methods, smeared methods, continuum disconnections, damage homogenization, and material point method. In this feast of science, ambitious goals are pursued such as towards understanding the nature of fracture, optimal design of structures with respect to fracture, failure time prediction and design of smart materials.

The event is planned as a series of weekly, invited talks by experts tackling the aforementioned problem from different viewpoints such as mechanics, material science, mathematics, physics, and chemistry. The weekly seminars will take place via Zoom with a 45 minute talk followed by discussion to allow scientific exchange amongst researchers around the world.

More information is available at: `frascal.research.eu/fvc`

The Research Training Group GRK 2423 FRASCAL

Within our Research Training Group, young researchers under the supervision of experienced principal advisors perform cutting-edge research on challenging scientific aspects of fracture. Our central aim is to improve the understanding of fracture in a broad variety of materials by developing methods able to capture the multiscale nature of failure. Various simulation approaches describing fracture exist for particular types of materials and specific time and length scales, an integrated and overarching approach that is able to capture fracture processes in different – and in particular heterogeneous – materials at various length and time resolutions is still lacking. We are a group of interdisciplinary experts from mechanics, materials science, mathematics, chemistry, and physics and contribute within twelve projects to the necessary methodology to investigate the mechanisms underlying fracture and how they are influenced by heterogeneities in various materials. The insights obtained together with the methodological framework allow tailoring and optimising materials against fracture. A representative spectrum of materials and their composites, together with granular and porous materials is covered. We study these on length and time scales relevant to science and engineering, ranging from sub-atomic via atomic and molecular over mesoscale to macroscopic dimensions. Our modelling approaches and simulation tools are based on concepts from quantum mechanics, molecular mechanics, mesoscopic approaches, and continuum mechanics.

Invited Talks

Bridging the scales in fracture and damage mechanics

Alexander Hartmaier

ICAMS, Ruhr-Universität Bochum, Germany

On the engineering scale, continuum mechanics provides an efficient way to model brittle fracture based on stresses, stress intensity factors, and energy release rates. On the atomic scale, in contrast, brittle fracture occurs by the breaking of atomic bonds, which is caused by exceedingly high interatomic forces. To describe ductile failure in metals, typically damage models are employed that mimic the physical process of nucleation, growth and coalescence of voids that is driven by plastic deformation and small-scale diffusion of monoatomic vacancies. In both, brittle fracture and ductile failure, the microstructure of the material plays a dominant role to determine the failure mechanism and the loading conditions at which failure occurs. Hence, it is seen that a comprehensive understanding and a consistent description of brittle fracture and ductile failure involves a number of length and time scales. The length scales are ranging from the atomic over the microstructural to the component scale, thus, covering roughly nine orders of magnitude; the involved time scales range from atomic oscillations to diffusive times, which poses and even more severe scale bridging problem, as more than twelve orders of magnitude need to be considered. To accomplish this, scaling methods are required that allow for the transfer of fundamental atomistic information and knowledge about the mechanisms occurring within the microstructure to models that solve engineering problems.
In this lecture, focusing on the implications of bridging several length scales, an overview is provided on methods that are used to describe damage and fracture on the macroscale, i.e. cohesive zone models for brittle and semi-brittle fracture and damage models for ductile failure. In a top-down scale bridging approach, these engineering models are augmented with information on atomic and microstructural processes, to capture the essence of the physical mechanisms occurring on the relevant length scales. In this way, atomistically and microstructurally informed continuum models are introduced and examples for their applications are given. In these applications, atomistically informed cohesive zone models for fracture in brittle ceramics with a heterogeneous microstructure are discussed [3], together with a physically motivated scaling scheme to transfer atomistic data into continuum fracture models [2]. Ductile failure models are introduced on the microstructural scale [1] and ways of homogenizing the material's damage behavior to the macroscale are revealed [4].

References

[1] M. Boeff, F. Gutknecht, P. S. Engels, A. Ma, and A. Hartmaier. "Formulation of nonlocal damage models based on spectral methods for application to complex microstructures". *Engineering Fracture Mechanics* 147 (2015), pp. 373–387.

[2] J. J. Möller, E. Bitzek, R. Janisch, H. ul Hassan, and A. Hartmaier. "Fracture ab initio: A force-based scaling law for atomistically informed continuum models". *Journal of Materials Research* 33.22 (2018), pp. 3750–3761.

[3] M. Prechtel, P. L. Ronda, R. Janisch, A. Hartmaier, G. Leugering, P. Steinmann, and M. Stingl. "Simulation of fracture in heterogeneous elastic materials with cohesive zone models". *International Journal of Fracture* 168.1 (2011), pp. 15–29.

[4] D. Reimann, K. Nidadavolu, N. Vajragupta, T. Glasmachers, P. Junker, and A. Hartmaier. "Modeling macroscopic material behavior with machine learning algorithms trained by micromechanical simulations". *Frontiers in Materials* 6 (2019), p. 181.

Brief Biosketch of Alexander Hartmaier

Dr. Alexander Hartmaier is currently Professor of Materials Science (Chair in Mechanics of Materials) at Ruhr-Universität Bochum/Germany and Director at the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), heading the department Micromechanical and Macroscopic Modelling. Since 2016 he is guest professor at the Harbin Institute of Technology/China, from 2016-2019 within the Jang Chiang Scholar Program. From November 2005 to May 2008, he has been Professor of Materials Science at Friedrich-Alexander-Universität Erlangen-Nürnberg/Germany. Prior to this position, he headed the group "Nanostructured Materials" in the department "Theory of Mesoscopic Phenomena" of Prof. Huajian Gao at the Max Planck Institute for Metals Research in Stuttgart/Germany. This is the same institute where he worked on his PhD thesis, which has been awarded the Otto-Hahn-Medal of the Max Planck Society in 2000. In between his stays at the Max Planck Institute in Stuttgart, Dr. Hartmaier spent three years in industrial research in responsible functions as project leader and group leader. The focus of his research work lies on micromechanical and scalebridging modeling of deformation, fracture and fatigue of heterogeneous materials and, more recently, on data-oriented methods and applications of machine learning in materials science. Besides his academic activities, Dr. Hartmaier served the Deutsche Gesellschaft für Materialkunde (DGM), the German Materials Society, as chairman in the term 2017/18, as board member from 2013 to 2018, and as speaker of the program for young scientists from 2011 to 2014.

Computational Modeling and Design Optimization of Structures using the Phase Field Fracture Method

Haim Waisman

Columbia University, USA

The phase field fracture method has been widely adopted due to its ability to handle crack initiation/propagation, and complex crack topologies without the need for explicit tracking fracture surfaces. I will discuss several applications related to fracture modeling and design optimization of structures which relies on the phase field method.

The first part of the presentation will focus on dynamic fracture of metals that often result in brittle and/or ductile fracture, depending on loading rates, geometry and material type. Further, at high strain rates, a material instability known as shear banding, may also occur and lead to narrow localization bands which reduce the stress bearing capacity of the material. I will present a model that can simultaneously account for these two failure processes through a novel phase-field formulation coupled to a temperature-dependent viscoplasticity for shear bands. I will also propose a material stability analysis to determine the onset of localization, which can be employed for adaptive mesh refinement.

The second part of the talk will be devoted to optimal design of structures for enhanced fracture resistance. I will present two topology optimization formulations, in which low weight designs are achieved with substantially increased fracture resistance. In contrast to the majority of the current relevant literature which favors stress constraints with linear elastic physics, we explicitly simulate brittle fracture using the phase field method during the topology optimization procedure. Subsequently, design for ductile failure and buckling resistance is addressed through an efficient numerical approach. The optimized structures are also subjected to a post-optimization verification step which show significant gains in structural strength and toughness.

Brief Biosketch of Haim Waisman

Haim Waisman
Associate Professor
Department of Civil Engineering and Engineering Mechanics
Columbia University

Haim Waisman is an Associate Professor of Civil Engineering and Engineering Mechanics at Columbia University. His research interests are in computational fracture mechanics, for which he develops advanced finite element methods for modeling and design-optimization of structures under extreme conditions. Dr. Waisman obtained his Bachelor and Master degrees in Aerospace Engineering from the Technion-Israel Institute of Technology, and a Doctorate in Civil Engineering from Rensselaer Polytechnic Institute in 2005. He was a post-doctoral fellow at the Scientific Computing Research Center (SCOREC) at RPI and at the Mechanical Engineering department at Northwestern University, before joining Columbia University in 2008. Dr. Waisman is the recipient of the 2012 Department of Energy Early Career Award, the 2014 Leonardo Da Vinci Award from the Engineering Mechanics Institute of ASCE, and several best paper awards. He is currently serving as an associate editor of the ASCE journal of Engineering Mechanics, the executive council US Association for Computational Mechanics, and is the past chair of the ASCE-EMI computational mechanics committee.

More information is available at: http://www.columbia.edu/cu/civileng/waisman/index.html

Predictability of failure in disordered solids using fiber bundle models

Soumyajyoti Biswas

Department of Physics, SRM University - AP, Andhra Pradesh 522502, India

The fiber bundle model is a simple model for breakdown in disordered materials. In this talk, we will discuss the formulation of the model and show how it can reproduce generic breakdown properties of disordered materials. Using those properties, it is possible to make predictions about the failure time for such materials. We will discuss how the predictability of the model changes when the disorder strength and the range of interaction are varied in the model.

Brief Biosketch of Soumyajyoti Biswas

Soumyajyoti Biswas is currently an Assistant Professor in the department of Physics at the SRM University – AP, India. He has received his Ph. D. in 2015 from the Saha Institute of Nuclear Physics in Kolkata. Following this, he carried out postdoctoral research work in the Institute of Mathematical Sciences, Chennai; University of Tokyo; Max Planck Institute for Dynamics and Self-Organisation in Göttingen and Friedrich-Alexander-University in Fürth. He has received the Alexander von Humboldt fellowship and the JSPS fellowship.

His main research interests include statistical physics of driven disordered systems; models of earthquakes; agent based models for societies and economies.

How disorder affects the failure: Fractures on models inspired by Bamboo Guadua angustifolia

José-Daniel Muñoz

Simulation of Physical Systems Group, Department of Physics, Universidad Nacional de Colombia, Bogotá

Guadua angustifolia is an Andean Bamboo extensively employed in Colombia as building material and in the elaboration of furniture and handicrafts that uses to develop cracks in the parenchymatous tissue as a consequence of either a poor drying process or mechanical stresses like traction or bending. This talk discusses statistical-mechanics models of fracture inspired on of *G. angustifolia*, both for the drying processes and the mechanical stresses. Our first set of models resembles the cellular structure of the parenchymatous tissue on a transversal cut and are employed to model both the initial drying stage – dominated by capillarity – and the final one – dominated by uniform contraction – with finite-element and discrete-element methods [1]. Our results for the initial drying stage suggest that these fractures are driven by invasion percolation, as the drying front advances from cell to cell. In contrast, our models for the final drying stage show a critical behavior for specific values of the structural disorder, represented either by random cells or as unequal values of braking thresholds [3, 4, 6]. In fact, a phase transition between two well-defined behaviors was clearly identified: the setting of a large initial crack at low structural disorder levels and, the slow aggregation of small cracks and better resistance to failure at large disorder levels [5]. The average size of the larger avalanche can be identified as the transition order parameter and the associated susceptibility, with the average ratio between the second and the first moments of the distribution of avalanche sizes. Our second set of models resembles with discrete elements the parenchymatous tissue on the axial longitudinal direction, where large cells alternate with smaller ones at random [2]. We also found that wider distributions of breaking thresholds give better resistance to failure by bending. In addition, the random sequence of large and shorter cells increases that resistance at narrow threshold distributions. The overall conclusion is that structural disorder, whether represented in broader failure thresholds or in diverse element sizes or shapes, increases the resistance to failure, a quality that has been adopted by the parenchymatous tissue of *G. angustifolia*.

References

[1] G. V. Camargo. "A statistical model of drying-induced fractures applicable to the bamboo Guadua angustifolia". Ph.D. dissertation in Physics (Summa Cum Laude). Universidad Nacional de Colombia, 2012.

[2] J. A. Pérez Rangel. "A Molecular Dynamics study of the resistance to failure under traction for a statistical model inspired by Bamboo Guadua angusifolia". M.Sc. dissertation in Physics. Universidad Nacional de Colombia, 2016.

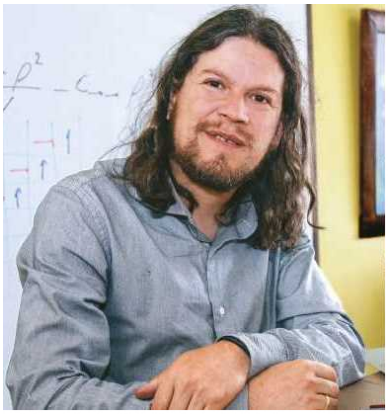
[3] G. Villalobos. "Acoustic emission signals resulting from the drying-induced fractures of *Phyllostachys pubescens* bamboo: evidence of scale-free phenomena". *Wood Sci. and Technol.* 50.3 (2016), p. 489. DOI: 10.1007/s00226-016-0798-0.

[4] G. Villalobos, F. Kun, D. L. Linero, and J. D. Muñoz. "Size distribution and waiting times for the avalanches of the Cell Network Model of Fracture". *Comp. Phys. Comm.* 182 (2011), p. 1824.

[5] G. Villalobos, F. Kun, and J. D. Muñoz. "Effect of disorder on temporal fluctuations in drying-induced cracking". *Phys. Rev. E* 84 (2011), p. 041114.

[6] G. Villalobos, D. L. Linero, and J. D. Muñoz. "A statistical model of fracture for a 2D hexagonal mesh: The Cell Network Model of Fracture for the bamboo Guadua angustifolia". *Comp. Phys. Comm.* 182 (2011), p. 188.

Brief Biosketch of José-Daniel Muñoz



Dr. José-Daniel Muñoz is Titular Professor in Physics at the National University of Colombia (UNAL), Bogotá, where he started teaching in 1994. He received his B.Sc. (1991) and M.Sc. (1996) in Physics from UNAL and his Ph.D. in Physics from the University of Stuttgart in 2001, under the advice of Prof. Hans J. Herrmann. Since then, he has been director of the Simulation of Physical Systems Group at UNAL. His research interest focuses on the numerical modeling and analysis of granular media, building materials, acoustics, fluid mechanics, vehicular traffic and statistical mechanics by using discrete elements, lattice Boltzmann, cellular automata and Monte Carlo methods, including the developing of novel simulation techniques. In those areas he has been advisor of 4 Ph.D., 24 M.Sc. and 32 B.Sc. students in Physics and Engineering. Some of his works have been reviewed in *Nature*, *Scientific American* and *New Scientist*, and he has established active collaborations with groups in Switzerland, Australia, USA, Spain, France, Hungary and Colombia. Along with his research and academic activities, Prof. Muñoz served as director of the Academic Programs in Physics from 2008 to 2012, director of the Department of Physics from 2018 to 2020 and co-founder of the M.Sc. program on Exact and Natural Sciences Teaching at UNAL, where he has been advisor of 27 students. Since 2014 he is member of the IUPAP C13 commission, *Physics for Development*.

From sub-Rayleigh anticrack to supershear crack propagation in snow slab avalanche release

Bertil Trottet[1], Ron Simenhois[2], Grégoire Bobillier[3], Alec van Herwijnen[3], Chenfanfu Jiang[4], and Johan Gaume[1,3]

[1] Snow and Avalanche Simulation Laboratory (SLAB), Swiss Federal Institute of Technology (EPFL), CH-1015 Lausanne, Switzerland

[2] Colorado Avalanche Information Center, Boulder, CO, USA

[3] WSL Institute for Snow and Avalanche Research SLF, CH-7260 Davos, Switzerland

[4] Computer and Information Science Department, University of Pennsylvania (UPenn), PA-19104 Philadelphia, USA

Snow slab avalanche release can be separated in four distinct phases: (i) failure initiation in a weak snow layer buried below a cohesive snow slab, (ii) the onset and, (iii) dynamic phase of crack propagation within the weak layer across the slope and (iv) the slab release. The highly porous character of the weak layer implies volumetric collapse during failure which leads to the closure of crack faces followed by the onset of frictional contact. To better understand the mechanisms of dynamic crack propagation, we performed numerical simulations, snow fracture experiments, and analyzed the release of full scale avalanches. Simulations of crack propagation are performed using the Material Point Method (MPM), finite strain elastoplasticity and constitutive models based on critical state soil mechanics. Experiments consist of the so-called Propagation Saw Test (PST). Concerning full scale measurements, an algorithm is applied to detect changes in image pixel intensity induced by slab displacements. We report the existence of a transition from sub-Rayleigh anticrack to supershear crack propagation following the Burridge-Andrews mechanism. In detail, after reaching the critical crack length, self-propagation starts in a sub-Rayleigh regime and is driven by slab bending induced by weak layer collapse. If the slope angle is larger than a critical value, and if a so-called super critical crack length is reached, supershear fracture occurs. The corresponding critical angle may be lower than the weak layer friction angle due to the loss of frictional resistance during volumetric collapse. The sub-Rayleigh regime is driven by mixed mode anticrack propagation while the supershear regime corresponds to a pure mode II propagation with intersonic fracture velocities. This intersonic regime thus leads to pure tensile slab fractures initiating from the bottom of the slab as opposed to surface initiations induced by slab bending in the sub-Rayleigh regime. Key ingredients for the existence of this transition are discussed such as the role played by friction angle, collapse height and slab secondary fractures.

Brief Biosketch of Johan Gaume

Johan Gaume received his PhD from the Grenoble University in 2013. He was then a postdoc at ETH Zürich and at the WSL Institute for Snow and Avalanche Research SLF in Davos, Switzerland. In 2016, he joined EPFL as a research and teaching associate. He was a visiting scholar in the Department of Mathematics of UCLA (2017) and in the Computer and Information Science Department of UPenn (2018). In 2019, he became Assistant Professor at EPFL and head of SLAB, the Snow and Avalanche Simulation Laboratory. His research focuses on the initiation and propagation of gravitational mass movements with a particular focus on snow and avalanche mechanics which includes the development of multiscale numerical methods. He developed, in collaboration with Prof. Joseph Teran at UCLA and Prof. Chenfanfu Jiang at UPenn, new constitutive snow models to simulate avalanche release and flow at the slope scale in a unified manner using the Material Point Method. He received the Excellence Scholarship from the Swiss Government and was awarded the Ambizione grant and Eccellenza Professorial fellowship from the Swiss National Science Foundation.

Modelling fracture with eigenerosion versus phase-field

Anna Pandolfi

Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133 Italy

Eigenerosion (EE) is a discretization approach to fracture alternative to the popular phase-field (PF) method. Phase-field is a very general method that can be used to model material discontinuities and interfaces. Contrariwise, eigenerosion has been developed to model fracture. Phase-field and element erosion methods have a common variational structure: an elastic energy-release mechanism, namely, progressive damage in the case of PF and abrupt damage in the case of EE; and an energy cost of damage, derived from the phase-field and its gradients in the case of PF and from an estimate of the fracture area in the case of ER. In both cases, the static equilibrium configurations of the solid follow from global energy minimization. In addition, crack propagation is modeled in both cases by means of a rate-independent gradient flow that balances elastic energy-release rate and dissipation. This presentation wants to compare eigenerosion and phase-field in a very general form, pointing out similarities and differences, and focusing on the accuracy and convergence properties to reveal the advantages and the drawbacks of both approaches. This research has been developed in collaboration with Michael Ortiz and Kerstin Weinberg.

References

[1] A. Pandolfi, B. Li, and M. Ortiz. "Modeling fracture by material-point erosion". *International Journal of Fracture* 184.1-2 (2013), pp. 3–16.

[2] A. Pandolfi, K. Weinberg, and M. Ortiz. "A comparative accuracy and convergence study of eigenerosion and phase-field models of fracture". *Submitted* (2021).

[3] A. Pandolfi and M. Ortiz. "An eigenerosion approach to brittle fracture". *International Journal for Numerical Methods in Engineering* 92.8 (2012), pp. 694–714.

[4] B. Bourdin, G. A. Francfort, and J.-J. Marigo. "Numerical experiments in revisited brittle fracture". *Journal of the Mechanics and Physics of Solids* 48 (2000), pp. 797–826.

[5] B. Schmidt, F. Fraternali, and M. Ortiz. "Eigenfracture: an eigendeformation approach to variational fracture". *SIAM Multiscale Modeling & Simulation* 7.3 (2009), pp. 1237–1266.

[6] M. Negri. "Finite element approximation of the Griffith's model in fracture mechanics". *Numerische Mathematik* 95.4 (2003), pp. 653–687.

Brief Biosketch of Anna Pandofli

Professor of Structural Mechanics and Solid Mechanics at the Politecnico di Milano, where she has been hired in 1995 as assistant professor, since 1996 Anna Pandolfi holds an intermittent Visiting Associate Position at Caltech, Pasadena CA, USA. She has been advising 10 PhD students and 4 post-docs. She is currently Elected Member of the Euromech Council. She has been serving as coordinator of the Italian Group of Computational Mechanics (GIMC) from 2015 to 2019. She is the editor in Chief of Meccanica (Springer) and she serves in the Editorial Boards of the International Journal of Fracture, PLOS ONE, ASME Journal of Journal of Engineering Materials and Technology, and Journal of Theoretical, Computational and Applied Mechanics. Reviewer for more than 90 scientific journals in the field of mechanics, biomechanics and physics, she has delivered 22 plenary or keynote lectures in international conferences and has been invited to give research seminars in international Scientific Institutions in more than 80 occasions. She is author or coauthor of 90 publications in international peer-reviewed journals and of other 50 scientific works. Her major scientific contributions to the scientific research are in the field of computational mechanics, with the development of advanced fracture tracking techniques (cohesive elements, eigenerosion), particle methods for the discretization of solids and fluids, a new concept concrete with attenuation properties (metaconcrete), multiscale material models for porous brittle materials (brittle damage) used to simulate fracking. A second field of intensive research is biomechanics of soft tissues, applied in particular to the behavior of active tissues, muscles, intestines, and eyes. She has been developing several successful models of the human cornea, used to model and assist patient specific refractive surgery, in strong connection with ophthalmologists. She has developed an active network of collaborators in Italy, Germany, France, and USA, with interaction and exchange of students.

Fracture of random media from atoms to the continuum

Lars Pastewka

Department of Microsystems Engineering, University of Freiburg, 79110 Freiburg, Germany

Almost all materials around us exhibit quenched disorder: Glasses are extreme cases where individual atomic positions are disordered, but even crystalline materials have disorder at a microstructural level and interfaces of common materials have surface roughness. This talk discusses computational aspects of cracks in such disordered media, starting from atomic-scale simulations of fracture toughness in amorphous carbon, over mesoscale simulations of the formation of crack morphologies in heterogeneous elastic media, to the depinning of contact lines in the adhesion of elastic spheres on rough surfaces. The calculations will employ a variety of techniques, from molecular scale simulations over phase-field approaches to line tension models for the crack front.

Brief Biosketch of Lars Pastewka

Lars Pastewka is Professor for Simulation in the Department of Microsystems Engineering at the University of Freiburg. He uses computer simulations at atomic and mesoscopic scales to study mechanical processes. He is particularly interested in unraveling the fundamental mechanisms underlying contact, adhesion and friction. Prof. Pastewka received his PhD in Physics from the University of Freiburg for research carried out at Fraunhofer IWM. He held a postdoctoral position at Johns Hopkins University and headed a junior research group at the Karlsruhe Institute of Technology before joining the University of Freiburg as faculty in 2017. Prof. Pastewka has held Fulbright and Marie Skłodowska-Curie fellowships. He is the recipient of an Emmy-Noether award of the Deutsche Forschungsgemeinschaft and a Starting Grant of the European Research Council.

Discrete and smeared approaches in computational fracture mechanics

René de Borst

University of Sheffield, Department of Civil and Structural Engineering, Sheffield S1 3JD, UK

The first attempts to simulate fracture numerically date back to the late 1960s, when the discrete and smeared crack models were introduced. In the discrete crack approach fracture initiation and propagation is modelled by changing the topology of the domain and cracks have a clearly defined width. This approach is physically intuitive, but requires tracking of each individual crack, including the concomitant topological changes of the domain. Different from this approach, smeared or diffuse methods for simulating fracture distribute the crack over a finite width, and the kinematic quantities of the discrete approach, namely the crack opening and crack sliding, are replaced by crack strains. While this can be computationally advantageous, in particular for three-dimensional simulations, it retains certain drawbacks which are less straightforward to resolve, such as the proper incorporation of traction-relative displacement relations as occur in cohesive-zone models, and dealing with flow and mass transport in cracks when considering multi-physics problems.

Over the years, strong opinions have been expressed regarding both approaches. In this presentation, we will discuss discrete and smeared crack models in a historical perspective and will attempt to dispel some misunderstandings. We will start at the origins of the discrete and smeared approaches to fracture, and discuss the improvements which have been applied to both methods in order to make them more versatile and more closely simulates the underlying physical processes. For discrete crack models an important step was the introduction of re-meshing, which enabled the approach to become mesh-objective in the sense that the crack path became independent from the underlying finite element discretisation. The extended finite element method can be viewed as an intelligent form of re-meshing, although it suffers from the disadvantage that the total number of degrees of freedom remains constant, thus limiting the mesh densification that is desirable around crack tips.

A fundamental problem with smeared approaches turned out to be that strain softening is introduced in the continuum to represent the degrading processes around the crack tips. Nonlocal and gradient approaches have been proposed successfully to remedy the severe mesh sensitivity that results from the introduction of strain softening, but some open issues persist such as the determination of the additional material parameters and the additional boundary conditions.

Recently, new discretisation methods, such as isogeometric analysis, and a new diffuse formulation, the phase-field approach, have been proposed. The final part of the lecture will examine the possibilities and limitations of these technologies for accurately and efficiently simulating fracture, including extensions to cohesive fracture and fracture in fluid-saturated porous media, and relations to preceding approaches like gradient-enhanced damage models.

Brief Biosketch of René de Borst

René de Borst received an MSc in civil engineering and a PhD from Delft University of Technology. He has been a Distinguished Professor at the Delft University of Technology, and Dean of the Faculty of Mechanical Engineering at the Eindhoven University of Technology. He has been the 10^{th} Regius Professor of Civil Engineering and Mechanics at the University of Glasgow, and is currently the inaugural holder of the Centenary Chair of Civil Engineering at the University of Sheffield.

René de Borst is Editor-in-Chief of the International Journal for Numerical Methods in Engineering, of the International Journal for Numerical and Analytical Methods in Geomechanics, and of the Encyclopedia of Computational Mechanics.

He is recipient of the Max-Planck Research Prize, the IACM Computational Mechanics Award, the NWO Spinoza Prize, a Royal Society Wolfson Research Merit Award, the JSCES Grand Prize, and the PACM O.C. Zienkiewicz Medal. He has been inducted in the Royal Netherlands Academy of Arts and Sciences, the Royal Society of Edinburgh, the European Academy of Sciences and Arts, and the Royal Academy of Engineering in London. He is an Officer in the National Order of Merit [France], and has been awarded an honorary doctorate by the Institut National des Sciences Appliquées de Lyon (INSA-LYON). He currently holds an ERC Advanced Grant on fracture in porous media.

Phase-field fracture models for linearized and finite elasticity

Kerstin Weinberg

University of Siegen, Germany

The phase-field approach to fracture simplifies sharp cracks by smooth transitions between broken and unbroken regions. The evolution of the phase-field follows an equation where the driving forces of crack growth are derived from an energy minimization principle, typically based on an Ambrosio-Tortorelli type functional. Modifications allow accounting for the no-healing irreversibility constraint of crack evolution and for the asymmetry of fracture, i.e., the fact that cracks only grow under tensile loadings but not under compression. Further modifications consider the crack evolution under pressure and at finite strains using energy densities, which are polyconvex functions of the deformation, [2, 3].

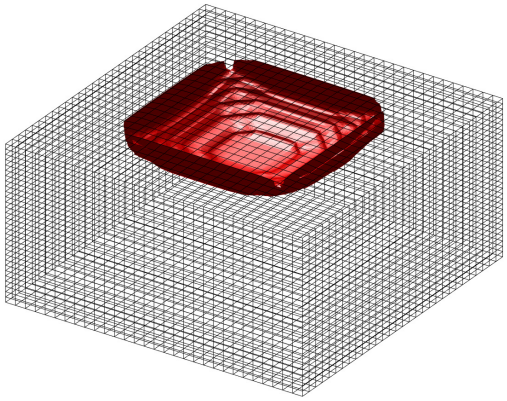


Figure 1: Crack surface in conchoidal fracture [1].

In this contribution different decompositions of the elastic energy and the pros and cons of variational and ad hoc formulations for the crack driving forces will be discussed. The latter may be based on positive principal stresses or strains for example. We compare models in linearized and in finite elasticity and present recent results on the mathematical analysis for a finite strain phase-field model. To illustrate the capability of a phase-field fracture approach, finite element simulations of brittle fracture are presented and in part compared to experimental results. The main challenge of our fracture simulations is that they require the ability of a numerical method to predict crack nucleation and fracture without stress concentration at a notch or at an initial crack.

References

[1] C. Bilgen, A. Kopaničáková, R. Krause, and K. Weinberg. "A phase-field approach to conchoidal fracture". *Meccanica* 53 (2018), pp. 1203–1219.

[2] C. Bilgen and K. Weinberg. "On the crack-driving force of phase-field models in linearized and finite elasticity". *Comp. Meth. in Appl. Mech. and Engng.* 353 (2019), pp. 348–372.

[3] M. Thomas, C. Bilgen, and K. Weinberg. "Analysis and simulations for a phase-field fracture model at finite strains based on modified invariants". *ZAMM - Journal of Applied Mathematics and Mechanics* (2020), e201900288.

Brief Biosketch of Kerstin Weinberg

Kerstin Weinberg received her PhD. in 1996, from the University of Magdeburg, with an emphasis on applied mechanics. She later worked as a research associate at the University of Kiel, the Medical University of Lübeck, and the California Institute of Technology. She was an assistant professor at the Technical University of Berlin from 2003 to 2008. Since 2008, she heads the Chair of Solid Mechanics at the University of Siegen.

She is currently elected member of the managing board of the International Association of Applied Mathematics and Mechanics (GAMM) and also serves on the editorial boards of Technische Mechanik, Continuum Mechanics and Thermodynamics, and Journal of Mechanics and Physics of Solids. She is also an associate editor of Mechanics of Materials.

She is broadly interested in numerical computations, from microstructural modeling of materials to engineering applications. Along with her group, she often works on non-linear problems in a multi-field setting. They range from dynamic fracture simulations, damage in soft polymers, diffusive phase decompositions in multi-component alloys to stochastic approaches, and high order finite element methods.

Continuum modeling of grain boundary plasticity using dislocations and disconnections

Nikhil Chandra Admal

Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, Illinois, USA

The macroscopic thermomechanical response of a polycrystalline material depends on its microstructure, which itself evolves. The focus of this talk is on the mesoscale modeling of the evolution of grain boundaries, which is a fundamental open problem relevant to technologically important processes such as additive manufacturing.

Traditionally, grain boundary (GB) evolution was modeled as motion by curvature (Mullins model [3]) which is a consequence of minimizing the GB energy. On the other hand, molecular dynamics simulations demonstrate that grain boundaries not only respond to stress but also plastically deform a material as they move resulting in a coupling between GB motion and deformation in phenomena such as stress-induced GB motion, and grain rotation. This observation, and the necessity to study large aggregates of grains motivate us to generalize the Mullins model.

In this talk, I will describe two approaches to model GB evolution and the accompanying plasticity. In the first approach [1], GBs are constructed using geometrically necessary dislocations (GNDs), and the GB energy is included in the constitutive law via the norm of the GB-GNDs. The simplicity of the model, and its ability to describe the coupled phenomena mentioned above are the highlights of the model. On the other hand, its major shortcoming arises from the non-uniqueness of GNDs to describe a grain boundary.

Next, motivated by the recent work of [2], I will describe our ongoing work on a second approach wherein GB evolution is modeled using continuum disconnections, which are dislocations with a step character. While the disconnections-based approach addresses the shortcomings of the GND-based approach, it is limited to specialized (Σ) grain boundaries. Finally, I will close with a proposal of a model that combines ideas from the two approaches and will enable us to model GB evolution in arbitrary polycrystals.

References

[1] N. C. Admal, G. Po, and J. Marian. "A unified framework for polycrystal plasticity with grain boundary evolution". *International Journal of Plasticity* 106 (2018), pp. 1–30.

[2] J. Han, S. L. Thomas, and D. J. Srolovitz. "Grain-boundary kinetics: A unified approach". *Progress in Materials Science* 98 (2018), pp. 386–476.

[3] W. W. Mullins. "Two-dimensional motion of idealized grain boundaries". *Journal of Applied Physics* 27.8 (1956), pp. 900–904.

Brief Biosketch of Nikhil Chandra Admal

Nikhil Admal is an Assistant Professor in the Department of Mechanical Science and Engineering at the University of Illinois at Urbana–Champaign. He is broadly interested in the multiscale modeling of materials at various length and times scales ranging from the atomic scale to the continuum scale. Currently, the focus of his research is on the study of recrystallization in refractory materials to increase their operating temperature, and development of first-principles strain gradient elastic models to include non-local effects relevant in micromechanical systems, and systems with defects.

He obtained his Ph.D. in Aerospace Engineering and Mechanics from the University of Minnesota under the guidance of Prof. Ellad Tadmor. Subsequently, he was a Postdoc in the Materials Science and Engineering department at UCLA working with Prof. Jaime Marian.

More information is available at: https://publish.illinois.edu/admal/people/

Ionic polymer nanocomposites under deformation

Ahmad Moghimikheirabadi[1], Martin Kröger[1], and Argyrios V. Karatrantos[2]

[1] Polymer Physics, Department of Materials, ETH Zurich, Switzerland

[2] Materials Research and Technology, Luxembourg Institute of Science and Technology, Luxembourg

Polymer nanocomposites have received special attention from academia and industry during the last 30 years, due to their improved properties in comparison to polymer blends. Nanoparticle (NP) dispersion is necessary for effective reinforcement in the matrix and is a prerequisite for property "tuning" and enhancement. One way to provide NP dispersion is to let the interaction between NPs and chains to be of an ionic nature. The presence of oppositely charged ions at the polymer/nanofiller interphase can promote dispersion. This relatively new class of ionic nanocomposites combines filler reinforcement with the reversibility of ionic interactions. Despite the improved mechanical performance, the reversible feature of ionic bonds, that can break and reform under certain conditions has led to smart materials for self-healing, shape-memory, piezoelectric, and mechanochromic applications due to their ability to respond directly under a certain chemical or physical stimulus [1, 3].

We set out to investigate the dynamics, structure, entanglements, and viscoelastic properties of ionic nanocomposites by means of coarse-grained molecular dynamics simulations. To this end, we study model systems consisting of bead-spring polymer chains and spherical nanoparticles –roughly with the same size as polymer radius of gyration– both in equilibrium [2] and subject to a deformation field.

References

[1] A. Crosby and J. Lee. "Polymer nanocomposites: The nano effect on mechanical properties". *Polym. Rev.* 47 (2007), pp. 217–229.

[2] A. Moghimikheirabadi, C. Mugemana, M. Kröger, and A. Karatrantos. "Polymer Conformations, Entanglements and Dynamics in Ionic Nanocomposites: A Molecular Dynamics Study". *Polymers* 12.11 (2020), p. 2591.

[3] M. Supova, G. Martynkova, S. Grazina, and K. Barabaszova. "Effect of nanofillers dispersion in polymer matrices: A review". *Sci. Adv. Mater* 3 (2011), pp. 425–431.

Brief Biosketch of Ahmad Moghimikheirabadi

Ahmad Moghimikheirabadi received his B.Sc. (2011) and M.Sc. (2013) degrees in mechanical engineering from the Sharif University of Technology in Iran. He holds a Ph.D. in Materials sciences (2020) from ETH Zurich. He is currently a postdoctoral researcher in the Computational Polymer Physics group in the department of Materials of ETH Zurich. His current research interests include computational modeling with Monte Carlo- and molecular dynamics simulation techniques with applications to the area of soft matter physics.

A molecular simulation approach of epoxy resins: from curing to deformation and fracture

Robert Meißner[1,2]

[1] Insitute of Polymers and Composites, Hamburg University of Technology, 21073 Hamburg, Germany
[2] Institute of Surface Science, Helmholtz-Zentrum Geesthacht, 21502 Geesthacht, Germany

Thermoset polymers are the first choice for a matrix material used in carbon and glass fibre reinforced plastics in high-performance applications. The simple manufacturing process, combined with a relatively low price and adaptive design possibilities, represents the major advantage over thermoplastic matrices. However, already the curing of thermosets is a complex and non-equilibrium process, which eventually explains why a comprehensive understanding of the interplay of the basic linking processes and the collective organization of a complex polymer network is still lacking. However, this is a prerequisite for rationalizing the material reaction and macroscopic properties of thermosetting polymers. Previously, it was shown that a hybrid quantum mechanical and molecular mechanical approach to cross-link a thermoset polymer is capable of reproducing experimentally determined mechanical and thermodynamic properties of an equivalent system [2]. To cross-link the thermoset, a new method was developed, which we call "smooth topology transfer". This method allows a smooth transition from one molecular topology to another by mixing forces and energies in molecular dynamics simulations, achieving as a top-score a degree of cross-linking of 93%. Reactive attempts are further controlled by Monte Carlo selection criteria—which also take quantum mechanical corrections into account—allowing at the same time a polymer network with a minimum of residual stress. This is in-line with mechanical properties found in the literature and which are otherwise often overestimated by other cross-linking approaches. A good agreement between cross-linking degree and heat of formations at different curing temperatures was additionally found when comparing the results of the simulation with results from a Differential Scanning Calorimetry (DSC) of a commercially available similar thermosetting polymer. Only recently has it become known that thermoset polymers can undergo significant plastic deformation at certain conditions [1]. In an attempt to explain this fundamentally, based on the previously developed models for cured thermosets and a newly developed reactive force field based on a coarse-grained approach, we were able to show for the first time that plastic deformation is associated with a fairly large bond reorganization before material fractures actually occur.

References

[1] A. Doblies, C. Feiler, T. Würger, E. Schill, R. H. Meißner, and B. Fiedler. "Mechanical degradation estimation of thermosets by peak shift assessment: General approach using infrared spectroscopy". *Polymer* 221 (2021), p. 123585.

[2] R. H. Meißner, J. Konrad, B. Boll, B. Fiedler, and D. Zahn. "Molecular Simulation of Thermosetting Polymer Hardening: Reactive Events Enabled by Controlled Topology Transfer". *Macromolecules* 53.22 (2020), pp. 9698–9705.

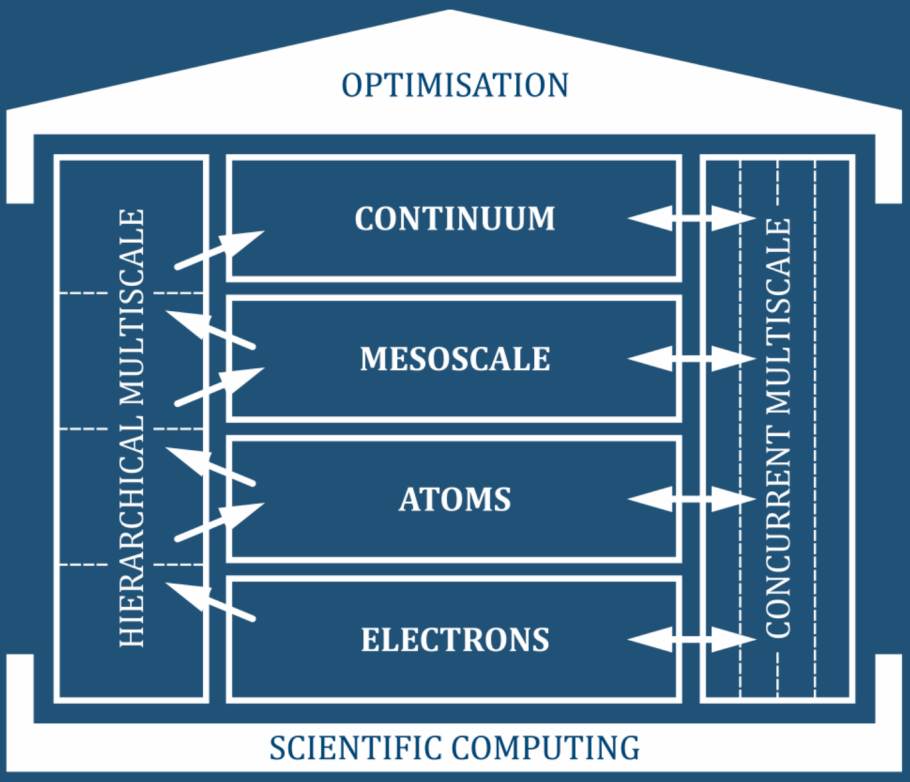
Brief Biosketch of Robert Meißner

Dr.-Ing. Robert Meißner is currently a professor at the Hamburg University of Technology (TUHH). He is affiliated with the Institute of Polymers and Composites at the TUHH and the Institute of Surface Science at the Helmholtz-Zentrum Geesthacht (HZG). He received his diploma in physics from the University of Bremen and his doctorate from the same university in the group of Prof. Lucio Colombi Ciacchi. However, he conducted his research at the Fraunhofer Institute for Manufacturing Technology and Applied Materials Research (IFAM) in Bremen, where he also was a postdoctoral research associate. During his time at IFAM, he completed courses to become a certified European Adhesives Specialist and a Fiber Reinforced Plastic Specialist. When he felt that the time had come for a professional change, he moved to Switzerland and worked in Prof. Michele Ceriotti's group at the École polytechnique fédérale de Lausanne (EPFL). Shortly after joining Michele Ceriotti's group, he received an appointment to a tenure-track junior professorship in soft matter simulations at TUHH. He is a long-standing member of the German Physical Society (DPG) and a deputy representative for the TUHH in the Topic Selection and Evaluation Committee of the Helmholtz Graduate School for the Structure of Matter (DASHH). His research focuses mainly on the application and development of advanced molecular dynamics simulation techniques to study interfaces between (bio)polymers as well as aqueous electrolytes and ionic liquids to inorganic surfaces such as amorphous carbons or ceramics. At the same time, he is interested in a fundamental atomistic understanding of magnesium corrosion processes, for which he is conducting research with colleagues at the Magnesium Innovation Center using machine learning methods and quantum chemical calculations based on ab initio approaches.

FRASCAL
GRK 2423

FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG

GRK 2423 FRASCAL
Fracture across Scales



Zentralinstitut
ZISC SCIENTIFIC COMPUTING

frascal.research.fau.eu/fvc