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Annual Report 2019

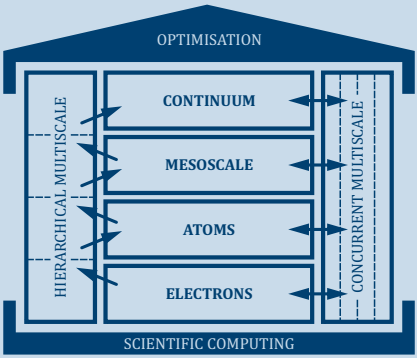
of the Research Training Group GRK 2423

FRASCAL

GRK 2423

Fracture across Scales:

Integrating Mechanics, Materials Science, Mathematics, Chemistry, and Physics



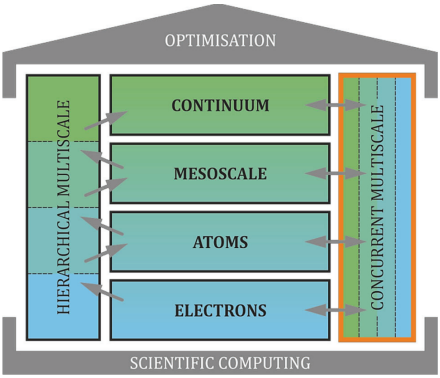
Annual Report
of the Research Training Group GRK 2423

FRASCAL
Fracture across Scales:

Integrating Mechanics, Materials Science, Mathematics, Chemistry, and Physics

at the
Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

Prof. Dr.-Ing. Paul Steinmann (spokesperson)
Prof. Dr.-Ing. Erik Bitzek (co-spokesperson)



2019

www.frascal.fau.de

Impressum

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Preface

The first year of our Research Training Group GRK 2423 FRASCAL has past.

This is a good opportunity to look back and thank all FRASCAL members, the doctoral and postdoctoral researchers together with the principal advisors and, last but not least, the coordinator and administrator, for their great engagement with the Research Training Group.

To date, the accomplished scientific and qualification achievements are already very impressive and, with further intense commitment, promise to result in successful doctoral theses.

The following report provides a detailed overview on the first research results, the already completed multidisciplinary qualification concept and other selected highlights, for example the participation of FRASCAL at the *Lange Nacht der Wissenschaften* as an independent program partner.

I am looking forward to see FRASCAL flourishing further.

Erlangen, December 2019

Paul Steinmann

Content

1 General Information

1.1 Title in German and English

Skalenübergreifende Bruchvorgänge:
Integration von Mechanik, Materialwissenschaften, Mathematik, Chemie und Physik
Fracture across Scales:
Integrating Mechanics, Materials Science, Mathematics, Chemistry, and Physics

1.2 Participating researchers

Prof. Dr.-Ing. Paul Steinmann (spokesperson), Prof. Dr.-Ing. Erik Bitzek (co-spokesperson)

Table 1: Participating supervisors

Principal Advisors (PAs)	Chair, Department, Work Address	Contact Data (Tel / Fax, Email, Web)	Research Area
Bitzek, Erik, Prof. Dr.-Ing.	General Material Properties, Dep. of Mat. Science and Engineering, Martensstraße 5, 91058 Erlangen	+49 9131 85-27 507 / -504, erik.bitzek@fau.de, gmp.ww.uni-erlangen.de	Material Properties Simulation
Leyendecker Sigrid, Prof. Dr.-Ing.	Applied Dynamics, Dep. of Mechanical Engineering, Immerwahrstraße 1, 91058 Erlangen	+49 9131 85-61 001, sigrid.leyendecker@fau.de, ltd.tf.uni-erlangen.de	Computational Dynamics
Mergheim, Julia, PD Dr.-Ing.	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-28 505 / -503, julia.mergheim@fau.de, www.ltm.tf.fau.eu	Computational Mechanics
Meyer, Bernd, Prof. Dr. rer. nat.	Computational Chemistry, Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen	+49 9131 85-20 403 / -404, bernd.meyer@fau.de, chemistry.nat.fau.eu/ccc/groups	Surface Science
Moretti, Paolo, Dr.	Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65 071 / -066, paolo.moretti@fau.de, matsim.techfak.uni-erlangen.de	Complex Microstructures
Pfaller, Sebastian, Dr.-Ing.	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-28 507/ -503, sebastian.pfaller@fau.de, www.ltm.tf.fau.eu	Scale Coupling Methods
Pöschel, Thorsten, Prof. Dr. rer. nat.	Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraße 3, 91058 Erlangen	+49 9131 85-70 501, thorsten.poeschel@fau.de, mss.cbi.fau.de	Granular Media
Smith, Ana-Sunčana, Prof. Dr. rer. nat.	Theoretical Physics, Dep. of Physics, Cauerstraße 3, 91058 Erlangen	+49 9131 85 70 565 / -518, smith@physik.uni-erlangen.de, puls.physik.fau.de/	Soft Matter
Steinmann, Paul, Prof. Dr.-Ing.	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-28 501 / - 503, paul.steinmann@fau.de, www.ltm.tf.fau.eu	Continuum Mechanics
Stingl, Michael, Prof. Dr. rer. nat.	Mathematical Optimisation, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen	+49 9131 85-67 141 / -20785, michael.stingl@fau.de, mso.math.fau.de	Optimization
Zahn, Dirk, Prof. Dr. rer. nat.	Theoretical Chemistry, Computer-ChemistryCenter, Nägelsbachstr. 25, 91052 Erlangen	+49 9131 85-20 205 / 404, dirk.zahn@fau.de, chemistry.nat.fau.eu	Condensed Matter
Zaiser, Michael, Prof. Dr. rer. nat.	Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65 060 / -066, michael.zaiser@fau.de, matsim.techfak.uni-erlangen.de	Statistical Mechanics of Materials

Table 2: Doctoral researchers

Doctoral Researchers	Chair, Department, Work Address	Contact Data (Tel / Fax, Email, Web)	Research Area
Bauer, Christof	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-28 508/ -503, christof.bauer@fau.de www.ltm.tf.fau.eu	Fracture in Thermoplastics: Discrete-to-Continuum
Birang Oskouei, Seyedeh Elmira	Central Institute for Scientific Computing, ZISC, Martensstraße 5a, 91058 Erlangen	+49 9131 85-20 783 / - 785, elmira.birang@fau.de, www.zisc.fau.de	Configurational Fracture/Surface Mechanics
Esfandiary, Nosaibeh	Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65 065 / -066, nosaibeh.esfandiary@fau.de, matsim.techfak.uni-erlangen.de	Collective Phenomena in Failure at Complex Interfaces
Konrad, Julian	Theoretical Chemistry, Computer-ChemistryCenter, Nägelsbachstr. 25, 91052 Erlangen	+49 9131 85-20 425 / -404, julian.konrad@fau.de chemistry.nat.fau.eu	Fracture in Polymer Composites: Nano to Meso
Kumar, Paras	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-20 323 / -503, paras.kumar@fau.de, www.ltm.tf.fau.eu	Fracture in Polymer Composites: Meso to Macro
Lakshmipathy, Tarakeshwar	General Material Properties, Dep. of Mat. Science and Engineering, Martensstraße 5, 91058 Erlangen	+49 9131 85-27 486 / -504, tara.ll.lakshmipathy@fau.de, gmp.ww.uni-erlangen.de	Atomistics of Crack-Heterogeneity Interactions
Müller, Tobias	Computational Chemistry, Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen	+49 9131 85-20 421 / -404, tobias.tm.mueller@fau.de, chemistry.nat.fau.eu/ccc/groups	Chemistry at the Crack Tip
Phansalkar, Dhananjay	Applied Dynamics, Dep. of Mechanical Engineering, Immerwahrstraße 1, 91058 Erlangen	+49 9131 85-61 019 / -011, dhananjay.phansalkar@fau.de, ltd.tf.uni-erlangen.de	Adaptive Dynamic Fracture Simulation
Ritter, Jonas	Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65 064 / -066, jonas.ritter@fau.de, matsim.techfak.uni-erlangen.de	Compressive Failure in Porous Materials
Singh, Sukhminder	Mathematical Optimisation, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen	+49 9131 85-67 048 / -20785, sukhminder.singh@fau.de, mso.math.fau.de	Fracture Control by Material Optimization
Velasco Sabogal, Ali Mauricio	Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraße 3, 91058 Erlangen	+49 9131 85-70 506, mauricio.as.velasco@fau.de, mss.cbi.fau.de	Fragmentation in Large Scale DEM Simulations

Table 3: Postdoctoral researchers

Post Docs	Chair, Department, Work Address	Contact Data (Tel / Fax, Email, Web)	Research Area
Davydov, Denis, Ph.D.	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-28 502 / 503, ltm-sekretariat@fau.de, www.ltm.tf.fau.de/	Multi-Scale Modelling and Simulation
Duchstein, Patrick, Dr. rer. nat.	Theoretical Chemistry, Computer-ChemistryCenter, Nägelsbachstr. 25, 91052 Erlangen	+49 9131 85-20 425 / 404, patrick.duchstein@fau.de, chemistry.nat.fau.eu	Fracture in Polymer Composites: Nano to Meso
Floros, Dimosthenis, Dr.	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-20 783 / - 785, dimosthenis.floros@fau.de, www.ltm.tf.fau.eu	Configurational Fracture/Surface Mechanics
Karewar, Shivraj, Dr.	General Material Properties, Dep. of Mat. Science and Engineering, Martensstraße 5, 91058 Erlangen	+49 9131 85-27 486 / -504, shivraj.karewar@fau.de gmp.ww.uni-erlangen.de	Modelling Fracture on the Atomic Scale
Wick, Christian, Dr. rer. nat.	Theoretical Physics, Dep. of Physics, Cauerstraße 3, 91058 Erlangen	+49 9131 85 70 566 / -518, christian.wick@fau.de, puls.physik.fau.de/	Quantum-to-Continuum Model of Thermoset

Table 4: Associated doctoral researchers

Associated Doctoral Researchers	Chair, Department, Work Address	Contact Data (Tel / Fax, Email, Web)	Research Area
Atila, Achraf	General Material Properties, Dep. of Mat. Science and Engineering, Martensstraße 5, 91058 Erlangen	+49 9131 85-27 468 / -504, achraf.atila@fau.de, gmp.ww.uni-erlangen.de	Crack nucleation and propagation in anisotropic oxide glasses
Esfandiary, Samaneh	Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65 063 / -066, samaneh.esfandiary@fau.de, matsim.techfak.uni-erlangen.de	Robustness and failure of brain activity patterns
Hosseini, Seyyed Ahmad	Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65 065 / -066, ahmad.hosseini@fau.de, matsim.techfak.uni-erlangen.de	Modelling Fracture of Hierarchically Structured Materials
Ries, Maximilian	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-67 619/ -503, maximilian.ries@fau.de, www.ltm.tf.fau.eu	Multiscale Simulation of Amorphous Polymers
Schmidt, Ina	Faculty of Mechanical Engineering Kesslerplatz 12 90489 Nürnberg	+49 911 5880-1327 ina.schmidt@th-nuernberg.de	Computational Bone Remodelling
Spannraft, Lucie	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-67 620 / - 503, lucie.spannraft@fau.de, www.ltm.tf.fau.eu	Grain Boundary Mechanics
Wullschläger, Florian	Computational Chemistry, Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen	+49 9131 85-20 424 / -404, flo.wullschlaeger@fau.de, chemistry.nat.fau.eu/ccc/groups	Atomistic Simulations of 2D Materials
Zhao, Wuyang	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-28 511/ -503, lwuyang.zhao@fau.de www.ltm.tf.fau.eu	Small-Scale Informed Constitutive Modelling

Table 5: Student assistants

Students Assistants	Project, Supervisors	Course / Field of study	Member of RTG (from - to)
Dhamo, Kevin	P1, Tobias Müller, Bernd Meyer	Molecular Science	Jan 2019 – Dec 2019
Gitizadeh, Mohammad	P6, Sebastian Pfaller	Computational Engineering	Sep 2019 – Dec 2019
Jahnel, Stefanie	P3, Julian Konrad, Dirk Zahn	Molecular Science	Mai 2019 – Oct 2019
König, Filip	P3, Julian Konrad, Dirk Zahn	Molecular Science	Jan 2019 – Mar 2019
Lengger, Michael	P10, Paul Steinmann	Mechanical Engineering	Jan 2019 – Mar 2019
Livraghi, Mattia	P12; Christian Wick, Ana-S. Smith	Integrated Life Sciences (ILS)	Mai 2019 – Dec 2019
Moerman, Evgeny	P1, Bernd Meyer	Chemistry	Jul 2019 – Sep 2019
Polzer, Markus	P2, Tarakeshwar Lakshmipathy	Materials Science and Engineering	Jan 2019 – Dec 2019
Pominov, Arkadii	P3, Julian Konrad, Dirk Zahn	Materials Physics	Mar 2019 – Apr 2019, Oct 2019 – Dec 2019
Rohracker, Maurice	P8, Paras Kumar	Computational Engineering	Sep 2019 – Dec 2019
Singh, Jatandeep	P11, Michael Stingl	Computational Engineering	Sep 2019 – Dec 2019
Weber, Felix	P10, Christof Bauer, Paul Steinmann	Mechanical Engineering	Apr 2019 – Jun 2019, Nov 15, 2019 – Dec 2019
Weigand, Marcia	P6,Maximilian Ries, Sebastian Pfaller	Mechanical Engineering	Dec 2019
Wolf, Stefan	P4, Ali Mauricio Velasco Sabogal	Physics	Nov 2019 – Dec 2019

Table 6: Mercator Fellows

Mercator Fellows	Affiliation	Expertise
Aifantis, Elias C., Prof.	Aristotle University of Thessaloniki, Greece	Generalized continuum models with internal length and time scales
Ortiz, Michael, Prof.	California Institute of Technology, Pasadena, CA, USA	Physical models of fracture and their mathematical analysis
Ponson, Laurent, Dr.	Pierre et Marie Curie University, Paris, France	Analytical and numerical treatment of 3D cracks in heterogeneous media

Table 7: External Advisory Board

External Advisory Board	Affiliation	Expertise
Kolk, Karsten, Dr.-Ing.	Siemens AG	Fracture Mechanics
Meske, Ralf, PD Dr.-Ing.	Federal Mogul Nürnberg GmbH	Optimization
Münz, Thomas, Dr.	DYNAmore GmbH	Computational Methods
Russwurm, Siegfried, Prof. Dr.-Ing.	Former CTO of Siemens AG	Fracture Mechanics

1.3 Coordination and administration

Table 8: Coordination and administration of GRK 2423 FRASCAL

	Work Address	Contact Data (Tel / Fax, Email, Web)	Work Area
Dakkouri-Baldauf, Andrea, Dr. rer. nat.	Central Institute for Scientific Computing, ZISC, Martensstraße 5a, 91058 Erlangen	+49 9131 85-20782 / -20785, andrea.dakkouri@fau.de, www.frascal.fau.eu	FRASCAL Coordination
Deserno, Julia	Central Institute for Scientific Computing, ZISC, Martensstraße 5a, 91058 Erlangen	+49 9131 85 20780 / -20785, julia.deserno@fau.de, www.zisc.fau.de	ZISC Administration
Güthlein, Nicole	Central Institute for Scientific Computing, ZISC, Martensstraße 5a, 91058 Erlangen	+49 9131 85 20780 / -20785, guethlein@math.fau.de, www.zisc.fau.de	ZISC Administration
Lanig, Harald, PD Dr. rer. nat.	Central Institute for Scientific Computing, ZISC, Martensstraße 5a, 91058 Erlangen	+49 9131 85 20781 / -20785, harald.lanig@fau.de, www.zisc.fau.de	ZISC Managing Director

Figure 1: Members of FRASCAL at the Kick-Off Meeting on April 2, 2019 (image: Georg Pöhlein).

1.4 Reporting period

01 January 2019 to 31 December 2019

2 Research Programme

2.1 Research projects

FRASCAL comprises 11 doctoral projects (P1-P11) and an overarching postdoctoral project (P12), which reach from quantum mechanics (P1) via atomistic and particle-based methods (P1-P4) to the continuum scale (P8-P11). Several projects (P5-P7, P12) are dedicated to bridging between particle-based approaches (indicated in blue) and continuum-based techniques (indicated in green), whereby the postdoctoral project P12 integrates the results and the expertise developed in the doctoral projects in order to realise a concurrent multiscale modelling approach for fracture. The effect of heterogeneities on fracture behaviour is a common scientific question underlying all projects. Heterogeneities can exist at the atomic scale in the form of locally changed bonding (P1) or density (P2, 12), or at larger scales, where heterogeneities include second phases as in composites (P3, P6, P8, P11), and porous structures (P5), as well as interfaces and surfaces (P7, P10) or (micro) cracks (P4, P9).

In projects P2, P3 and P10, additional research was carried out by postdocs for a limited time (see page 40-46)

P1: Chemistry at the Crack Tip

Tobias Müller and Bernd Meyer

Objectives and status

Silicon was chosen as first model system. It has simple crystal and surface structures and extensive literature data on its fracture properties (from experiment and simulation) is available, making it an ideal candidate for first fracture simulations.

At the beginning, density functional theory calculations were performed with the PWscf code of the Quantum Espresso package. The lattice parameters, bulk elastic constants and surface energies of relaxed surfaces were determined. These calculations were done in generalized-gradient approximation with the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional using a plane wave basis set, Vanderbilt ultrasoft pseudopotentials and the semi-emprical Grimme D3 dispersion correction for including van der Waals forces. This data is needed to determine the long-range strain field of a crack tip, which was provided for us from project P2 together with an initial crack structure. The strain field serves as boundary condition for our *ab initio* simulations. Cutouts of the “pacman” structures are taken, the boundaries are saturated with hydrogen atoms, outer atoms are fixed and the inner part including the crack surfaces are relaxed.

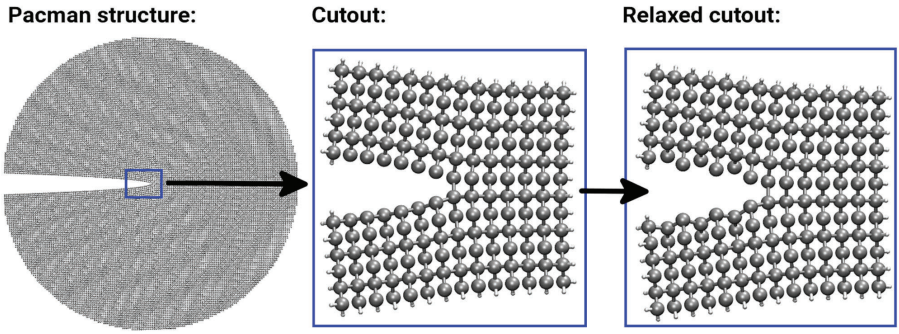


Figure 2: General procedure to create the structure of a crack.

For the structure shown in Figure 2, different series of Car-Parrinello molecular dynamics simulations (CPMD) were performed: without adsorbates, with different loads, and for crack tips exposed to H_2, O_2 or water. The simulation cell was heated to room temperature and equilibrated. Adsorbate molecules with random initial velocities were placed inside the crack and propagated in order to initiate stress corrosion cracking under subcritical load. For O_2 and water spontaneous dissociation events are observed, whereas the dissociation barrier for H_2 is too high for a chemical reaction to occur on the timescale of the simulations. Adding more and more adsorbate molecules to the simulation cell results in the formation of an initial silicon oxide/hydroxide monolayer (see Figure 3). While for water spontaneous reactions stop at this point, oxygen continues to break Si bonds and penetrates deeper into the silicon.

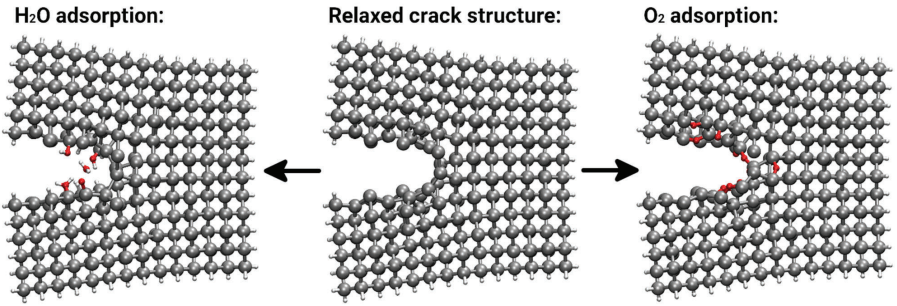


Figure 3: First CPMD simulations.

Recently, project P2 provided us with their “pacman” scripts for performing anisotropic elasticity calculations of the strain field around a crack. This enables us to create independently new crack structures for varying loads (stress intensity factors *K*, see Figure 4). Right now, the described simulations are repeated to examine the influence of an increased load.

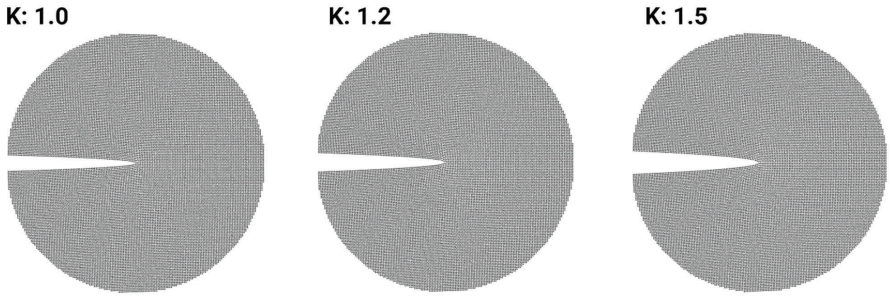


Figure 4: Crack structures with different initial load (stress intensity factor K).

Conclusions, main achievements and outlook

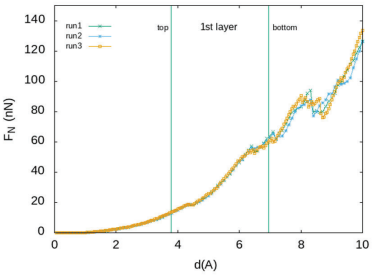
A first test system was established to investigate stress corrosion cracking by subcritical loads. Bond breaking events are observed for oxygen, while water only dissociates and hydroxylates the crack surfaces. To enforce also reactions of more inert adsorbates like hydrogen, acceleration methods like umbrella sampling and metadynamics are needed and will be used in future simulations. Furthermore, the present approach based on the elastic strain field from the “pacman” structures is only valid up to the first bond breaking. Then the strain field has to be adjusted. Thus, for studying crack propagation, an automated procedure for recalculating the strain field needs to be established, possibly by switching to a QM/MM approach.

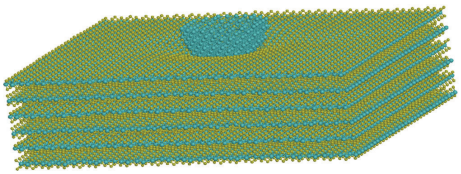
P1: Mechanical and Chemical Properties of 2D Materials

Florian Wullschläger and Bernd Meyer

Objectives and status

In the last six months, I started to work on a new project, which aims at a fundamental understanding of the elementary atomistic mechanisms of damage, wear and failure in solid lubricants for ball bearings. Specifically, I am interested in wear, fracture and chemical modification of MoS_2 films under extreme loads. As first steps, I had to choose an appropriate reactive atomic interaction potential for MoS_2, get it incorporated into the LAMMPS molecular dynamics code and setup a MoS_2 model system for first atomistic simulations (see below). In my first molecular statics calculations for a model of six MoS_2 layers (about 26000 atoms) and a hollow spherical tip, I encountered many different problems with the minimization methods available in LAMMPS, which lead to either non-converged results or computationally expensive relaxations. Therefore, I changed strategy from geometry relaxations to using averages over molecular dynamics trajectories. With the new approach at hand I was able to perform first initial indentation simulations, where I pressed a tip into the MoS_2 layers to investigate the deformation and fracture of the lubricant (see below). Further simulations were performed for dragging the indented tip over the layers (scratch tests), for the compression of the layered material and the sliding of the layers against each other.





Conclusions, main achievements and outlook

Up to now, I only used rather small model systems, which may show severe finite size effects. The aim is to be able to compare the indentation and scratch simulations with results from nanoindentation and nanoscratch experiments in the group of Benoit Merle (WW1/FAU). New simulations will be done for larger systems and for films with different textures, for which I will analyse damage and fracture mechanisms depending on load and gliding speed.

P2: Influence of Structure and Anisotropy on Deformation and Fracture of Oxide Glasses

Achraf Atila and Erik Bitzek

Objectives and status

Metaphosphate glasses, defined as the composition in which the ratio O/P is three, have a chain-like structure made of PO_4 tetrahedra.

It is commonly known that glasses produced by melt-quenching are isotropic. However, anisotropy can be introduced in glasses during the glass making process, e.g., by fibre drawing. This anisotropy influences remarkably the mechanical properties. Additionally, we point out that there is a need to distinguish between (i) transient anisotropy, which is only exhibited by a material under load and (ii) persistent anisotropy, which is reversible only upon thermal annealing. For this reason, molecular dynamics simulations were performed to study the origins of the structural anisotropy in metaphosphate (Na_2O-P_2O_5, MgO-P_2O_5 and CaO-P_2O_5) glasses. The atomistic view of the glass structure showed us that the anisotropy seen in the mechanical properties of the predeformed glasses is linked to an anisotropic structure due chains orientation. Our results helps in the understanding of the origin and effect of the structural anisotropy on the mechanical behaviour of metaphosphate glasses.

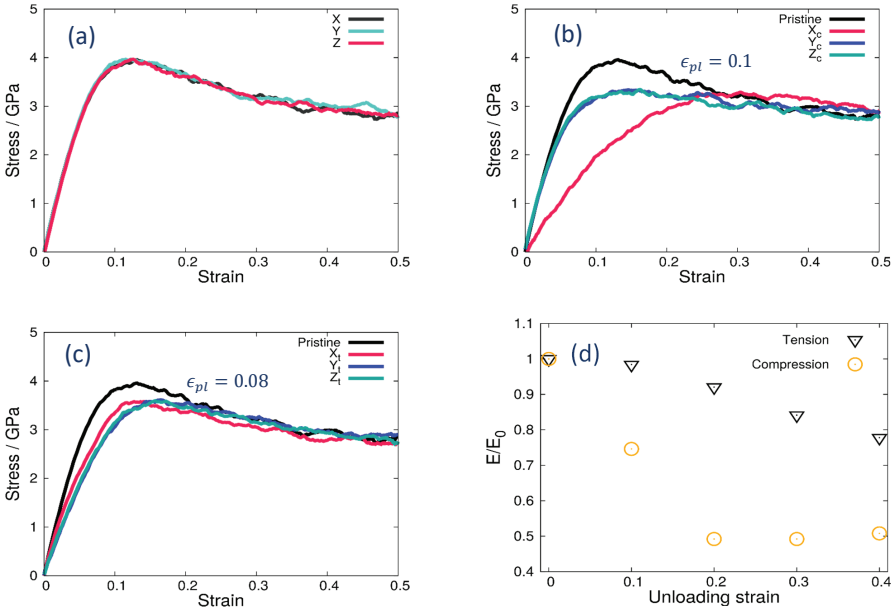


Figure 5: Tensile stress-strain curves along X, Y, and Z directions in (a) isotropic magnesium metaphosphate glass, (b) anisotropic magnesium metaphosphate glass where the anisotropy was induced by pre-compression along X, (c) anisotropic metaphosphate glass where the anisotropy was induced by pre-tension along X. (d) Normalized Young's modulus as a function of the unloading strain of pre-deformed anisotropic MgP_2O_6 glass.

Conclusions, main achievements and outlook

The results show that the type of the modifier (e.g., Na^+) have an effect on the degree of the persistent anisotropy in the metaphosphate glasses, which was linked to the cation-oxygen bond strength (field strength). Cations with higher field strength show higher degree of the persistent anisotropy and higher elastic moduli. It is planned to start working on some preliminary results on the fracture and crack propagation in different oxide glasses with different network connectivity.

P2: Influence of Crack Tip Radius on Fracture Behaviour: An Atomistic Study

Tarakeshwar Lakshmipathy and Erik Bitzek

Objectives and status

The influence of finite blunting radii on fracture behaviour was studied using quasistatic simulations at the atomic scale. The calculations were performed using various embedded atom method (EAM) potentials for tungsten (bcc) for different crack systems. All calculations were performed with the open source code IMD.

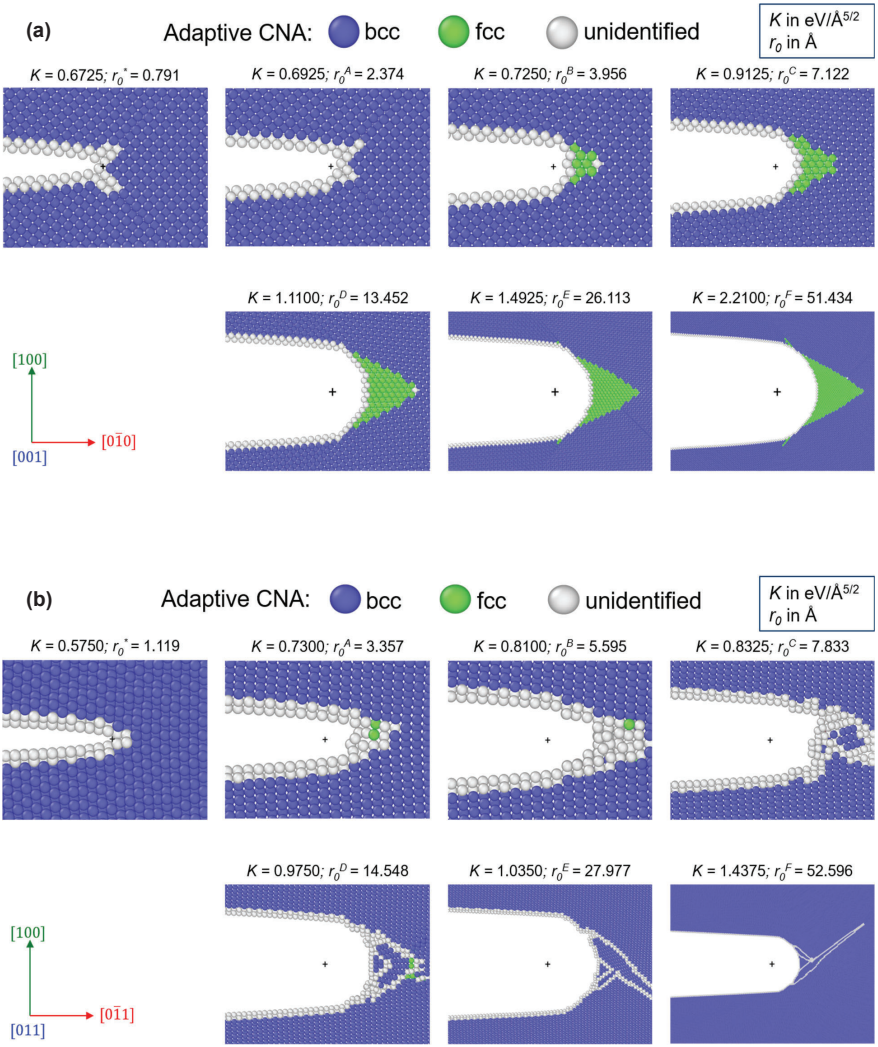


Figure 6: Atomic rearrangements in (a) crack system (100)[001] and (b) crack system (100)[011] at loads (K) below the critical value for sharp crack reinitiation with blunted cracks (crack tip radii r_0^A to r_0^F), in contrast to the behaviour with an atomically sharp crack (crack tip radius r_0^*). Crystal structures were identified using adaptive Common Neighbor Analysis (CNA) tool in Ovito.

In the crack system (100)[001], it was observed that a region ahead of the crack tip transformed to a distorted fcc structure before a sharp crack was reinitiated from the pre-existing blunted crack (see Figure 6(a)). In addition, it was found that the volume of the transformed region played a significant role in determining the fracture toughness, which was a linear function of the blunting radius.

In the crack system (100)[011], the crack tip underwent reconstruction with small blunting radii, re-orientation with intermediate blunting radii and twinning with large blunting radii (see Figure 6(b)). The fracture toughness was a non-linear function of the blunting radius, with the fracture mechanisms depending on the degrees of freedom offered by the magnitude of blunting.

Conclusions, main achievements and outlook

Earlier works have shown that EAM potentials for bcc metals like tungsten could be problematic. To check whether the aforementioned results are correct, it is planned to perform calculations using density functional theory (DFT) and a bond order potential (BOP), and compare them to the results using EAM potentials. Due to the computationally expensive nature of DFT and BOPs, cutouts at selected loads will be used for the comparisons.

Furthermore, plasticity and transformations at the crack tip make the results ill suited for comparisons with linear elastic fracture mechanics. Hence, calculations with harmonic potentials will be performed where the fracture behaviour is expected to be perfectly brittle.

P3: Fracture in SiO_x Polymer Composites: from Nano to Meso Scale

Julian Konrad and Dirk Zahn

Objectives and status

A MD/MC approach based on quantum mechanics was used to form epoxy resins with high crosslinking degrees (η = 96 %) with mechanical properties close to experimental data.

Δ E values from DFT calculations were fed into the Monte Carlo decision tree and a sigmoidal function made a smooth topology transfer from the reactants to the product [in collaboration with. Prof. Dr.-Ing. R. Meißner TUHH]. The curing process was performed at different temperatures which yielded in different η's and therefore resulting in slightly various mechanical properties. These specifications are here shown for a crosslinking degree of 91%.

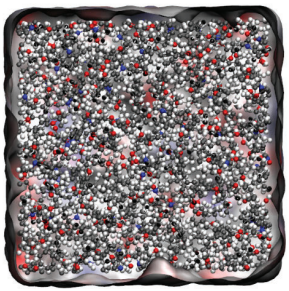


Figure 7: Epoxy resin before elongation.

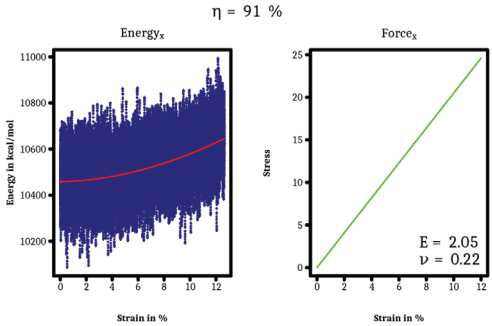


Figure 8: Mechanical properties derived from the total energy during elongation.

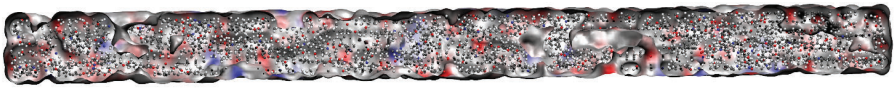


Figure 9: Epoxy resin after elongation.

Furthermore, fracture mechanics are going to be discovered, which requires a dissociative force field of the epoxy resin.

The development of this FF again is based on DFT calculations, where the product was pulled apart between the bonds of the reactants. A potential function was fitted into this computation neglecting the activation barrier because of its kinetic manner. The reacting atoms were treated as united atoms to mimic the proton transfer, the bond of those with the new potential and the topology of the thermoset describes the epoxy resin. The resulting model reflects the properties of the thermoset and the resin and is additionally reactive to facilitate fracture mechanics.

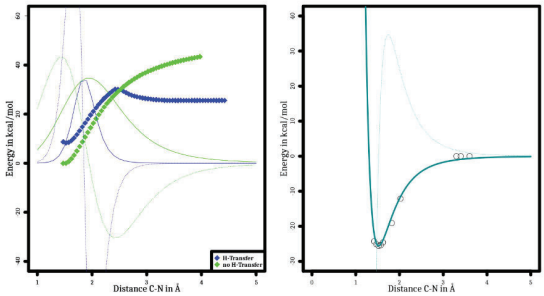


Figure 10: QM-based development of the dissociative Force Field.

First tensile tests verified the possibility of fracture of epoxy resins with the reactive FF in contrast to the OPLS-AA FF for the initial system.

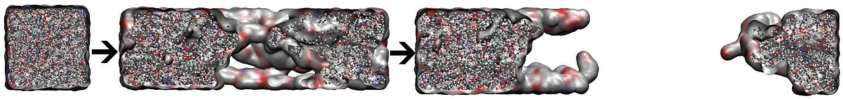


Figure 11: Fracture of the epoxy resin with reactive Force Field.

Conclusions, main achievements and outlook

Creation of a model of epoxy resins with high crosslinking degrees and mechanical properties in agreement with the experiment. Development of a force field for the dissociation of the decisive atoms for fracture mechanic investigations was achieved. Further studies will focus on the mechanical properties of different shapes and crack propagation.

P4: Multi-sphere algorithm for Large Scale DEM simulations with fractures

Ali Mauricio Velasco Sabogal and Thorsten Pöschel

Objectives and status

One of the main project objectives is to computationally represent grains with any arbitrary shape. This representation should be done in such a way that the generated grains can be used in a DEM simulation i.e. the DEM contact laws, defined mainly for spheres, must be still applicable. Furthermore, the used algorithm should be capable to track the appearing of new fragments and complex shapes after the grain breakage. The correct computation of the inertia tensor and mass and volume conservation was an additional challenge of the model.

A common representation of irregularly shaped grains in DEM is by clumps of spheres (Multi-sphere approach). However, past multi-sphere creation methods were computationally slow and expensive and, concavities and holes present in the shapes could not be represented.

To solve this, we create a novel multi-sphere algorithm that is able to represent any shape, even when concavities, holes and discontinuities are present. The iterative algorithm locates spheres only inside the surface of the shape to represent. As a result, hollow multi-sphere particles of an optimal reduced number of spheres are obtained. The computational time is one order of magnitude less than the previous tested algorithm.

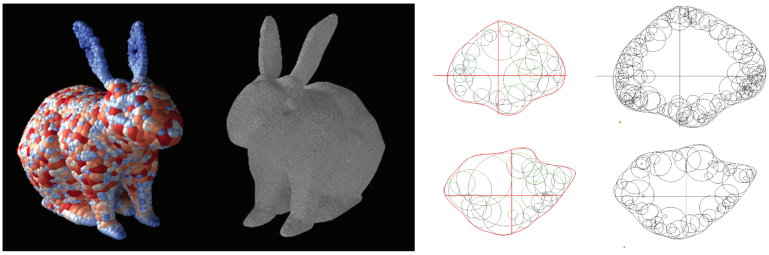


Figure 12: Complex shape represented by multi-sphere clump (left). Comparison of slices of represented shapes: previous algorithm in red, our proposal in black (right).

In addition, a coupled algorithm to compute the inertia tensor from the original shape, represented via a triangulated point cloud, is proposed and tested.

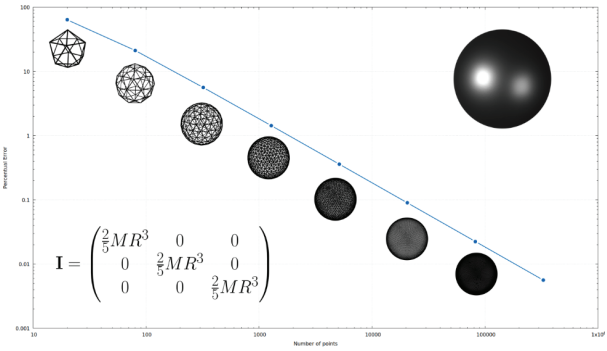


Figure 13: Inertia tensor computation method. Convergence study.

Conclusions, main achievements and outlook

A novel algorithm for representing any complex 3D shape by a clump of spheres was developed and tested. In addition, a methodology for computing the inertia tensor of the irregular grains and assure mass and volume conservation after the breakage was proposed.

Once the geometrical representation of the grains is suitable for a DEM simulation. The next step is modelling the fracture occurrence under stress conditions. The proper definition of the crack geometry, the size distribution of the fragments and the fracture criteria is the current work of the project.

P5: Modelling Failure and Flaw Tolerance of Hierarchically Structured Materials

Ahmad Hosseini and Michael Zaiser

Objectives and status

Our aim is to develop Beam network models (BNM) and employ it in our research on fracture and flaw tolerance of hierarchically structured fibrous (bio)materials. BNM serves as a paradigmatic modelling approach which despite its simple structure captures key features of fracture as a multiscale process: The existence of local failure thresholds which reflect properties of the material microstructure, the existence of an internal length above which the material can be described as a continuum, and the long-range coupling of different material elements by long-range stress fields that emerge in response to local failure. By abstracting from the bewildering detail of real material microstructures, such models achieve a degree of simplicity that makes them amenable to large-scale simulations and systematic studies over a wide range of system sizes, using ensembles of a size that allows for meaningful statistical predictions.

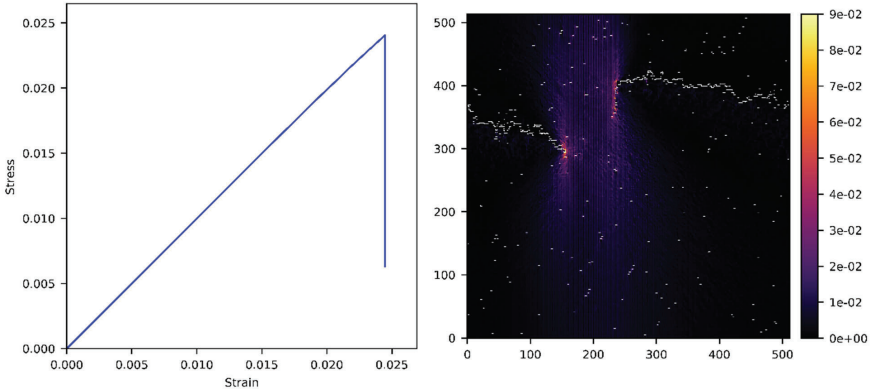


*Figure 14: Damage propagation and stress-strain curve in a typical randomly cross-linked beam network model of size 512*512, with cross-linking ratio = 0.667. The failure thresholds of network beams elements are statistically distributed with a Weibull distribution exponent of 4 and a mean of 0.1.*

We have used our model to study the nucleation and propagation of cracks in materials consisting of randomly cross-linked fibres with statistically distributed failure thresholds (Figure 14). We investigated failure behaviour of such materials and determined the fraction of cross-links, which is required to achieve an optimal strength-to-weight ratio for different degrees of disorder.

Conclusions, main achievements and outlook

Our exercise demonstrated that, for materials whose failure strength may be subject to a large statistical scatter, even very simple design questions might have answers that depend critically on parameters characterizing the statistical scatter of material properties. Thus the question 'is it beneficial to introduce statically redundant cross links into a net-work of parallel load-carrying fibres' has opposite answers when we are dealing with a very reliable material (low statistical scatter: cross links are superfluous or even detrimental to performance) and with a very unreliable material (cross links significantly improve structural performance).

To explore how hierarchical organization affects the precursor activity in the run-up to failure and ultimately changes the mode of failure, we formulate for the first time hierarchical generalizations of beam network model (BNM).

P5: Compressive Failure in Porous Materials

Jonas Ritter and Michael Zaiser

Objectives and status

At first, time was invested to establish an elaborate organizational structure of the PhD project (documentation, gathering and organize of information, etc.). In parallel, requirements for an appropriate approach to simulate microstructural compaction were evaluated. At this, it turned out that for the planned simulations the peridynamics theory could be more beneficial rather than the discrete element method. It is also considered to be better suited for simulating realistic microstructures with complexed shaped geometries. Moreover, to the author's knowledge, peridynamics was never used to simulate resolved snow or sandstone microstructures. In addition, research cooperation partners at the WSL-Institut für Schnee- und Lawinenforschung SLF and the SLAB institute at EPFL utilize the Finite Element Method (FEM) respectively Material Point Method (MPM) in similar projects. Therefore, and in agreement with our partners at SLF and EPFL the decision was made to use this non-local continuum theory on the microscale.

To obtain a deeper understanding and knowledge of the theory itself the fundamental literature on peridynamics was worked through. Moreover, a one-dimensional peridynamics code was implemented in C++. It has been written to gain deeper insight into the issues of peridynamic codes and shall be extended to two dimensions in future. This code will be then used for testing more complex material models. As a productive peridynamic code as a means the simulation of realistic microstructures Peridigm of the Sandia National Laboratories is used. It provides an extensible and comprehensive code framework based on Sandia's Trillions project. This library collection is also used by the molecular dynamics code LAMMPS.

In the further course of the project, a set-up for first peridynamic simulations based on real microstructure has been designed. Computed tomography (CT) images of snow specimen, provided by the WSL-SLF, served therefore as a simulation data base. It turned out pre-processing of the input data seems to be a challenging part of it. The geometrical data for the simulation must be given in an appropriate data format, which has to be extracted from CT-images first. Furthermore, raw CT-data need to be prior post-processed to make them accessible as a volumetric representation of the microstructure. Beside reconstruction of the volumetric shape this contains also the generation of a volume mesh for discretizing the microstructure in finite sub volumes. These are the basis for input of the geometry to the simulations.

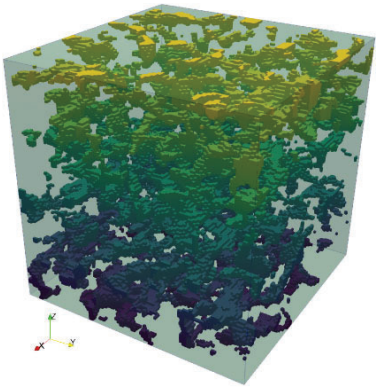


Figure 15: Highly porous snow microstructure discretized by voxel representation. Colours indicate the voxel number.

Relating to the extraction of relevant information from already post-processed CT-data, great progress could be made during a two-week research stay at the SLAB institute of EPF Lausanne (Switzerland). Based on the voxel-discretized snow CT-data, shown in Figure 15, the hexahedrons position and volume have been determined. These were used as an input for a very first successful peridynamic simulation of a highly porous snow microstructure. A state-based elastic material served as material model in the displacement controlled compression simulation. The elastic constant where chosen such that it mimics those of ordinary ice. A critical bond-stretch approach simulated damage of the ice material matrix.

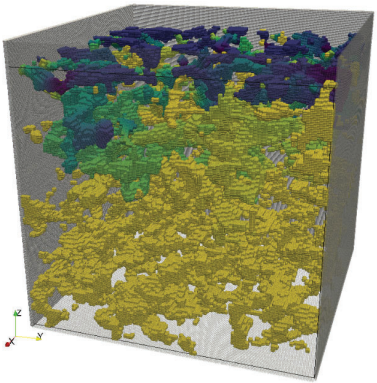


Figure 16: Magnitude of the displacement field at an early stage of confined, displacement-controlled compression simulation with the confinement indicated in grey.

Beside a first simulation, attempts with varying set-up were performed to gain first experiences with the Peridigm code. It included confined compression tests (Figure 16), simulations with and without gravitational load as well as various combination of input parameters. Confinement of the specimen was achieved by introducing walls represented by plates made of steel. It is depicted as the grey domain in Figure 16. As a result, the number of computational integration points highly increased which end up in rising computational time.

Conclusions, main achievements and outlook

Overall, the results revealed the requirements for improvements in the peridynamic simulation code and the need of a higher geometrical resolution. To overcome the deficiency of the confinement representation by plates, walls like in discrete element codes must be implemented. Apart from that, extension of existing contact models need to be made as well as mechanism for natural dissipation should be included into the set-up. This could be achieved by applying a visco-plastic material model and adding friction in the contact. The adequate choice of the horizon and its physical counterpart as well as a solution for problem of material weakening at surfaces remains an open question so far.

In summary, with the first fruitful peridynamic simulations of realistic snow microstructures important experiences have been gained. In addition, the simulations showed first promising results as well as the aforementioned challenges. However, these objections might be overcome with justifiable expenditure and changes in the existing code. Furthermore, the cooperation with our research partners opens new perspectives. Thus, successful progress could be made in the project's first year.

P6: Fracture in Thermoplastic Polymers: Discrete-to-Continuum Coupling

Christof Bauer and Sebastian Pfaller

Our project aims to extend the Capriccio method to adaptive particle-based regions moving within the continuum. This is an essential precondition for our long-term research on multiscale fracture simulation: There, the individual levels of resolution will be chosen such that the moving crack tip can be fully described by MD. Hence, the remaining parts, which are typically exposed to low stresses and strains, can be modelled with significantly less computational effort by continuum mechanics. That far, it can be stated that no suitable approach for thermoplastic materials exists. One reason for this is the amorphous structure of thermoplastics without any lattice structure, which makes such an approach much more difficult. Thus, the development of a new method is required.

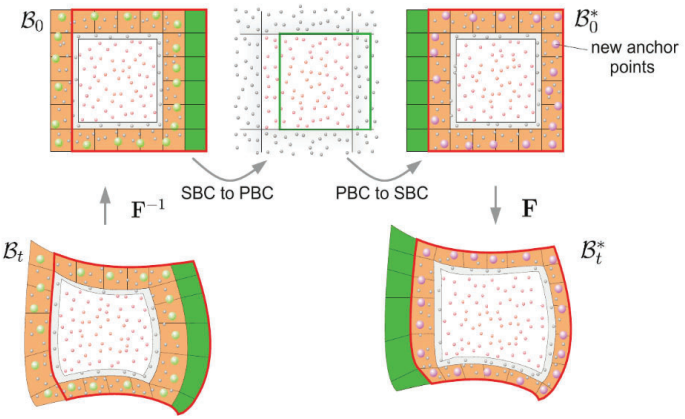


Figure 17: PBC moving approach.

Within the scope of project P6, two basic methods are being acquired and investigated. The one under the working title "PBC moving approach" (Figure 17, PBC: periodic boundary conditions, SBC: stochastic boundary conditions), the other under "machine learning expansion approach" (Figure 18). One of the main challenges is to adapt the particle region without generating a new initial system in each adaptation step and to avoid expensive re-computations by using an MD system built beforehand.

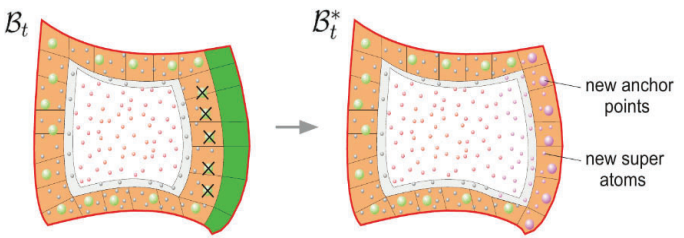


Figure 18: Machine learning expansion approach.

The MD system and thus the initial configuration of the considered polymer below glass transition temperature is derived from pure MD simulations. For this purpose, the Capriccio group currently uses the MD code IBIsCO, which is provided by TU Darmstadt. In order to open up further possibilities, the transfer to the widely used MD code LAMMPS was carried out and the polymer was derived in the initial configuration in coarse-grained resolution. Figure 19 and Figure 20 show the polymer chains (300 chains with chain length of 200 beads) with Figure 19 illustrating the polymer chains created by a random walk algorithm at lower density in the starting configuration. Figure 20 depicts the polymer in the final solid state after the equilibration.

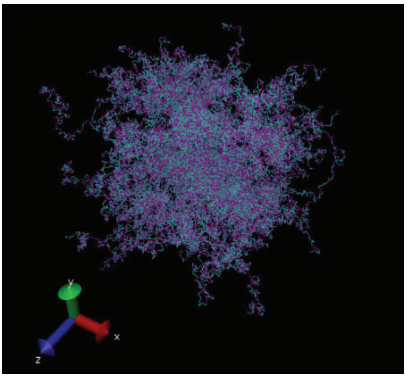


Figure 19: Coarse-grained polystyrene (PS) in starting configuration.

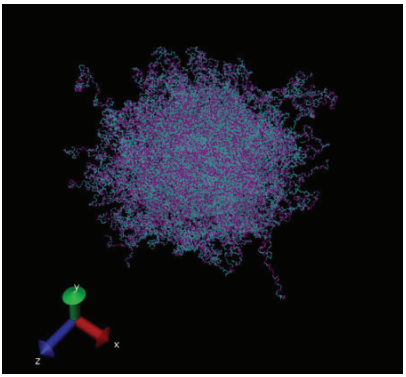


Figure 20: Coarse-grained PS in initial configuration in solid state.

The definition of the switching from FE to MD resolution and vice versa is highly challenging and the core part for later moving the MD domain throughout the continuum along a predefined path. The peculiarities arising from the switching between MD and continuum descriptions have to be investigated, whereby the focus lies on the particle domain under different load cases. In particular, it should be discussed how and to what extend the deformation of the continuum can be related to the according movements of the particles in the polymer bulk. In a first step, uniaxial deformation simulations are performed and the tendencies of the individual particle movements are evaluated.

P6: Extensive CGMD Simulations of Atactic PS Providing Pseudo Experimental Data to Calibrate Nonlinear Inelastic Continuum Mechanical Constitutive Laws

Maximilian Ries, Gunnar Possart, Paul Steinmann and Sebastian Pfaller

In [1] we present a characterization methodology to obtain pseudo experimental deformation data from CGMD simulations of polymers as an inevitable prerequisite to choose and calibrate continuum mechanical constitutive laws. Without restriction of generality, we employ a well-established CG model of atactic polystyrene as exemplary model system and simulate its mechanical behavior under various uniaxial tension and compression load cases.

To demonstrate the applicability of the obtained data, we exemplarily calibrate a viscoelastic continuum mechanical constitutive law. We conclude by a thorough discussion of the findings obtained in the numerical pseudo experiments and give an outline of subsequent research activities. Thus, this work contributes to the field of multiscale simulation methods and adds a specific application to the body of knowledge of CG MD simulations.

Furthermore, this work is strongly interconnected with DFG project 'Identifikation von Interphaseneigenschaften in Nanokompositen' (cf. W. Zhao) and FRASCAL project P6 (cf. C. Bauer).

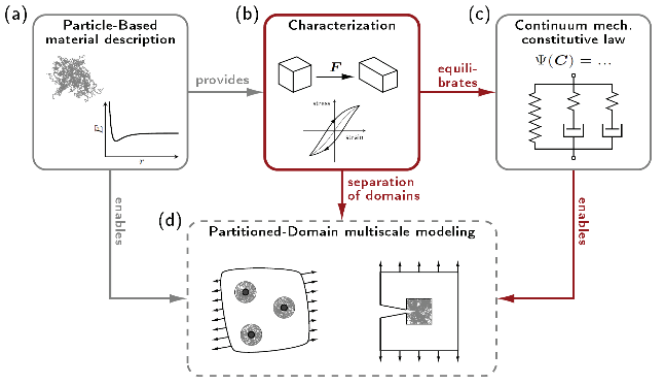


Figure 21: Schematic overview: Particle-based material description a, characterization procedure b, continuum mechanical constitutive law c, and partitioned-domain multiscale investigations d.

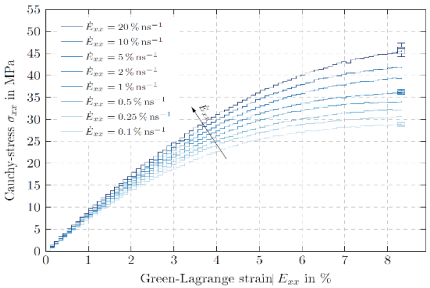


Figure 22: Influence of strain rate: stress over strain for time proportional uniaxial tension tests with varying strain rates.

Reference

[1] M. Ries, G. Possart, P. Steinmann, and S. Pfaller. “Extensive CGMD Simulations of Atactic PS Providing Pseudo Experimental Data to Calibrate Nonlinear Inelastic Continuum Mechanical Constitutive Laws". *Polymers 11* (2019), p. 1824.

P6: An Elasto-Viscoplastic Constitutive Model for Polymers Based on Molecular dynamics Simulation Under Uniaxial Finite Deformation

Wuyang Zhao, Maximilian Ries, Paul Steinmann and Sebastian Pfaller

Partitioned domain multiscale simulation methods, which combine a particle and a continuum region, have shown great potential for studying the mechanical properties of amorphous materials as e.g. polymers and polymer-based composites, because they are able to combine the spatial scales. Such methods require identical mechanical behaviour in all resolutions, thus the constitutive model used in the continuum has to fit the mechanical behaviour of the particle level in molecular dynamics (MD) simulations. The material can exhibit elastic, viscous and plastic behaviour, together with compressibility. In contrast to experiments, the low load rates are hard to reach due to the current computational capability. Our contribution [1] presents a methodology for constitutive modelling of polymers based on MD simulations and gives an elasto-viscoplastic constitutive model with nine parameters as an example to fit the coarse-grained MD simulations of polystyrene under uniaxial deformation. We employ the parallel networks framework, then decompose the mechanical behaviour of the polymer of the MD simulations into volumetric and isochoric parts and model them separately. A criterion for evaluating the volumetric inelasticity is introduced by comparing the dissipated energy density due to the volumetric change and due to the total deformation. Within this framework, we present a constitutive model that can accurately fit the MD results, which is expected to be further used for other polymers under various loading conditions and in partitioned domain multiscale simulations of polymers.

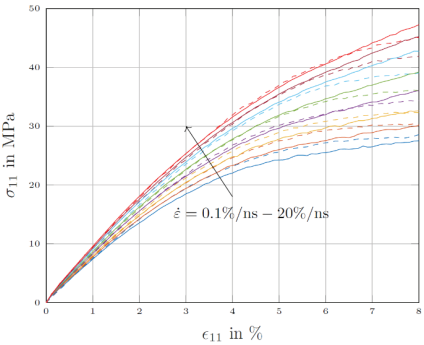


Figure 23: Comparison between the constitutive model (solid curves) and the MD simulation (dashed curves) in time proportional deformation with different constant strain rates.

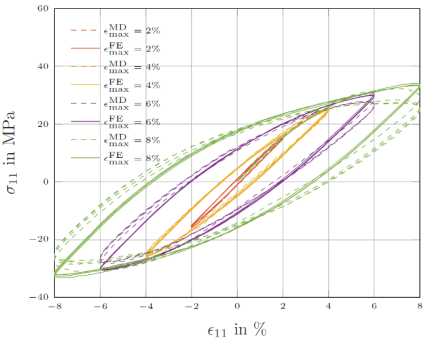


Figure 24: Comparison between the constitutive model and the MD simulation in time periodic deformation with different amplitudes and the same maximum strain rate.

Reference

[1] W. Zhao, M. Ries, P. Steinmann, and S. Pfaller. “An elasto-viscoplastic constitutive model for polymers based on molecular dynamics simulation under uniaxial deformation”. Manuscript in preparation.

P7: Collective Phenomena in Failure at Complex Interfaces

Nosaibeh Esfandiary and Paolo Moretti

Objectives and status

Hierarchical materials are characterized by modules that repeat several times on different length scales in a self-similar fashion. Biological materials provide examples of hierarchical systems. Collagen protein, for instance, exhibits a hierarchical fibre organization in different scales from Angstroms to centimetres, comprises molecules, microfibrils, fibres, and fibre bundles. This structure provides enhanced toughness, which isolated collagen molecules cannot show. Hierarchical structures play also a key role in adhesion, as it is evident in the case of the gecko. The peculiarity of this reptile is its ability to walk on ceilings and vertical walls, despite its comparably high weight. This is due to the hierarchical structure of the gecko toes. This structure optimizes the ability of the gecko to use van der Waals forces to adhere to a rough surface, to detach in a controlled manner and to resist the effect of flaws.

In this work, we study failure and failure precursors of hierarchical structures in contact with heterogeneous surfaces, as a model for adhesion and detachments of such biomimetic systems. To this end, we employ the well-known random fuse model (RFM), which, in spite of its simplicity, allows us to explore the role of hierarchical structures retaining the basic aspects of continuum elasticity, at reduced computational costs. Our large-scale simulations are currently running in the RRZE Emmy cluster in Erlangen and are producing large amounts of data, aimed at the study of crack surface morphology and fracture strength.

Conclusions, main achievements and outlook

Our results indicate that interface fracture (detachment) of hierarchical fuse network structures proceeds according to a novel failure mode, in which no crack propagation occurs and scale invariant crack surfaces are observed throughout the loading curve (i.e. not just at the failure point), as shown in Figure 25. This property is robust against structural changes of the hierarchical fuse network and

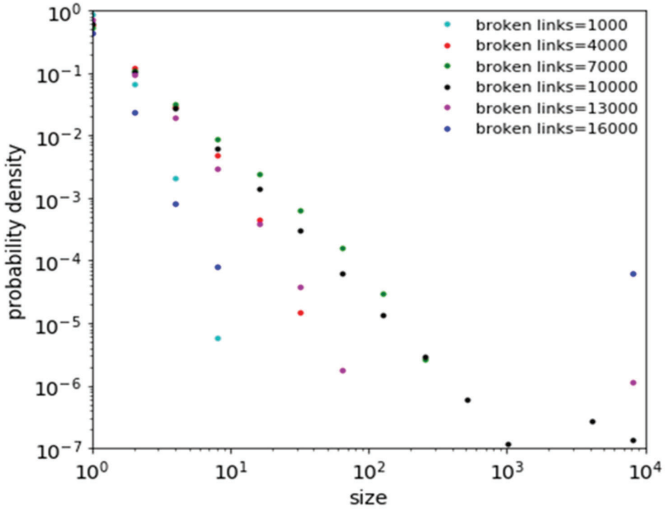


Figure 25: Crack surface morphology for the detachment of a hierarchical structure in contact with a heterogeneous surface. Probability density of crack surface areas, measures as the number of contiguous broken bonds, when modelling interface heterogeneity with a Weibull distribution of interface bond strengths. Different data sets correspond to different numbers of broken bonds, for increasing applied load.

against different choices of heterogeneity strength at the interface. The absence of crack propagation suggests that the adhesion strength of hierarchical structures is much more resilient in the presence of pre-existing flaws than that of the non-hierarchical material counterparts. We have already verified this hypothesis in the case of 2D bulk fracture and our goal now is to explore its implication in the 3D adhesion case.

Summary

We study crack area size during detachment, the result shows us, in hierarchical systems, the structure breaks according to a fracture mode that precludes crack growth and favours crack localization. These results are in agreement with the spatio-temporal avalanche behaviour we previously explored in 2D systems and points to a promising scenario, in which hierarchical materials can offer increased flaw tolerance and tuneable fracture behaviour.

P7: Activity Patterns in Brain Networks

Samaneh Esfandiary and Paolo Moretti

Objectives and status

Activity in the human brain displays features of localization, allowing for multiple tasks at the same time, and slow relaxation, which means that in localized regions activity is sustained for long times. This phenomenology can be explained starting from the structure of brain connectivity patterns, which is that of a hierarchical modular network (HMN). In this work, we address the study of these two features, localization and anomalous dynamics. To achieve this objective, we use a minimal computational model for diffusion, as a simple dynamic protocol, able to capture the essence of the dynamic slowing down due to the hierarchical organization. Diffusion and random walk simulations are tightly related to the concept of spectral dimension of a network. Hierarchical modular networks are known to have a finite intrinsic dimension. The spectral dimension (D_s), for instance, can be computed measuring the return probability (P_{ii}) of a simple random walk simulation, providing a direct connection between structure and function (diffusive dynamics in this case). If P_{ii} behaves asymptotically as $P_{ii}(t) \sim t^{-\frac{D_s}{2}}$ then D_s is the spectral dimension of the network.

In the broader context of FRASCAL, damage in structural network models is associated with reductions in dimensionality. The techniques that I develop are thus relevant in the context of Project P7, where dimensionality measures can be used to assess the state of damage of a hierarchically structured material under mechanical load. Our approach thus consists in running very-large-scale simulations (network sizes up to 30 million nodes), for the accurate computation of spectral dimension in HMNs. Our results show that the dynamic slowing down in such systems can be related to the surprising fact that the spectral dimension for such systems is undefined, i.e. the return probability for HMNs does not decrease in time as a simple power law, and it rather exhibits a stretched exponential correction which is created an exponent for the function of return probability, $P_{ii} \sim \{-(\frac{t}{t0})^{\beta}\}$.

The exponent $0.5 < \beta < 1$ is found to depend on the connectivity strength α: lower values of α produce lower values of β (and more significant slowing down). For higher α instead, β approaches 1 and the standard behaviour is recovered.

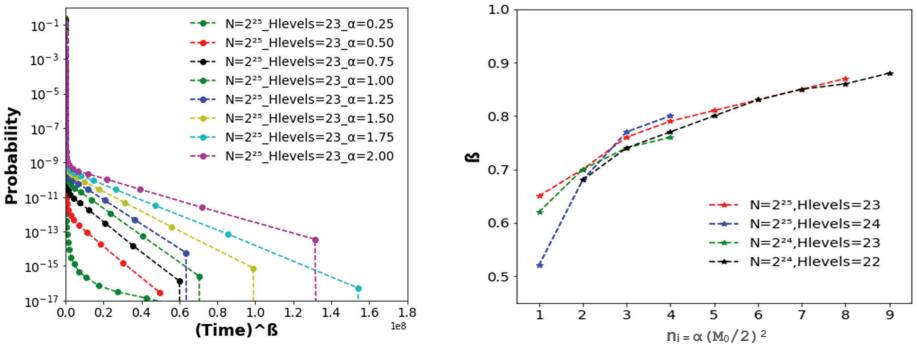


Figure 26: Stretched exponential form of the return probability for random walk simulations in HMN (left) and dependence of the anomalous exponent β on the connectivity strength α (right).

Since several brain pathologies are associated with a dimension reduction and/or anomaly (as in a breaking process), our results may serve as the foundation for topology-based diagnostic tools, in the broader context of network physiology and medicine.

Conclusions, main achievements and outlook

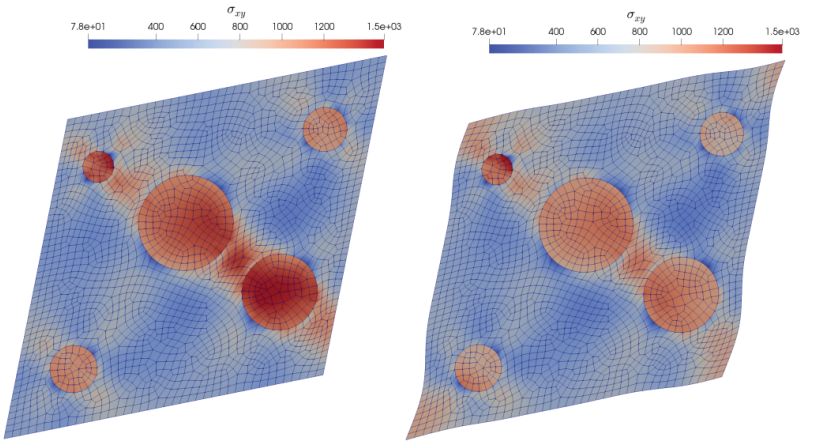
Our results point to a novel scenario, in which features of structural localization in hierarchical networks lead to ultra-slow diffusion modes. This phenomenon is the classical analogue of Anderson localization in condensed-matter low dimensional systems, and is expected to contribute to the ability of the brain to conduct multiple tasks at the same time. How this scenario evolves under damage (for instance, in percolation) would allow us to identify structural patterns which can be attributed to pathological conditions. In the next year, we will focus on these issues, by coupling random walk and percolation simulations.

P8: Modelling Size Effect in Polymer Nano-Composites

Paras Kumar and Julia Mergheim

The usage of nano-sized inorganic reinforcements culminates in much better improvement in the fracture properties of polymers in comparison to micro-sized filler particles [1]. The goal of the sub-project P8 is the development of a multiscale simulation framework for *continuum mechanics* based modelling of fracture in polymer nano-composites. The interphase layer being formed around the filler particles possesses properties that are considerably different from those of the bulk polymer. This phenomenon is more prominent in case of nano-sized filler particles owing to their much higher specific surface area (SSA) and thus the interphase layer dominates the properties of the nanocomposite [2]. Standard continuum mechanics based models are unable to capture this so-called *size effect* and thus suitable modifications are necessary.

Within the scope of this project, computational homogenization scheme is being employed for modelling the effective mechanical behaviour of the composite material present in the region far away from the crack tip. In this approach, a representative volume element (RVE) of the material is subjected to a prescribed macroscopic deformation gradient and the corresponding macroscopic stress is determined through averaging over the volume of the RVE. The choice of boundary conditions, i.e. linear (LBC) or periodic (PBC) has considerable effect on the overall response of the RVE as depicted in Figure 27.



(a) σ_{xy} contour for LBC (b) σ_{xy} contour for PBC

Figure 27: Contours for the shear component σ_{xy} of the Cauchy stress σ for 2D RVE containing circular inclusions. The RVE is subjected to a shear loading and is modelled using different boundary conditions. i.e. (a) LBC and (b) PBC.

However, this classical homogenization approach does not involve a length scale, which is necessary to model the above-mentioned size effect. In this work, two enhancements for capturing the size effect are being explored. The first approach involves the modeling of a finite thickness interphase around the filler particles and the other one is based on the idea of interface energetics [3].

In order to implement the methodologies being developed during the course of this project, a modular software framework written in *C++* and based on the open source finite element library *deal.II* [4] is being developed. The code provides all the necessary building blocks for solving generic problems in finite deformation solid mechanics in a dimension independent manner through application of C++ templates. The framework also supports an easy extension to include different constitutive models including hyperelasticity and viscoelasticity. Furthermore, a module providing the functionality for interface enhanced computational homogenization has been implemented.

Additionally, the development of a workflow for automated generation of finite element meshes for RVEs (both 2D as well as 3D) comprising of randomly placed inclusions of different sizes and shapes is under process.

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P9: Challenges Associated with Quasi-Static Phase-Field Model for Brittle Fracture

Dhananjay Phansalkar and Sigrid Leyendecker

The existence of micro-cracks and flaws further leading to fracture cannot be prevented in engineering structures. The requirement for an accurate estimate for the failure of load-bearing components of all kinds is evident. Traditionally, cracks are studied as an evolving internal discontinuous boundary$\Gamma(t)$ that represents a discrete crack. Alternatively, a phase-field model represents, the fracture as a smooth interface between broken and undamaged material, namely a diffusive crack. According to Griffith's theory of fracture, the energy needed to construct a fracture surface unit area is equal to the critical energy density of the fracture $\mathcal{G}_c$. The total potential energy of the body $\mathcal{E}$ is the sum of the elastic energy ψ_e and the fracture energy, given by $\mathcal{E}(\mathbf{u},\Gamma) = \int_\Omega \psi_e(\boldsymbol{\varepsilon}(\mathbf{u}))\mathrm{d}\mathbf{x} + \int_\Gamma \mathcal{G}_c\,\mathrm{d}\mathbf{x}$. Instead of applying the classical Griffith criterion to predict the evolution of crack, a variational formulation of the model is proposed in [1]. In order to make this variational formulation suitable for numerical implementation, [2] proposes a regularized version of this variational formulation and it reads

$$E(\boldsymbol{\varepsilon}(\boldsymbol{u}),c) = \int_\Omega (c^2+\eta)\psi_e(\boldsymbol{\varepsilon}(\boldsymbol{u}))d\boldsymbol{x} + \frac{\mathcal{G}_c}{4}\int_\Omega \left(\frac{(1-c)^2}{\epsilon} + \epsilon|\nabla c|^2\right)d\boldsymbol{x} \qquad (1)$$

where $\mathbf{u}, c, \varepsilon$ and ϵ are the displacement, phase-field, strain and regularisation parameter respectively. It can be shown that this regularized formulation approximates the variational formulation of brittle fracture in the sense of Γ-convergence [3]. Minimizing the energy functional (1) with respect to $\mathbf{u}$ and c we obtain the following Euler-Lagrange equations

$$\begin{aligned} \nabla\cdot\boldsymbol{\sigma} &= \mathbf{0} \quad \text{in} \quad \Omega \\ \left[\frac{4\epsilon\psi_e(\boldsymbol{\varepsilon}(\boldsymbol{u}))}{\mathcal{G}_c}+1\right]c - 4\epsilon^2\Delta c &= 1 \quad \text{in} \quad \Omega \end{aligned} \qquad (2)$$

In addition to equations of motion (2), the typical boundary conditions for phase-field problem are $\mathbf{u} = \mathbf{u_0}$ on $\partial\Omega_\mathrm{d}$ and $\nabla c\cdot\mathbf{n} = 0$ on $\partial\Omega$. First, we restrict ourselves to a one-dimensional domain $\Omega \in (-L, L)$ to understand various characteristics of the phase-field formulation for brittle fracture. Figure 28 shows the problem configuration. The analytical solution of the phase-field for the above-mentioned boundary value problem can be shown to be

$$x(c) = \int_{c_{crack}}^{c(x)} \left[\frac{\overline{c}^2}{2} - \overline{c} - \frac{\epsilon\sigma^2}{\mathbb{C}\mathcal{G}_c[\eta+\overline{c}^2]} + a\right]d\overline{c} \qquad (3)$$

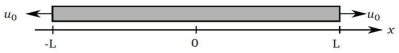
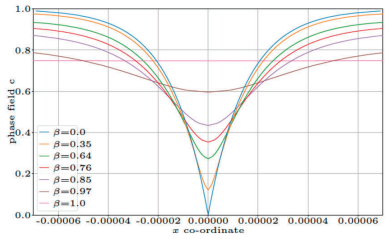
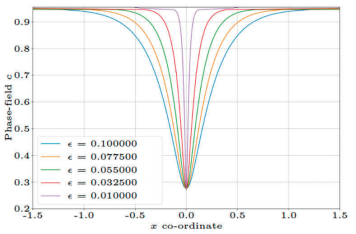


Figure 28: 1D problem set-up.

Evaluating this integral numerically for $\sigma = \beta\sigma_c$ with various values of $\beta \in [0,1]$ and critical stress σ_c we get Figure 29 (a).



(a) Phase field solution for various values of the stress with $\epsilon = 7.5\times10^{-6}$



(b) Phase field solution for various values of the ϵ with $\beta = 0.64$

Figure 29: Analytical solution of the stationary evolution equation in 1D.

Nonetheless, it is quite tricky to solve this 1D problem numerically using the non-linear finite element method. When we solve the equations (2) simultaneously, typically called a monolithic approach, the residual from the Newton method explodes even with very small load steps. We can reformulate the energy functional (1) with an additional evolution law. However, it does not resolve this convergence issue. It can be improved by damping the Newton update as suggested in [4]. This improvement is limited i.e., the residual decreases and then stagnates. Alternatively, the equations (2) can be solved one after the other for a fixed-point solution; this is typically called staggered approach. However, for all the load steps greater than the critical load, the resulting solution does not coincide with the analytical solution. Also weakening the fracture toughness ($\mathcal{G}_c$) at the center does not help to obtain the predicted analytical solution.

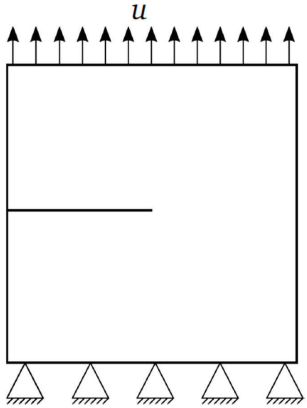


Figure 30: 2D problem set-up.

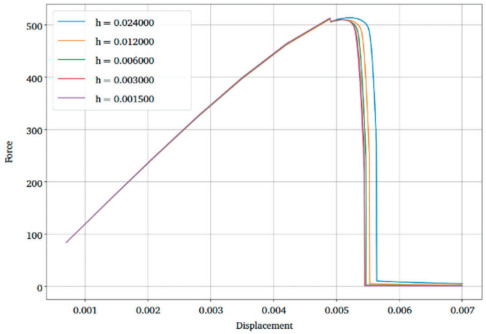


Figure 31: Force vs displacement with ϵ = 0.1.

These problems make it quite difficult to simulate the 1D problem. Hence, we move on to a 2D problem with the set-up as depicted in Figure 30. We try to solve this problem with the staggered approach and study the behaviour with respect to two parameters, ϵ and the mesh size h. The force vs displacement plot Figure 31 provides a good measure to understand the behaviour. This study also provides an upper bound for the mesh size with respect to regularization parameter i.e. $h = \epsilon/17$ to obtain a reliable solution.

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P10: Configurational Fracture Mechanics

Elmira Birang and Paul Steinmann

In this work, we study the atomistic fracture mechanism of metal crystals by means of the theory of configurational mechanics for discrete structures [5]. Following the mathematical concept of configurational forces that is already provided for atomistic systems modelled by Lennard-Jones potential energy, we could derive the configurational forces for Embedded-Atom Model potential energy. Next, a computational framework is developed here to investigate in the application of configurational forces in atomistic fracture mechanics. To this aim, two- and three-dimensional small-size lattice crystals including pre-defined static crack under quasi-static loading are simulated. In these simulations, firstly, configurational forces are calculated in a post-processing computationally efficient step. According to these results, configurational forces can namely, (i) detect the location of defect in the crystals, (ii) track precisely the crack emission into the lattice, as illustrated in Figure 32. Secondly, configurational forces are directly embedded into molecular static algorithm, to that extent, we propose configurational forces as an energy based fracture criterion. To this aim, the length of pair-wise configurational force $K_{\alpha\beta}$ is compared with a material-dependent criterion K^{cr}, termed as *configurational force criterion*, to release the pair-wise bond whenever $K_{\alpha\beta}$ met the criterion. Configurational force criterion is in fact higher than the length of cohesive force between an atomistic pair, therefore we can assure that by approaching to the criterion, required energy to break the interatomic bond is also releasing (see Figure 33). Consequently, the criterion is suitable for simulation of highly brittle crack propagation and according to our knowledge, this is the first work to introduce it.

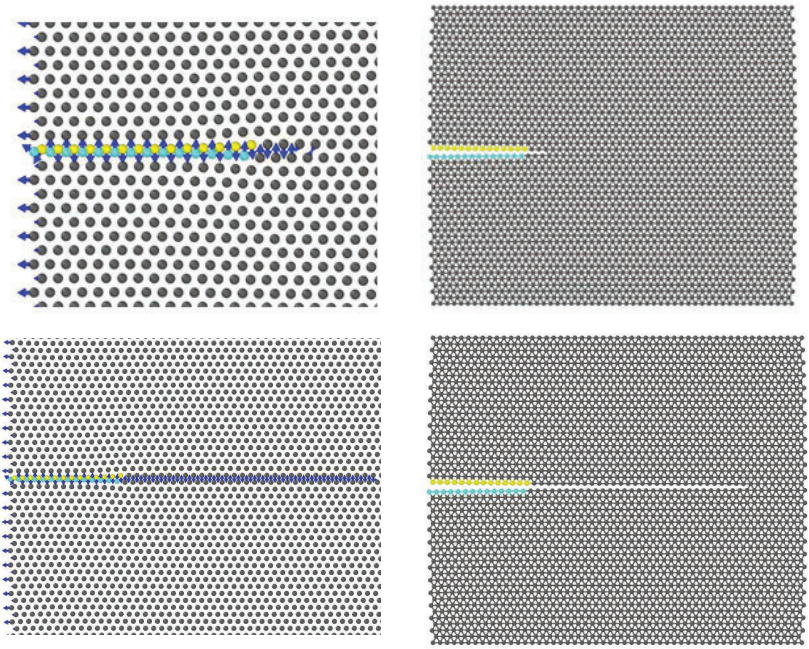

Figure 32: Emission of crack into the lattice along with the emergence of configurational forces atom-wisely on the crack path, propagation of crack is based on configurational force criterion. Configurational forces are also observed on crystal boundaries.

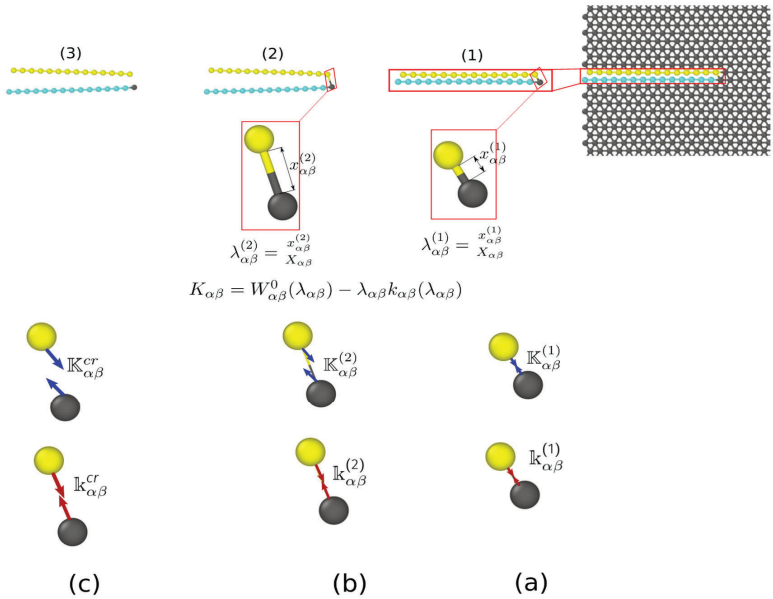

Figure 33: The process of bond release at the crack tip. Length of configurational force depends on the internal potential energy and work of interatomic force. Whenever configurational force as crack driving force met configurational force criterion, the bond is released and crack moves forward, consequently the crack tip atoms are changed and process of bond releasing will be repeated again.

Furthermore, we are developing the theory of configurational mechanics for the case of fast running crack under constant loading, in order to investigate in the capabilities of configurational forces in tracking the variations of kinetic energy due to structural changes in the course of defect evolution. At this stage, in addition to our molecular dynamics implementation, we also extend the theory of atomistic configurational mechanics to Fast Parallel Algorithms for Short-Range Molecular Dynamics (LAMMPS) [6], which may facilitate performing various atomistic fracture examples.

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P10: Biomechanics of Bones

Ina Schmidt and Paul Steinmann

Objectives and status

Osteoporosis is one of the most significant diseases in the steadily aging population. Also younger people may be affected by bone degeneration due to poor movement and nutrition. The consequence of decreasing bone density is a reduced stiffness and thus an increased risk in fracture. The main goal of this project is to create a tool, which calculates the development of human bone under mechanical loading using finite element methods and therefore predicts fractures and their local origin. An important aspect is the so-called remodelling process, which shall be modelled as realistic as possible. Therefore, different extensions were created for a macroscopic model based on continuum mechanics.

Since long bones are divided in different areas, a program was created which automatically performs the local assignment of the corresponding material parameters of cortical and spongiosa. Simulations in this setting were carried out and evaluated.

Age dependency was added to the simulation by varying the attractor stimulus, the driving parameter in this context, over time. A step type function and a saturation type function were compared to the classical approach including a constant stimulus. This modification was validated via a series of numerical examples.

A recent model extension contains the availability of nutrition and hormones. Therefore different availability functions were created and implemented e.g. on the humerus (see Figure 34).

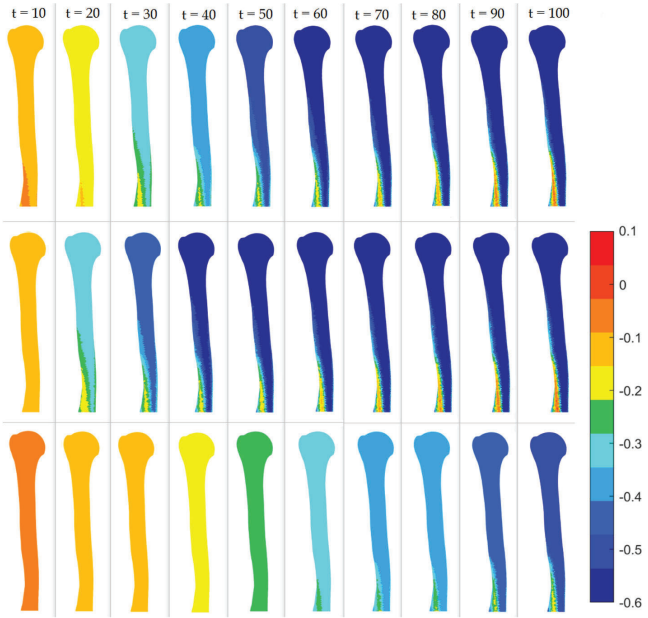

Figure 34: Sufficient, reduced and exploited availability at the humerus.

Conclusions, main achievements and outlook

With the created model extensions, further aspects could be included to make the simulation more realistic. A combination of all modifications should also be tested and compared with clinical data.

P10: Grain Boundary Mechanics

Lucie Spannraft and Paul Steinmann

The constitutive properties of a polycrystalline metal depend, inter alia, on the interaction along the grain boundaries. A geometrically non-coherent grain boundary interaction model must be able to account for the mismatch of crystal orientation of the neighbouring grains as well as decohesion. In an on-going cooperation with international research partners Magnus Ekh, Frederik Larsson and Kenneth Runesson from Chalmers University of Technology, Gothenburg, Sweden a gradient-extended crystal inelasticity model accounting for grain boundary interaction including decohesion is developed. The prime novelty is the incorporation of a coupling between the gradient (microtraction) interaction and decohesion via a damage variable, compare Spannraft et al. [1]. The damage variable d_Γ equals zero prior to damage initiation and approaches unity at complete decohesion. As a consequence, decohesion exerts an impact on the standard tractions and on the microtractions along the grain boundaries. The appropriate modelling framework is assessed in terms of numerical results obtained by Finite Element Method simulations utilizing the deal.II library.

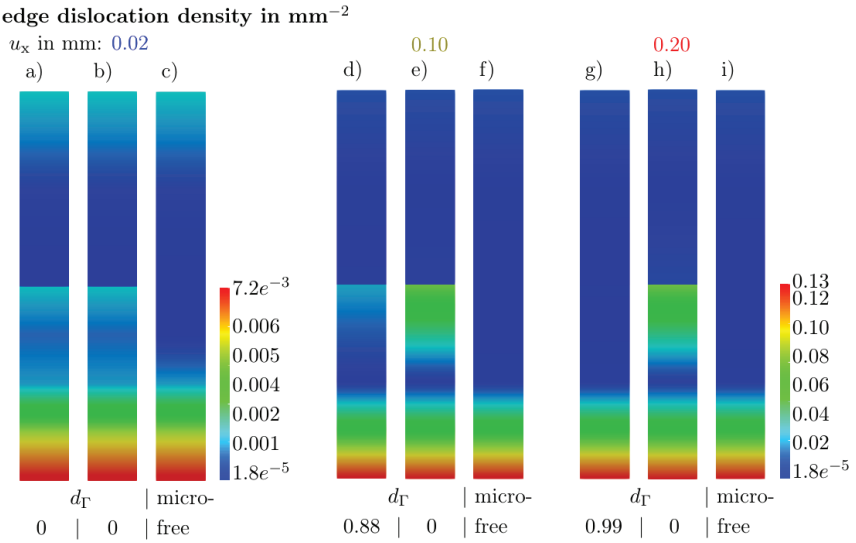

Figure 35: Edge dislocation density (in mm^{-2}) for simple shear (u_x = 0.02, 0.10 and 0.20 mm) of a bicrystal. (a,d,g). Damage coupled to microtractions. (b,e,h). No coupling of damage to microtractions. (c,f,i). Microfree condition along grain boundary [1].

Figure 35 visualizes the numerically computed edge dislocation density in a bicrystal with a crystallographic misfit at the grain boundary subjected to simple shear for three different applied displacements. Figure 35 a,d,g illustrate the different stages for increasing displacement jump and, accordingly, rising damage. A comparison with the situation without such coupling effect, cf. Figure 35 b,e,h, shows that the microtractions along the grain boundary reduce for increasing damage and a microfree boundary is approached when the damage approaches unity, compare Figure 35 g,i. The reason for this behaviour is that the microtractions along the grain boundary will eventually vanish as a result of the damage.

Reference

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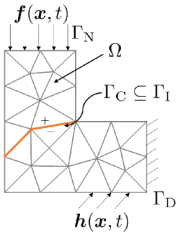
P11: Fracture Control by Material Optimization

Sukhminder Singh and Michael Stingl

Objectives and Status

The project started with an aim to develop a gradient-based material optimization model for the control of crack growth along a desired path in linear elastic composite structures. However, structural optimization problems involving quasi-static crack growth are, though, ill-posed as they include nonlinear and discontinuous responses. This limits the applicability of gradient-based optimization algorithms without incorporating any special regularization techniques. In order to use the same, the original optimization problem is modified to contain state problem, which involves rate dependent crack growth with respect to time. This eliminates the discontinuities and non-uniqueness of the crack state with respect to small perturbations in the control parameters. In this work, the crack propagation problem is solved using initially elastic cohesive interface elements in a finite element setting under monotonically increasing displacement loads. Cohesive forces and energy dissipation are dependent on the interface openings both in the normal as well as in the tangential directions.



The strong form of the governing equations in the underlying model of quasi-static crack growth assuming small deformations is written as:

$$
\begin{aligned}
\boldsymbol{u} :& \mathbb{R}^2 \times [0,T] \to \mathbb{R}^2, \\
\operatorname{div} \boldsymbol{\sigma}(\boldsymbol{u}(\boldsymbol{x},t)) &= \boldsymbol{0}, && \text{in } \Omega, \\
\boldsymbol{u}(\boldsymbol{x},t) &= \boldsymbol{h}(\boldsymbol{x},t), && \text{on } \Gamma_{\mathrm{D}}, \\
\boldsymbol{\sigma}(\boldsymbol{u}(\boldsymbol{x},t)) \cdot \boldsymbol{n}(\boldsymbol{x}) &= \boldsymbol{f}(\boldsymbol{x},t), && \text{on } \Gamma_{\mathrm{N}}, \\
\boldsymbol{\sigma}(\boldsymbol{u}(\boldsymbol{x},t))^- \cdot \boldsymbol{n}(\boldsymbol{x})^- &= \boldsymbol{\tau}(\llbracket \boldsymbol{u}(\boldsymbol{x},t) \rrbracket) + \eta \llbracket \dot{\boldsymbol{u}}(\boldsymbol{x},t) \rrbracket, && \text{on } \Gamma_{\mathrm{I}}, \\
\boldsymbol{\sigma}(\boldsymbol{u}(\boldsymbol{x},t))^+ \cdot \boldsymbol{n}(\boldsymbol{x})^+ &= -\boldsymbol{\tau}(\llbracket \boldsymbol{u}(\boldsymbol{x},t) \rrbracket) - \eta \llbracket \dot{\boldsymbol{u}}(\boldsymbol{x},t) \rrbracket, && \text{on } \Gamma_{\mathrm{I}}, \\
\llbracket \boldsymbol{u}(\boldsymbol{x},t) \rrbracket &= \boldsymbol{u}(\boldsymbol{x},t)^+ - \boldsymbol{u}(\boldsymbol{x},t)^-, && \text{on } \Gamma_{\mathrm{I}}, \\
t &\in [0,T], \\
\boldsymbol{u}(\boldsymbol{x},0) &= \boldsymbol{u}_o, \\
\eta &> 0,
\end{aligned}
$$

where $\boldsymbol{u} \in \mathrm{R}^2$ is displacement field, $\boldsymbol{\sigma}$ is the second order symmetric stress tensor given by

$$\boldsymbol{\sigma}(\boldsymbol{u}(\boldsymbol{x})) = \mathbb{C}(\boldsymbol{x}) : \nabla^{\mathrm{sym}} \boldsymbol{u}(\boldsymbol{x}),$$

where $\boldsymbol{C(x)}$ is fourth-order elasticity tensor. $\boldsymbol{h}$ and $\boldsymbol{f}$ are the applied, time-dependent, displacement and force loads at the Dirichlet and Neumann boundaries, respectively. $\boldsymbol{\tau}$ is the first-order cohesive traction tensor which depends upon the jumps in the displacement field at the finite elements' interfaces, Γ_{I}. The regularization term, controlled by parameter η, appears with cohesive traction in the form of additional rate dependent force, which can be chosen sufficiently small that it does not lose its effect.

The weak form of the above system can be written by multiplying it with a test function $\boldsymbol{v}$ and integrating over the domain Ω:

$$
\begin{aligned}
\int_{\Omega \setminus \Gamma_{\mathrm{I}}} \boldsymbol{\epsilon}(\boldsymbol{v}(\boldsymbol{x})) : \mathbb{C}(\boldsymbol{x}) : \boldsymbol{\epsilon}(\boldsymbol{u}(\boldsymbol{x},t))\, \mathrm{d}\Omega + \int_{\Gamma_{\mathrm{I}}} \llbracket \boldsymbol{v}(\boldsymbol{x}) \rrbracket \cdot \boldsymbol{\tau}(\llbracket \boldsymbol{u}(\boldsymbol{x},t) \rrbracket)\, \mathrm{d}\Gamma + \int_{\Gamma_{\mathrm{I}}} \eta \llbracket \boldsymbol{v}(\boldsymbol{x}) \rrbracket \cdot \llbracket \dot{\boldsymbol{u}}(\boldsymbol{x},t) \rrbracket\, \mathrm{d}\Gamma \\
= \int_{\Gamma_{\mathrm{N}}} \boldsymbol{v}(\boldsymbol{x}) \cdot \boldsymbol{f}(\boldsymbol{x},t)\, \mathrm{d}\Gamma, \quad \forall \text{ test functions } \boldsymbol{v}
\end{aligned}
$$

$$\boldsymbol{u}(\boldsymbol{x},t) = \boldsymbol{h}(\boldsymbol{x},t) \text{ on } \Gamma_{\mathrm{D}}, \qquad \boldsymbol{u}(\boldsymbol{x},0) = \boldsymbol{u}_o(\boldsymbol{x}).$$

The above equation can be discretized in space to form a system of non-linear ordinary differential equations:

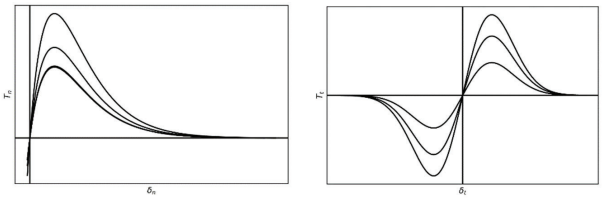
$$K \underset{\sim}{u}(t) + g(\underset{\sim}{u}(t)) + \eta M \dot{\underset{\sim}{u}}(t) = \underset{\sim}{f}(t), \quad \dot{\underset{\sim}{u}}(0) = \underset{\sim}{u}_o,$$

where $\underline{u}$ is the vector of displacement degrees of freedom in the finite element model. *K* is positive semi-definite stiffness matrix; *g* is a non-linear function, which represents the cohesive tractions with respect to displacement jumps at the interfaces. The viscosity parameter *η* comes with the mass matrix *M* together with the time rate of change of displacement.

A smooth optimization problem with an arbitrary objective function and the crack state problem can be written as:

$$\begin{aligned} &\underset{z\in\mathcal{Z}}{\text{minimize}} && J(z;T) = \int_0^T J_1(\underset{\sim}{u}(z,t),z)\,\mathrm{d}t + J_2(\underset{\sim}{u}(z,T),z) \\ &\text{where } \underset{\sim}{u}(z,t) = \underset{\sim}{u}(t) \text{ solves} && K(z)\underset{\sim}{u}(t) + g(\underset{\sim}{u}(t),z) + \eta M\dot{\underset{\sim}{u}}(t) = \underset{\sim}{f}(z,t), \\ & && \dot{\underset{\sim}{u}}(0) = \underset{\sim}{u}_o, \quad t\in[0,T] \end{aligned}$$

Here, the objective function *J(z; T)* can be split into two parts: J_1 and J_2. $J_1(\underline{u}(z,t))$ contributes to the cost at each time step whereas $J_2(\underline{u}(z,T),z)$ only depends on the final time step. The control variables are represented in a vector *z*. This is a bound-constrained optimization problem which can be solved using gradient-based optimization solvers.



Normal Traction *Tangential Traction*

In order to have the state and optimization problems well posed, the time-step can be chosen sufficiently small for a small positive viscosity parameter η. The condition can be described by an inequality:

$$\frac{\eta}{\Delta t} > -\min \mathrm{eig}\left\{\nabla^2 G(\boldsymbol{\delta})\right\}, \quad \forall\, \boldsymbol{\delta}\in\mathbb{R}^2$$

where *G* is the non-convex cohesive energy function which provides the constitutive law at the interfaces, dependent on crack opening field $\boldsymbol{\delta}$.

Conclusion and outlook

An important step towards material optimization is to check whether the crack state model provides results that are close enough to the experimental results cited in the literature. The current model uses interface cohesive elements, which restrict the crack to propagate only at the finite elements', interfaces, which makes the crack solutions dependent on the finite element mesh. Also, the use of initially elastic traction-separation laws leads to a high artificial compliance of the finite element model in the limit of mesh refinement. So, in order to stay as close as possible to reality, incorporating crack propagation models which are mesh independent, e.g. phase field method, XFEM, will be a challenge. Also shifting to extrinsic traction-separation laws introduces non-smoothness in the optimization problem for which further regularizations will have to be added or the optimization problem will have to be solved using non-smooth optimization algorithms.

P12: Development of a Quantum-to-Continuum Multiscale Model for the Fracture of Thermosets

Christian Wick and Ana-Sunčana Smith

Objectives and Status

The aim of the first post-doctoral project in P12 is the assessment of methods to enable the reliable modelling of covalent bond breaking in epoxy-based thermosets at the molecular scale. This starts with the correct treatment of electronical degrees of freedom and will ultimately lead to a physically solid hybrid quantum mechanical / molecular mechanical (QM/MM) treatment of epoxy thermosets in the framework of molecular dynamics (MD) simulations.

A priori, this also includes the reliable generation of molecular models for cured amorphous epoxy-based thermosets. The example system investigated was based on the epoxy resin diglycidyl ether of bisphenol A (DGEBA) and the curing agent 4,4'-diamino diphenyl sulfone (DDS). The actual curing reaction was simulated with an established method for modelling chemical reactions in MD simulations by Gissinger et al.,[1] which has been implemented in LAMMPS. The required time and length scales of such simulations, however, afford the use of a force field for the unreacted epoxy and curing agents, as well as the (partly) cured or reacted system. Due to the limited availability and transportability of commercial force field parameters, such as DREIDING or OPLS3, we investigated general and publicly available force fields of the AMBER type, which are well documented and tested.[2] We developed a fragment-based scheme for the unified derivation of atomic charges compatible with the AMBER force fields. This fragment-based scheme can be readily applied to DGEBA (covering all possible chain lengths n), as well as DDS, and can be easily expanded to all amine-based curing agents.

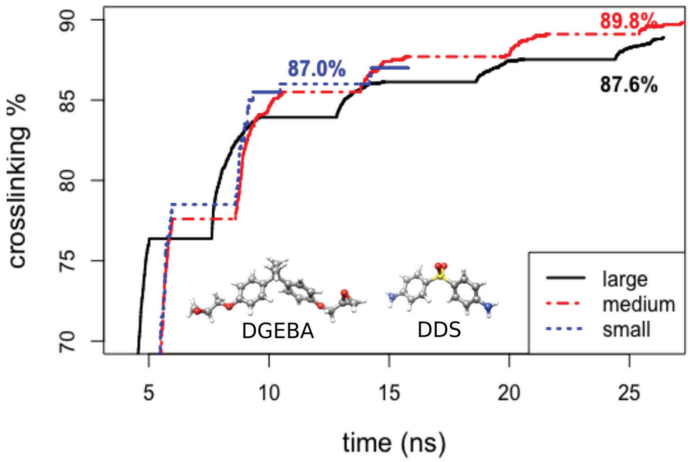


Figure 36: Crosslinking of three example model epoxy systems of different sizes (large: 120000 atoms, medium: 32000 atoms, small: 6400 atoms).

We tested our new AMBER type force field in curing simulations of DGEBA/DDS based thermosets with 3 different system sizes (small: 6400 atoms, medium: 32000 atoms and large: 120000 atoms). The overall conversion achieved during such simulations is shown in Figure 36: Crosslinking of three example model epoxy systems of different sizes (large: 120000 atoms, medium: 32000 atoms, small: 6400 atoms). The cured large model system is depicted in Figure 37. Most of the force field development and curing simulations was coupled to the combined supervision of Mattia Livraghi in Integrated Life Sciences (ILS) at FAU. A preliminary implementation of an ONIOM type QM/MM driver

to model a periodic epoxy thermoset with LAMMPS and Gaussian was investigated. This program allows the definition of a variable mechanical embedding ONIOM scheme for each bond type of the backbone of a cured epoxy thermoset and can perform optimizations as well as relaxed energy surface scans with the ONIOM system. This is connected to purely MM based molecular dynamics simulations within LAMMPS, which maintains different deformation mechanisms for mechanical testing of the cured thermoset at the molecular level.

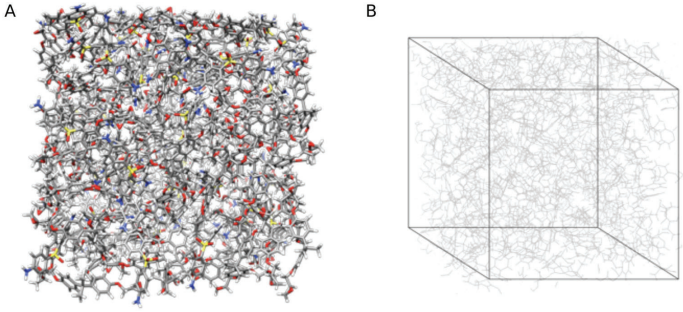


Figure 37: Final thermosets. Molecular structure (A) and a schematic representation of the periodic box used in the simulations (B).

Furthermore, several small model systems have been designed to investigate the accuracy of density functional and wave functional based methods with respect to homolytic bond cleavage of the backbone bonds of the epoxy thermoset. Those cheap methods have to be compared to high-level multi-reference ab initio calculations and are currently under investigation.

Conclusions, main achievements and outlook

A methodology for deriving sets of AMBER compatible atomic charges for amine and DEGEBA based epoxy resins has been established. Special emphasis has been taken on extendibility and general applicability in deriving the force field charges. We tested the final model chemistry in curing reactions with LAMMPS. Unfortunately, the largest systems suffer from “ring-spearing”, which necessitates further investigations of the simulation protocols applied. However, the small and medium systems could be used as starting points for the development of a preliminary driver for QM/MM simulations with LAMMPS and ONIOM. While those large model systems are important for the hybrid QM/MM description, smaller model systems are necessary to assess the quality of the QM methods, which should be applied in the actual simulations. This affords comparison to high-level multi-reference ab initio methods, which is currently under investigation.

Additionally, further force field validation will be necessary, e.g. testing mechanical or curing properties, to assess the overall quality and applicability.

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P10: Matrix-Free Locally Adaptive Finite Element Solution of Density Functional Theory

Denis Davydov and Paul Steinmann

Ultimately, properties of matter such as electric conductivity, magnetism and mechanical response upon applied loads are determined by its electronic structure. One of the most successful and widely used approaches to obtain the ground state electronic structure is the Density Functional Theory (DFT) [1,2].

The challenge in applying the DFT to real-life problems is that in traditional approaches the computational complexity of the solution scales cubically with respect to the number of electrons. Various methods have been proposed to address this issue. One promising formulation is the direct minimization of energy using orbital minimization (OM) approach, see [3,4] and references cited therein. Within the OM approach one searches for a minimum of the following functional

$$E(U) = \mathrm{tr}\left(\left[2I - U^T M U\right] U^T H U\right)$$

Here U denotes a set of orbitals, H and M are Hamiltonian and mass operators, respectively.

Different spatial discretization approaches have been used, such as finite differences, finite elements (FE) [3,4] or B-splines. The FE basis has the following advantages: (i) it is a locally adaptive basis with variational convergence; (ii) it has well-developed rigorous error estimates; (iii) a hierarchy of nested functional spaces can be used to formulate multigrid solvers and geometric multigrid (GMG) preconditioners [4] (iv) MPI parallel implementation of operators within the FEM is achieved by domain decomposition of the mesh and does not require global communication, apart from the implicit global communication in the multigrid V-cycle. (v) the real-space formulation of DFT is key to studying defects and fracture phenomena.

In order to study industrially relevant problems of fracture with quantum mechanics (QM) methods, based on [4] we aim to further improve the real space FE solution techniques of DFT. In that work we formulated DFT as a minimization problem with non-orthogonal orbitals and solved it with the quasi-Newton BFGS method with the GMG preconditioner and matrix-free operator evaluation. This formulation can take advantage of physical localization of the solution, namely that the solution can be sought in terms of non-orthogonal orbitals with local support. In order to incorporate this assumption into the FE solver, numerically efficient implementation of sparse FE vectors suitable for matrix-free multi-grid MPI parallel operators within the open-source Differential Equations Analysis Library (deal.II) [5] is required. The block compressed sparse row (BCSR) format was adopted to store sparse multivectors. BCSR matrix can be considered as an extension of compress sparse row (CSR) matrices where each element is a dense matrix. Figure 38 shows preliminary results of the roofline performance model for the various operations measured for quadratic FE basis on Intel Xeon 2660v2 “Ivy Bridge” chips. The matrix-free approach is additionally compared to dense column vectors with filtering of the FE operator based on support for each vector (denoted as “FE op. (dense filtered)”).

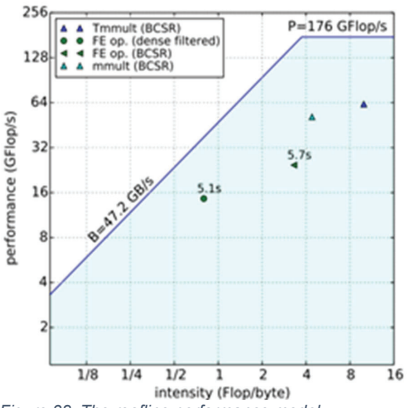

Figure 38: The roofline performance model.

For sparse matrix-matrix products (“mmult” and “Tmmult”) more than 90% of time spent in BLAS dense matrix-matrix product routines, suggesting efficient implementation of BCSR infrastructure. Column vector filtered approach is inferior both in terms of performance and measured computation intensity. We can conclude that BCSR is a promising data format to implement sparse FE multivectors for QM applications.

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P10: Development of a Computational Homogenization Framework of Atomistically-Induced Damage

Dimosthenis Floros and Paul Steinmann

Objectives and status

To be able to account for information on microstructural events at the atomic scale in simulations of engineering components at the macroscale, a computational homogenization framework of atomistically-induced damage is proposed.

As a first task, the continuum—atomistic multiscale setting was restated via a framework for variationally-consistent homogenization. This led to the development of an FE^2 scheme, in which atomistic RVEs are assumed to reside at each quadrature point of an assumed homogeneous macroscale, see Figure 39. Computational homogenization is thereafter performed over the RVE to obtain the macroscale response at the quadrature point. The framework was implemented on homogenization of a multitude of finescale atomistic problems with heterogeneities and the work is currently being documented in a report.

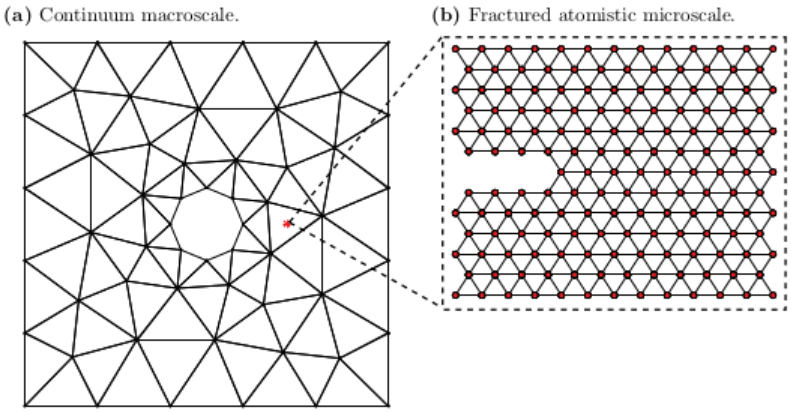

Figure 39: Coupled continuum-atomistic multiscale setting.

Conclusions, main achievements and outlook

The developed framework allows for concepts that are typical within the so-called FE^2 method to be extended in a natural manner to continuum—atomistic simulations. As an example, it was possible to identify as a special case of first-order homogenization, the scheme known to-date as the Cauchy-Born rules in continuum-atomistics.

Preliminary results show that first-order homogenization without allowing for microscopic fluctuations (atomic lattice relaxation) does not always provide with a well-posed homogenized macroscale problem. In this regard, the work will continue with consideration of first-order homogenization with microscopic fluctuations, as a remedy to obtain unconditionally solvable homogenized problems at the macroscale.

P2: Atomistics of crack-heterogeneity interactions

Shrivraj Karewar and Erik Bitzek

Initial hypothesis and aims of the project, current project status, description of results achieved to date, where applicable information on the anticipated work schedule, networking with other projects; option-al: references on the state of the art.

The influence of grain boundary (GB) morphology on fracture behaviour was studied using molecular dynamics simulations at the atomic scale. Crack propagation was studied for different GB misorientations and different GB curvatures, and compared to planar GBs. The atomistic fracture simulations were performed along symmetric and asymmetric tilt GBs in Tungsten using an embedded atom meth-od (EAM) type potential. All calculations were performed with the open-source code IMD.

The atomic structure of the planar GBs consist of periodically repetitive GB units whereas the curved GBs consists of GB steps or ledges. The crack propagates smoothly along planar GB without any hin-drance. In contrast, the crack propagation along curved GBs show stop-and-start type behaviour and crack arrest was also observed at the atomic ledges.

Our results help to understand the atomistic aspects of intergranular crack propagation with different GB morphologies. The results of crack propagation along tilt GBs with different morphologies show that the atomic ledges created by the GB curvature could locally hinder and slow down crack propagation. The kinetic criteria based on the local stress state indicated that high magnitudes of local compressive stress states created at the atomic steps could hinder crack propagation. Earlier works have shown that the boundary conditions used for these simulations could affect the results. Therefore, it is planned to use damping boundary conditions to check if the aforementioned results are correct.

P3: Employing Classical Force Fields to Model Chemical Reactions of a Duromer

Patrick Duchstein and Dirk Zahn

Famous algorithms to couple different simulation techniques over multiple scales are well established in the scientific community. The most-known algorithm is probably QM/MM [1], an approach where quantum chemistry calculations are coupled with classical molecular dynamics. This approach allows to extend the time and length scales of quantum calculations with minor effects on the accuracy. In contrast, however, a simple and efficient method to enable chemical reactions with classical force fields, such as AMBER, CHARMM or OPLS-AA is not available yet.

We propose in this work an alternative algorithm which allows to smoothly switch from one molecular topology to another by simply mixing the forces and energies of the new and old topology with a CHARMM-like switching function. By molecular topology we refer here to a molecular structure defined by bonded interactions, commonly described by harmonic bonds, angles, dihedrals and impropers and non-bonded interactions, e.g., van der Waals and Coulomb interactions.

The epoxy resin EPON 862 and the amino hardener DETDA are well-known molecules and have been studied extensively in literature, experimentally and in simulations. They present thus an ideal system to illustrate our approach to cross-link these two molecules to form a duromer.

Smooth transfer of topology

OPLS-AA topologies and partial charges on the semi-empirical 1.14*CM1A-LBCC level [2] for monomeric, single and double cross-linked bisphenol F diglycidyl ether (BFDGE) and 4,6-diethyl-2-methylbenzene-1,3-diamine (DETDA) are obtained using the online tool LigParGen [3]. In order to allow and model chemical reactions in classical molecular dynamics simulations, we developed a method to switch smoothly from one topology to another, e.g., by forming a chemical bond between an epoxide group and an amine where the epoxide ring is opened, a chemical bond between the epoxide carbon and amine nitrogen is created and the oxygen of the epoxide is hydroxylated in a typical addition reaction of an amino hardened epoxide duromer. In order to change from one chemical state to another, typically several bonds, angles, dihedrals and impropers need to be broken and others have to be created. Especially challenging in MD is when topologies from educts to products change and how non-bonded interactions between 1-2, 1-3 and 1-4 (so-called special neighbours) are treatable in a differentiable way. We present here an approach to circumvent this problem by smoothly turning off all bonded and non-bonded interactions (including special neighbours) of an old topology and at the same time smoothly turn on a new topology. This is achieved by simply switching old forces off and new forces on by multiplying them with the following function,

$$s(t) = 1.0 - \frac{(t_{end}^2 - t^2)^2 (t_{end}^2 + 2t^2 - 3t_0^2)}{(t_{end}^2 - t_0^2)^3} \qquad (1)$$

Starting from the energy of the smooth topology transfer algorithm, which is defined by

$$E_{A+B\rightarrow AB}^{topo}(t) = s(t) \cdot [E_{AB}^{mm}(X(t)) - E_{A+B}^{mm}(X(t))] \qquad (2)$$

In between a transition, $E_{A+B\rightarrow AB}^{topo}$ smoothly switches between the additional energy required for a transition from an unreacted topology (A+B) to a reacted topology (AB). At the end of a transition $E_{A+B\rightarrow AB}^{topo}(t_{end})$ thus stores the additional energy required to switch from the unreacted to the reacted state, if no atoms would move:

$$E_{A+B\rightarrow AB}^{topo}(t_{end}) = E_{AB}^{mm} - (E_{A}^{mm} - E_{B}^{mm}) \qquad (3)$$

We can derive from eq. 2 an expression for the force $\vec{F}(t) \equiv \vec{F}(\vec{r}_j(t))$ acting on atom *j* when the topology should be switched by simply adding the additional smooth topology transfer energy to the unreacted systems energy:

$$\vec{F}_j(t) = -\nabla_j [E^{mm}_{A+B}(X(t)) + E^{topo}_{A+B\rightarrow AB}(t)]$$
$$= -s(t)\cdot\nabla_j \cdot E^{mm}_{AB}(X(t)) - (1-s(t))\cdot\nabla_j \cdot E^{mm}_{AB}(X(t)) \quad (4)$$
$$= s(t)\cdot F_j^{AB} + (1-s(t))\cdot F_j^{A+B}$$

Where $\nabla_j = (\frac{\partial}{\partial x_j}, \frac{\partial}{\partial y_j}, \frac{\partial}{\partial z_j})$ is the nabla operator with respect to the position of atom *j*. F_j^{AB} and F_j^{A+B} are the forces from the reacted and unreacted topology on atom *j*, respectively. *X(t)* are the positions of all atoms in a Cartesian space at time *t*. If no atom types or charges are changed, it is enough to limit the additional force calculations for the new topology to atoms involved in new bonds, angles, dihedrals or impropers. However, if charges or atom types change, all interactions within the non-bonded cut-off of atoms involved in the reaction need to be calculated twice (for the old and new topology). After a transition, forces for all atoms are defined by the new topology The new topology is then permanently active and the old topology is fully removed from any force or energy calculations. In the reaction group R all atoms are stored which are involved in bonds, angles, dihedrals or impropers of the new topology and needed to be changed upon a chemical reaction. Figure 40 shows an example of atoms which need to be considered in the reaction group *R* for a two-step addition reaction of an epoxy resin. Atoms directly affected by the smooth topology transfer are indicated by green and atoms which are only indirectly affected by blue colours.

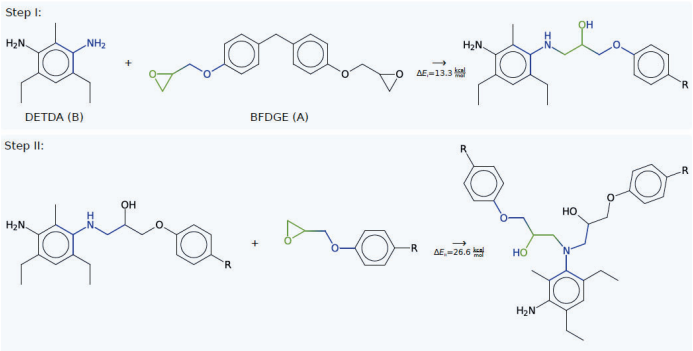

Figure 40: Chemical structures of DETDA (upper left) and BFDGE (upper middle). Illustration of the two-step curing reaction of BFDGE and DETDA.

During the reaction, the potential energy of the system can be corrected for the smooth topology transfer energies. By adding $E^{topo}_{A+B\rightarrow AB}$ to the potential energy of the system for each step in which the algorithm is applied during e.g. an NVT simulation, a smooth transition between states is achieved. The form of the switching function affects the shape of the potential energy in the transition region.

For a realistic polymerization behaviour, an additional Monte Carlo (MC) step is added to our method and the force field energies are corrected by a subtractive QM/MM scheme. By using a subtractive QM/MM approach, it is checked whether a chemical reaction at the respective temperature is energetically reasonable and whether bonds, angles, dihedrals or impropers are not subjected to excessive mechanical stress. Hence, energy corrections of a two-step cross-linking reaction are introduced in Figure 40 and used according to eq. 7 of our QM/MM approach for realistic modelling of the curing of an epoxy resin. The energy correction ΔE_I of the first step of the reaction, in which one epoxy of molecule (A) attaches covalently to an amine group of the hardener (B), is given by

$$\Delta E_I = E^{qm}_{AB} - (E^{qm}_A + E^{qm}_B) - E^{mm}_{AB} + (E^{mm}_A + E^{mm}_B) = (-25.5^{qm} + 38.8^{mm})kcal/mol \quad (5)$$

The energetic correction ΔE_{II} for a second epoxide that binds to the same amine is determined with the following equation

$$\Delta E_I = E^{qm}_{ABA} - (E^{qm}_{AB} + E^{qm}_A) - E^{mm}_{ABA} + (E^{mm}_{AB} + E^{mm}_A) = (-15.5^{qm} + 42.1^{mm})kcal/mol \quad (6)$$

E_{AB}^{qm} and E_{ABA}^{qm} are potential energies based on a DFT calculation on the B3LYP/6-11+G** level for a single or double-bonded amino group to epoxides. E_{A}^{qm} and E_{B}^{qm} are the potential energies of a monomeric resin and hardener molecule, respectively. Variables indicated with “mm" are the molecular mechanics equivalent.

In summary, a reaction is accepted with the following probability according to the Metropolis algorithm:

$$p = \min(1, e^{-\frac{\Delta E}{k_B T}}) \qquad (7)$$

where T is the temperature of the system, k_B is the Boltzmann constant, and

$$\Delta E = \left\langle E_{AB}^{mm} \right\rangle_{\tau} - \left\langle E_{A+B}^{mm} \right\rangle_{\tau} + \Delta E_{I/II}$$

with $\left\langle E_{AB}^{mm} \right\rangle$ and $\left\langle E_{A+B}^{mm} \right\rangle$ as respective total potential energies of the system averaged over τ =2.5 ps using solely the classical force field and without quantum corrections before and after the polymerization reaction.

Results

Initially, we performed MD simulations of the uncured resin in order to speed up the curing procedure by identifying an estimate for a cut-off to identify eligible reaction pairs. We analysed the radial pair distribution functions (RDF) between epoxy and amine groups in an uncured system at five different temperatures (see Figure 41). With increasing temperature we observed a negligible shift of the peak to greater distances which corresponds well with the decrease in overall density at elevated temperatures (from 1.05 g/cm³ at 300 K to 0.95 g/cm³ at 460 K). Furthermore, a decrease of the peak area is observed, indicating less reactive epoxy groups at higher temperatures around an amine. The cut-off was determined by the first shell of neighbours in the RDFs of reactive partners around an amine, which is shown in Figure 41. After all possible reaction sites have been identified, a random pair is chosen which is then cross-linked using the smooth transfer of topology algorithm. The monomers were thus cross-linked iteratively at different temperatures using the Monte Carlo algorithm mentioned above. The curing reaction was modelled at five different temperatures (300 K, 340 K, 380 K, 420 K and 460 K) which have been used in the thermostat as well as in the MC step. After the topology transition, the system is equilibrated in a 2.5 ps short NpT simulation and finally potential energies for the MC step are averaged from the second half of the NpT simulation. Those energy averages are used subsequently in the subtractive QM/MM approach in order to decide to accept a reaction or not. Finally, with this approach we could obtain duromer structures with a degree of cross-linking ranging between 83% and 93 %, depending on the temperature selected in the simulations.

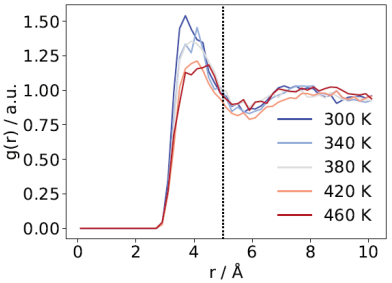

Figure 41: RDF g(r) of the epoxy carbon edge in the resin and nitrogen in the amine group of the hardener. The dashed black line at r_c = 5 Å marks the cutoff for finding reactive pairs.

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2.2 Publications

(in alphabetical order)

Journal Articles

Published

[1] **Seyyed Ahmad Hosseini, Paolo Moretti, Michael Zaiser**
A Beam Network Model Approach to Strength Optimization of Disordered Fibrous Materials
Adv. Eng. Mater. 2019, 1901013
DOI: 10.1002/adem.201901013

[2] **Maximilian Ries, Gunnar Possart, Paul Steinmann, Sebastian Pfaller**
Extensive CGMD Simulations of Atactic PS Providing Pseudo Experimental Data to Calibrate Non-linear Inelastic Continuum Mechanical Constitutive Laws
Polymers 2019, 11(11), 1824
DOI: 10.3390/polym11111824

[3] **Nikola Topic, Thorsten Pöschel**
Inelastic collapse of perfectly inelastic particles
Communications Physics 2, 85 (2019)
DOI: 10.1038/s42005-019-0184-y

FULL PAPER

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A Beam Network Model Approach to Strength Optimization of Disordered Fibrous Materials

Seyyed Ahmad Hosseini, Paolo Moretti, and Michael Zaiser*

A beam network model is used to study the nucleation and propagation of cracks in uniaxially loaded materials consisting of randomly cross-linked fibers with statistically distributed failure thresholds. The failure behavior of such materials is investigated and, for different degrees of disorder, the fraction of cross links required to achieve an optimal strength-to-weight ratio is determined. In the absence of disorder, this problem has a trivial analytical solution (no cross links), which however turns out the worst possible arrangement for strongly disordered materials and/or for large system sizes.

1. Introduction

Network models play an important role for investigating the mechanical properties, fracture, and failure of heterogeneous and disordered materials.[1] Beam network models (BNM) serve as a paradigmatic modeling approach which despite its simple structure captures key features of fracture as a multi-scale process: The existence of local failure thresholds which reflect properties of the material microstructure, the existence of an internal length above which the material can be described as a continuum, and the long-range coupling of different material elements by long-range stress fields that emerge in response to local failure. By abstracting from the bewildering detail of real material microstructures, such models achieve a degree of simplicity that makes them amenable to large-scale simulations and systematic studies over a wide range of system sizes, using ensembles of a size that allows for meaningful statistical predictions.[2] At the same time, BNM, as opposed to even more simplified models such as random fuse models, or random spring models, explicitly preserve fundamental features of continuum mechanics such as the tensorial nature of stress and strain, and the conservation of linear and angular momentum. This allows to "tune" them to reproduce, in principle, macroscopic elastic properties of any type of material.

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In turn, metamaterials with designed elastic properties often assume the physical form of beam networks. For instance, additively manufactured auxetic metamaterials[3,4] may often be considered fairly direct physical realizations of beam network structures. Similarly, beam networks may be additively manufactured to act as process-specific catalyst supports[5] or scaffolds for tissue engineering.[6]

In design and optimization of such structures, it is often assumed that materials properties of the matrix are completely known.[7] In contrast, it is well known that the quality of additively manufactured metal parts is subject to huge variations and this feature poses serious problems for application of manufactured parts in terms of reliability and predictability.[8] The problem is particularly relevant when considering mechanical failure, as failure loads may be strongly influenced by disorder.[4] Moreover, this influence is not trivial: While structural disorder at first glance is likely to promote crack nucleation and failure, it has also been reported that artificially introducing "flaws" in the form of geometric defects into periodic metamaterials may actually enhance damage tolerance.[9] For materials that fail by the formation of localized shear bands, it has been demonstrated that enhanced disorder may delay failure,[10] and for cellular materials, disorder has been shown to homogenize the deformation response and prevent formation of localized crushing bands.[11]

To ensure strength and reliability of materials that can be modeled as beam networks, design rules and paradigms need to be adapted to account for the statistical variability of materials properties. In the present investigation, we show this for an extremely simple design problem, namely the optimal configurations of a uniaxially strained bundle of load-carrying (LC) brittle fibers with variable amount of cross links. In the absence of structural disorder, this problem has a trivial solution which, however, turns out to be the worst possible solution if the system is large or the material is strongly disordered.

2. The Method: BNM

The basic structure of our BNM is a 2D square lattice that consists of interconnected beams that are clamped together at their intersections as shown in **Figure 1**. The points where beams are mutually connected are referred to as nodes; a BNM of size L has $L(L+1)$ nodes. At the top and bottom boundaries of the BNM, all degrees of freedom (DOFs) are fixed through two rigid bars which are used to apply an axial displacement along one of the two cubic axes of the lattice structure. Periodic boundary

polymers

MDPI

Article

Extensive CGMD Simulations of Atactic PS Providing Pseudo Experimental Data to Calibrate Nonlinear Inelastic Continuum Mechanical Constitutive Laws

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check for updates

Abstract: In this contribution, we present a characterization methodology to obtain pseudo experimental deformation data from CG MD simulations of polymers as an inevitable prerequisite to choose and calibrate continuum mechanical constitutive laws. Without restriction of generality, we employ a well established CG model of atactic polystyrene as exemplary model system and simulate its mechanical behavior under various uniaxial tension and compression load cases. To demonstrate the applicability of the obtained data, we exemplarily calibrate a viscoelastic continuum mechanical constitutive law. We conclude our contribution by a thorough discussion of the findings obtained in the numerical pseudo experiments and give an outline of subsequent research activities. Thus, this work contributes to the field of multiscale simulation methods and adds a specific application to the body of knowledge of CG MD simulations.

Keywords: molecular dynamics; simulation of polymers; mechanical properties of polymers; material characterization

1. Introduction and Outline

In contrast to continuum mechanics, particle-based simulation techniques provide insight into the processes taking place at the level of atoms or molecules. Thus, these approaches are well-suited to understand the behavior of material originating from the structures at very small length and time scales. However, when larger system sizes have to be employed, e.g., representative volume elements for composite materials with a representative number of inclusions, pure particle approaches may become computationally prohibitive due to the large number of degrees of freedom to be considered. In such problems, the combination of particle-based techniques with a continuum mechanical treatment has great potential to reduce the computational effort, but still allows for a sufficiently fine resolution in crucial regions of the domain of interest.

Figure 1 sketches potential set-ups where only regions of specific interest are treated at the atomistic or molecular level: (a) displays a polymer nanocomposite with atomistic resolution only in the vicinity of the filler particles; (b) shows a pre-cracked sample with atomistic treatment only around the crack tip. Beyond these, a variety of applications is possible for the symbiotic usage of fine and coarse resolutions. Typically, the coarse scale (i.e., continuum mechanics) is applied in regions that are exposed to only moderate deformations, whereas the fine scale is required in parts of the domain where the material is subjected to large strains and stresses, which might arise from, e.g., discontinuities as sketched in Figure 1. To realize this kind of simulations, so-called partitioned-domain coupling approaches [1] are required which combine continuum mechanics and particle-based approaches. In the recent decades, a large number of multiscale simulation schemes has been proposed. Prominent examples are, e.g., presented and assessed in [2], but with

COMMUNICATIONS PHYSICS

ARTICLE

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Inelastic collapse of perfectly inelastic particles

Nikola Topic[1] & Thorsten Pöschel[2]

One of the most intensively discussed subjects in the dynamics of dissipative hard sphere systems is the effect of inelastic collapse, where the entire kinetic energy of the relative motion of a set of particles is dissipated in finite time due to an infinite sequence of collisions. The known collapse scenarios imply two preconditions: inertia of the particles and at least some degree of elasticity. For completely inelastic particles, collapse scenarios degenerate to a single sticky contact. By considering the overdamped motion of a frictional particle along the steepest descent in a rigid landscape, here we show that there exist collapse scenarios of novel type even if neither of these preconditions hold true. By means of numerical simulations we show that such collapses are no rare events due to particular particle shape and/or initial conditions and, thus, may be considered as an alternative scenario of granular cluster formation.

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Under review

[1] **Areti Papastavrou, Ina Schmidt, Kefu Deng, Paul Steinmann**
On age-dependent bone remodeling
Journal of Biomechanics, submitted

[2] **Areti Papastavrou, Ina Schmidt, Paul Steinmann**
On biological availability dependent bone remodeling Computer Methods
Biomechanics and Biomedical Engineering, submitted

[3] **Lucie Spannraft, Magnus Ekh, Fredrik Larsson, Kenneth Runesson, Paul Steinmann**
Grain boundary interaction based on gradient crystal inelasticity and decohesion
Computational Materials Science, submitted

In preparation

[1] **Seyedeh Elmira Birang Oskouei, Paul Steinmann**
Computational Study of Configurational Forces with an Application in Atomistic Fracture Mechanics

[2] **Seyedeh Elmira Birang Oskouei, Paul Steinmann**
Configurational Forces in Molecular Dynamics: Case Study of Brittle Crack Propagation

[3] **Samaneh Esfandiary, Paolo Moretti, Miguel A. Muñoz**
Localization and dynamic slowing down in hierarchical network models of the brain

[4] **Seyyed Ahmad Hosseini, Paolo Moretti, Avraam Konstantinidis, Michael Zaiser**
Beam network model for fracture of materials with hierarchical microstructure

[5] **Ali Mauricio Velasco Sabogal, Thorsten Pöschel**
Fast Method for Multi-sphere Fitting of Complex Shapes

[6] **Ali Mauricio Velasco Sabogal, Thorsten Pöschel**
Fracture of Irregular Grains under Single Load Conditions

[7] **Wuyang Zhao, Maximilian Ries, Paul Steinmann, Sebastian Pfaller**
An elasto-viscoplastic constitutive model for polymers based on molecular dynamics simulation under uniaxial deformation

Conference papers

Under review

[1] **Maximilian Ries**
Characterization of polystyrene under shear deformation using Molecular Dynamics", Proceedings of ICoNSoM

2.3 Participation in conferences and workshops

Achraf Atila

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
31.03.2019 / 05.04.2019	DPG 2019	Regensburg, Germany	Poster: *Structural and mechanical properties of sodium, magnesium, and calcium metaphosphate glasses: insights from molecular dynamics simulations*
13.05.2019 / 15.05.2019	DGG	Nuremberg, Germany	Poster: *Atomistic insight into the mixed Alkaline earth modifier effect on mechanical properties of metaphosphate glasses*
05.08.2019 / 08.08.2019	ISAM4 2019	Erlangen, Germany	Talk: *Atomistic Study of Mechanical and Structural Anisotropy of Metaphosphate Glasses*
09.09.2019 / 12.09.2019	4th Glass & Entropy	Jena, Germany	Poster: *Atomic-Scale Study of Deformation-Induced Topological Anisotropy in Silica and Metaphosphate Glasses*

Christof Bauer

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
05.08.2019 / 08.08.2019	ISAM4 2019	Erlangen, Germany	Participation only

Elmira Birang

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
12.06.2019 / 14.06.2019	CFRAC 2019	Braunschweig, Germany	Talk: *Configurational Forces in Crystalline Systems*
05.08.2019 / 08.08.2019	ISAM4 2019	Erlangen, Germany	Talk: *Configurational Force Driven Crack Propagation*
09.09.2019 / 12.09.2019	Molecular and materials simulation at the turn of the decade: Celebrating 50 years of CECAM	Lausanne, Switzerland	Participation only

Nosaibeh Esfandiary

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
05.08.2019 / 08.08.2019	ISAM4 2019	Erlangen, Germany	Participation only
10.12.2019 / 12.12.2019	Complex Networks 2019	Lisbon, Portugal	Poster: *Network models of fracture in materials with hierarchical microstructure*

Samaneh Esfandiary

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
17.09.2019 / 20.09.2019	Computational and Statistical Physics	Granada/ Spain	Poster: *Slow and Anomalous Dynamic in Hierarchical Modular models of Human Brain*
10.12.2019 / 12.12.2019	Complex Networks 2019	Lisbon, Portugal	Talk: *Slow and Anomalous Dynamic in Hierarchical Modular models of Human Brain*

Ahmad Hosseini

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
01.09.2019 / 05.09.2019	EUROMAT 2019	Stockholm, Sweden	Talk: *Beam network models for optimizing failure properties of fibrous (bio)materials*
10.12.2019 / 12.12.2019	Complex Networks 2019	Lisbon, Portugal	Poster: *Strength optimization of materials with complex microstructure: Beam Network Model*

Shrivraj Karewar

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
31.03.2019 / 05.04.2019	DPG 2019	Regensburg, Germany	Talk: *Effect of Grain Boundary Morphology on Crack Propagation Behaviour in Tungsten*
05.08.2019 / 08.08.2019	ISAM4 2019	Erlangen, Germany	Talk: *Effect of Grain Boundary Morphology on Crack Propagation Behaviour in Tungsten*

Julian Konrad

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
05.08.2019 / 08.08.2019	ISAM4 2019	Erlangen, Germany	Participation only

Paras Kumar

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
05.08.2019 / 08.08.2019	ISAM4 2019	Erlangen, Germany	Participation only

Tarakeshwar Lakshmipathy

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
31.03.2019 / 05.04.2019	DPG 2019	Regensburg, Germany	Participation only
05.08.2019 / 08.08.2019	ISAM4 2019	Erlangen, Germany	Talk: *Influence of crack tip radius on fracture behaviour: An atomistic study*

Tobias Müller

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
31.03.2019 / 05.04.2019	DPG 2019	Regensburg, Germany	Poster: *Adsorption of organic molecules with high dipole moment on the Au(111) surface*
08.04.2019 / 10.04.2019	33rd MMWS	Erlangen, Germany	Poster: *Adsorption of organic molecules with high dipole moment on the Au(111) surface*
17.07.2019 / 19.07.2019	ICICP Summer School	Erlangen, Germany	Talk: *Chemistry at the crack tip: First MD simulations*
30.07.2019 / 31.07.2019	3rd Franconian Theory Meeting	Erlangen, Germany	Participation only
05.08.2019 / 08.08.2019	ISAM4 2019	Erlangen, Germany	Participation only

Dhananjay Phansalkar

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
05.08.2019 / 08.08.2019	ISAM4 2019	Erlangen, Germany	Participation only

Maximilian Ries

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
16.06.2019 / 19.06.2019	ICoNSoM 2019	Rome, Italy	Talk: *Characterization of polystyrene under shear deformation using Molecular Dynamics*
1.10.2019 / 4.10.2019	CMCS 19	Glasgow, Scotland	Poster: *Investigation of the Mechanical Behavior of Polystyrene under Uniaxial Deformation using the Capriccio method*

Jonas Ritter

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
05.08.2019 / 08.08.2019	ISAM4 2019	Erlangen, Germany	Participation only

Sukhminder Singh

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
05.08.2019 / 08.08.2019	ISAM4 2019	Erlangen, Germany	Participation only

Lucie Spannraft

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
26.06.2019 / 28.06.2019	ICMM6	Lund, Sweden	Talk: *Gradient-extended crystal inelasticity with grain boundary interaction coupled to classical decohesion*
03.09.2019 / 05.09.2019	COMPLAS	Barcelona, Spain	Talk: *Modeling of gradient-extended crystal inelasticity with grain boundary interaction including decohesion*

Christian Wick

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
08.04.2019 / 10.04.2019	33rd MMWS 2019	Erlangen, Germany	Talk: *From Force Fields to QM/MM and back: Modelling chemical change in coenzyme B12 dependent enzymes*
13.03.2019 / 15.03.2019	Katalytiker 2019	Weimar, Germany	Poster: *Mechanism of the Water-Gas Shift Reaction Catalysed by Efficient Ruthenium Based Catalysts*
16.06.2019 / 19.06.2019	ICoNSoM 2019	Rome, Italy	Poster: *Modelling Chemical Change in Epoxy Resins: What Can We Learn from Complex Biopolymer Systems?*
03.11.2019 / 05.11.2019	15th GCC 2019	Mainz, Germany	Poster: *Modelling Chemical Change in Epoxy Resins: What Can We Learn from Complex Biopolymer Systems?*

Florian Wullschläger

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
31.03.2019 / 05.04.2019	DPG 2019	Regensburg, Germany	Poster: *Atomistic simulations of chemical graphene exfoliation and carbon nanotubes*
08.04.2019 / 10.04.2019	33rd MMWS	Erlangen, Germany	Poster: *Atomistic simulations of chemical graphene exfoliation and carbon nanotubes*
08.07.2019 / 18.07.2019	CCP5 Summer School	Durham, United Kingdom	Poster: *Atomistic simulations of chemical graphene exfoliation and carbon nanotubes*
30.07.2019 / 31.07.2019	3rd Franconian Theory Meeting	Erlangen, Germany	Participation only
29.09.2019 / 02.10.2019	5th SFB Symposium	Erlangen, Germany	Poster: *Atomistic Modeling of the Synthesis of New Carbon Allotropes by Surface-Assisted Cyclodehydrogenation*

Wuyang Zhao

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
16.06.2019 / 19.06.2019	ICoNSoM 2019	Rome, Italy	Talk: *An elasto-viscoplastic polymer constitutive model based on molecular dynamics simulation under uniaxial finite deformation*

3 Qualification Concept

3.1 Qualification programme

The qualification programme comprises “Qualification Days”, “Alumni and Visitors Workshops”, and “RTG Retreats” as basic activities. These are accompanied by obligatory participations at international conferences and optional research stays abroad.

3.1.1 Qualification days

During each lecture period (typically from October to February and from April to July), one day per week is reserved for “qualification days” covering mini lectures, soft skills trainings, and RTG seminars.

Mini Lectures

The mini lecture programme consists of four pillars addressing Mathematical Skills, Modelling Approaches, Computational Methods, as well as Material Sciences Background. It thus covers the most important techniques and tools to be employed in the doctoral projects and ensures profound interdisciplinary education. For the doctoral researchers/associated doctoral researchers it is mandatory to attend at least ten/five of them within the doctorate.

The mini lectures were hold by PAs, their co-workers*, FRASCAL post docs**, members of the external advisory board*** and visiting guests****.

Table 9: Mini lectures

	Date	Title	Lecturer
01	22 March 2019	Introduction to Tensor Calculus (ITENS)	P. Steinmann
02	17 April 2019	Introduction to Continuum Mechanics (ICOME)	P. Steinmann
03	10 May 2019	Introduction to RTG's Software Platform deal.ii	D. Davydov**, J.-P. Pelteret*
04	17 May 2019	Introduction to the Finite Element Method (IFEM)	S. Pfaller
05	24 May 2019	Failure of Disordered Materials: Statistical Modelling	P. Ray****
06	05 July 2019	Introduction to Mathematical Optimization (IOPTI)	M. Stingl
07	12 July 2019	Introduction to Molecular Modelling: Classical and Hybrid (IMOMO)	C. Wick**, P. Duchstein**
08	16 July 2019	Introduction to Elastic Fracture Mechanics (IFRAC)	K. Kolk***
09	02 October 2019	Introduction to Numerics (INUMS)	H. Lang*
10	11 October 2019	Introduction to Homogenisation (IHOMO)	J. Mergheim
11	01 November 2019	Introduction to Configurational Continuum Mechanics (ICCM)	P. Steinmann
12	08 November 2019	Introduction to Deformation & Fracture Mechanisms in Crystalline & Amorphous Materials (IMECH)	E. Bitzek

Each lecture is also published as a printed script. This serves as a reference work for the doctoral students also after the lecture.

Figure 42: Impressions of some mini lectures and photo of the mini lecture notes (middle).

Soft Skills Trainings

Soft skills trainings (Table 10) are organised by FRASCAL coordination as well as in cooperation with the “FAU Graduate Centre”.

For the doctoral researchers it is mandatory to attend at least at the following three courses:

“Good Scientific Practice”, “Introduction to Research at FAU” and “Gender Equality in Research” within the doctorate.

Table 10: Soft skills trainings

	Date	Title	Lecturer
01	21 February 2019	Good Scientific Practice	C. Schmitt-Engel
02	25 April 2019	Time Management for Doctoral Researchers	A. Egeling
03	03 May 2019	Research Data Management	J. Rohrwild
04	07 June 2019	Introduction to Research at FAU	C. Schmitt- Engel
05	19 July 2019	Gender Equality in Research	S. Schnurbusch






Figure 43: Impressions of some soft skills seminars: "Good Scientific Practice" (top), "Time Management for Doctoral Researchers" (middle) and "Gender Equality in Research" (bottom).

RTG Seminars

In each lecture period, one qualification day is reserved for a RTG seminar mandatory for the doctoral researchers and associated doctoral researchers. Within the framework of this seminar, the current developments of each doctoral project is presented as talks of 15 min duration with 5 min subsequent discussion. Based on these seminars, the doctoral researcher and the mentoring team may evaluate the progress of the doctoral project also in comparison to the other projects.

Table 11: RTG-Seminars

	Date		**Mode**
01	27 June 2019	1. RTG Seminar	all doctoral researchers and postdoctoral researcher
02	13 December 2019	2. RTG Seminar	half doctoral researchers, half associated doctoral researchers and postdoctoral researcher

Programmes see Appendix 1 and Appendix 2

1st RTG Seminar

On June 27, 2019, the first RTG Seminar of the Research Training Group GRK 2423 FRASCAL took place in the Seminar Room of the Regional Computer Centre in Erlangen (RRZE)

Before the official lecture programme started, the spokesperson of the RTG, Prof. Paul Steinmann, gave an overview of all GRK 2423 FRASCAL activities that have already taken place and all upcoming events. After this relatively impressive presentation and the communication of some organizational issues, the scientific programme began.

All 11 doctoral researchers and one postdoctoral researcher have presented the results they have received in the first six months of their scientific work. After each lecture, some already considerable results were discussed. Partly very stimulating and detailed discussions took place, which then had to be interrupted even by the chairpersons and were continued in the coffee breaks.

Figure 44: Impressions of the 1st RTG Seminar.

2nd RTG Seminar

On December 13, 2019, the second RTG Seminar of the Research Training Group GRK 2423 FRASCAL took place in the Seminar Room of the Chair of Applied Mechanics in Erlangen (LTM).

In the morning, the participants were welcomed by RTG co-spokesperson Prof. Erik Bitzek. After a few introductory words, the scientific programme started.

This time, five doctoral researchers, two postdoctoral researchers and – unlike in the 1st RTG seminar - three associated doctoral researchers presented the latest results of their scientific work.

In addition to the multitude of materials examined (from epoxy resins and tungsten single crystals to glass and human bones), the lectures particularly highlighted the interdisciplinarity of the projects, which was also evident in the very stimulating and detailed discussions after the talks.

Figure 45: Impressions of the 2nd RTG Seminar.

Software Development Workshops

Since all 12 projects in FRASCAL require extensive programming knowledge, it is essential that the doctoral researchers acquire sound knowledge in the field of software development.

For this reason, FRASCAL offered a three-part software development workshop, which dealt with the basics and the development of software architectures (Table 12).

Similar to the mini lectures, the content of the workshops was made available to the students as a printed script.

Table 12: Software development workshops

	Date	Title	Lecturer
01	26 July 2019	**General Aspects:** Introduction to HPC Software using C++ Software Design Principles C++ and Object Oriented Programming Basics Git – Basics and Advanced Features GitLab for Continuous Integration Spack Package Manger Cmake – Introduction and Testing	H. Köstler / D. Thönnes
02	20 September 2019	**Advanced Topics I:** C++ Templates C++ Standard Library C++ Exceptions Docker Usage for Testing Testing in Software Development googletest framework GitHub Actions	H. Köstler / D. Thönnes
03	25 October 2019	**Advanced Topics II:** Introduction to Parallel Programming: C++ Threads Design Patterns C++20 Features	H. Köstler / D. Thönnes

Figure 46: Impressions of the Software Development Workshops and photo of the workshops notes.

English Language Coaching

Publications in international journals, presentations at international conferences, and scientific exchange with international researchers require profound knowledge of scientific English. Paul Gahman from the “FAU Language Centre”, a professional English language coach was available for the FRASCAL participants to train oral presentations, to proofread English publications, and to give English classes in each lecture period (120 min every second week). In the first lecture period, the writing skills were strengthened, the second part focused on speaking. The attendance of English classes is optional.

Figure 47: English Coaching with Paul Gahman.

Table 13: English coaching seminars

	Date	Subject	
01	02 May 2019	Introduction to Course; Text Feedback; Written Register	P. Gahman
02	16 May 2019	Creating Language Corpora; Collocations & Lexical Work; Research Tools; Paraphrasing	P. Gahman
03	23 May 2019	Hedging and Expressing Modality	P. Gahman
04	06 June 2019	Thematic Progression	P. Gahman
05	04 July 2019	Thematic Cues and Signposting Devices	P. Gahman
06	11 July 2019	Embedded Clauses (1) and Words of Degree	P. Gahman
07	18 July 2019	Embedded Clauses (2); Intro to Clause and Sentence Variation	P. Gahman
08	25 July 2019	Clause and Sentence Variation; Course Review	P. Gahman
09	24 October 2019	Establishing Baseline Pronunciation Tendencies	P. Gahman
10	7 November 2019	English Prosody 1	P. Gahman
11	21 November 2019	Advanced Pronunciation Techniques 1: Assimilation/Linking	P. Gahman
12	5 December 2019	English Prosody 2: Consonants & Telephoning Language	P. Gahman
13	19 December 2019	Advanced Pronunciation Techniques 2: Shadowing	P. Gahman

3.1.2 Alumni and visitors workshops

In addition to the RTG seminars, the annual alumni and visitors workshop enables scientific exchange with external experts and shall thus stimulate intense discussions. The RTG's Mercator fellows and additional visiting researchers from the fields encountered in the RTG, but also from other related research fields, are invited to these workshops.

Each doctoral researcher has to attend at least two workshops, typically at the end of her/his first and second year.

The first Alumni and visitors workshop was also the Kick-Off Meeting

Table 14: Alumni and visitors workshops

	Date	Subject	
01	02 April 2019	FRASCAL Kick-Off Meeting (1st Visitors Workshop)	

Programme see Appendix 3

On April 2, 2019, the first official joint meeting of doctoral researchers and principal advisors from the Research Training Group GRK 2423 FRASCAL took place in the Hans-Georg-Waeber-Saal of the Fraunhofer Institute (IISB) Erlangen and in the foyer in front of the hall.

Before the official beginning, the doctoral researchers carried out the election of their representatives. Elmira Birang has been elected as the "doctoral researchers' spokesperson" and Jonas Ritter as the "doctoral researchers' gender representative". Both were elected for one year and will be in permanent exchange with RTG spokespersons to represent the interests of the doctoral researchers in all matters. Congratulations!

At 2 pm, the Kick-Off Meeting started and Professor Paul Steinmann, the spokesperson, welcomed the guests to the event. In his opening speech, he described the scientific challenges the GRK 2423 FRASCAL has set itself in the next 4.5 years and how it developed from the idea of this Research Training Group to the application and commission by the German Research Foundation, DFG, and finally the approval of the application.

He then presented the scientific content of the Research Training Group and the challenging interdisciplinary and cross-linking project structure. Paul Steinmann highlighted the close cooperation between the FRASCAL's projects and clearly communicated that the focus of the various research activities within the Research Training Group is the development of simulation methods that capture the multi-scale nature of failure.

Thereafter, co-spokesperson of the RTG, Professor Erik Bitzek, addressed the audience and presented the organizational structure of the Research Training Group, which was initiated and is managed by the Zentralinstitut für Scientific Computing (ZISC). In addition to presenting available software platforms and data storage options, Erik Bitzek described the content of the qualification programme more detailed: Apart from their scientific work, the doctoral researchers have the opportunity to be part of an individualized qualification programme consisting of subject-specific mini lectures, soft skill trainings, alumni and visitors workshops, RTG seminars, retreats and more.

A particularly valuable aspect of the FRASCAL programme is the possibility of involving Mercator Fellows, outstanding scientists from abroad, which enables an intensive and long-term scientific exchange with the young FRASCAL researchers. Therefore, it was a great pleasure and honour that all three Mercator Fellows of the RTG, Prof. Michael Ortiz (California Institute of Technology, Pasadena, CA), Prof. Elias Aifantis (Aristotle University of Thessaloniki, Greece) and Dr. Laurent Ponson (Pierre et Marie Curie University, Paris, France), took the time to travel to the event and talk about their fields of research. In their lectures, the audience was able to experience how versatile and exciting the topic of fractures is. The GRK 2423 FRASCAL wholeheartedly thanks the speakers for sharing their knowledge.

During the coffee break and the welcome reception, the doctoral researchers presented their projects in poster sessions and in a relaxed atmosphere, culminating in intensive conversations with other visitors and particularly with the Mercator Fellows.

It was a great pleasure that Dr. Thomas Münz (DYNAmore GmbH) and PD Dr.-Ing. Ralf Meske (Federal Mogul Nürnberg GmbH) were able to participate in the Kick-Off Meeting as a part of the external advisory board. In this way, the FRASCAL doctoral researchers gained the chance to make initial contacts with industry partners with even the idea for a new subject of a mini lecture being born: It will deal with the possibility of solving industry-relevant fracture mechanical problems with the commercial software LS-DYNA. The lecture will then be held especially for the FRASCAL doctoral researchers by employees of DYNAmore GmbH.

All in all, the opening event highlights an already successful start to the research work of GRK 2423 FRASCAL based on an intensive cooperation between principal advisors, doctoral researchers, Mercator Fellows and members of the external advisory board.

Figure 48: Impressions of the Kick-Off Meeting (1st Visitors Workshop).

3.2 Visiting researcher programme

Table 15: Visiting researchers

From / to	Guest	Research Subject
02.04.2019 / 03.04.2019	**Prof. Michael Ortiz** California Institute of Technology, Pasadena, CA, USA	Invited lecture at Kick-Off Meeting and discussions with several FRASCAL doctoral researchers and PAs Host: Prof. Sigrid Leyendecker (LTD)
01.04.2019 / 03.04.2019	**Dr. Laurent Ponson** *Pierre et Marie Curie University, Paris, France*	Invited lecture at Kick-Off Meeting and participation in research activities particularly relevant to project P2 Host: Prof. Erik Bitzek (WW1)
01.4.2019 / 04.04.2019	**Prof. Elias Aifantis** Aristotle University of Thessaloniki, Thessaloniki, Greece	Invited lecture at Kick-Off Meeting and participation in research activities particularly relevant to project P5 Host: Prof. Michael Zaiser (WW 8)
20.5.2019 / 23.5 2019	**Prof. Kenneth Runesson** Material and Computational Mechanics, Department of Industrial and Materials Science Chalmers University of Technology, Gothenburg, Sweden)	During his stay, Prof. Runesson participated in our research activities in the area of Configurational Fracture Mechanics, which was particularly relevant to project P10. Prof. Runesson contributed his expertise in the corresponding computational setting and the associated area of analysis. Host: Prof. Paul Steinmann (LTM)
09.5.2019 / 10.06.2019	**Prof. Purusattam Ray** The Institute of Mathematical Sciences, Chennai, India	1. Research Seminar (22 May 2019): “Equivalence of the Burridge-Knopoff train model of earthquakes and the dynamics of driven Edwards-Wilkinson interfaces” 2. Mini Lecture (24 May 2019):"Failure of disordered materials: Statistical modelling" Host: Prof. Michael Zaiser (WW 8)
28.07.2019 / 02.08.2019	**Dr. Laurent Ponson** Pierre et Marie Curie University, Paris, France	Discussions with the FRASCAL doctoral researchers about their projects. The students benefited greatly from these fruitful discussions and constructive advice from the Mercator fellow. The new insights gained in their work certainly contribute to making rapid progress in further research. Host: Prof. Erik Bitzek (WW1)
06.08.2019 / 08.08.2019	**Dr. Laurent Ponson** Pierre et Marie Curie University, Paris, France	Participation with invited lecture at ISAM4 2019 (with FRASCAL as program partner) in Erlangen (Friedrich-Alexander-Universität Erlangen-Nürnberg, Wassersaal in der Orangerie) Host: Prof. Erik Bitzek (WW1)
14.11.2019 / 15.11.2019	**Prof. Michael Ortiz** California Institute of Technology, Pasadena, CA, USA	Discussions with S. Leyendecker and D. Phansalkar about P9-relevant questions Host: Prof. Sigrid Leyendecker (LTD)
18.12.2019 / 20.12.2019	**Prof. Michael Ortiz** California Institute of Technology, Pasadena, CA, USA	Discussions S. Leyendecker about • phase field models • dynamic fragmentation, branching of cracks • diffused cracks • mesh free methods • variational derivation of Liouville equation • numerical solution of Liouville equation • mesodynamics Discussion with E. Birang (P10) about her research project. Host: Prof. Sigrid Leyendecker (LTD)

3.3 Additional qualification measures

3.3.1 Research stays or internships at other research institutions

Christof Bauer

From / to	Institute visited	Local supervisor (if applicable)	Research activities performed and skills acquired during stay
10.09.2019	Theoretical Physical Chemistry Group, TU Darmstadt, Germany		Presentation of the Capriccio Group and definition of the planned cooperation
23.09.2019	Institut Jean le Rond d'Alembert, Sorbonne University, France	Laurent Ponson	Solid mechanics seminar, own presentation
24.09.2019 / 25.09.2019	Equipe de Mécanique, Université Paris-Est Marne-la-Vallée, France	Fabrice Detrez	Multiscale Modelling and Simulation seminar, own presentation

Ahmad Hosseini

From / to	Institute visited	Local supervisor (if applicable)	Research activities performed and skills acquired during stay
15.03.2019 / 16.05.2019	ESTIA, Thessaloniki, Greece	Elias Aifantis, Avraam. Konstantinidis	Fracture of disordered beam systems

Julian Konrad

From / to	Institute visited	Local supervisor (if applicable)	Research activities performed and skills acquired during stay
26.08.2019 / 28.08 2019	Technische Universität Hamburg, Germany	Robert Meißner	Discussion/Collaboration for the curing process of epoxy resins

Maximilian Ries

From / to	Institute visited	Local supervisor (if applicable)	Research activities performed and skills acquired during stay
23.09.2019	Institut Jean le Rond d'Alembert, Sorbonne University, France	Laurent Ponson	Solid mechanics seminar, own presentation
24.09.2019 / 25.09.2019	University of Paris-Est, Laboratoire de Modélisation et Simulation Multi-Échelle, France	Fabrice Detrez	Multiscale Modelling and Simulation seminar, own presentation

Jonas Ritter

From / to	Institute visited	Local supervisor (if applicable)	Research activities performed and skills acquired during stay
30.05.19 / 31.05.19	WSL-Institut für Schnee- und Lawinenforschung SLF, Davos		Meeting and discussion of planned cooperation with Prof. Dr. Johan Gaume (SLF and EPFL), Dr. Henning Löwe (SLF) and Prof. Dr. Michael Zaiser (FAU and FRASCAL)
11.11.19 / 23.11.19	SLAB Institute at EPFL, Lausanne	Prof. Dr. Johan Gaume	Discussion and work on compression simulations of snow microstructures; Presentation of the own work; Exchange of data

Ina Schmidt

From / to	Institute visited	Local supervisor (if applicable)	Research activities performed and skills acquired during stay
20.10.2019 / 15.11.2019	University of Capetown	Daya Reddy	Further work and public presentation of model extensions

Lucie Spannraft

From / to	Institute visited	Local supervisor (if applicable)	Research activities performed and skills acquired during stay
16.09.2019 / 23.09.2019	Chalmers University of Technology, Gothenburg, Sweden	Kenneth Runesson	Joint work on a paper with Magnus Ekh, Fredrik Larsson and Kenneth Runesson; Discussion on decohesion models for grain boundary interaction and on recent numerical results; Gaining insight in related work performed at Chalmers University of Technology

Christian Wick

From / to	Institute visited	Local supervisor (if applicable)	Research activities performed and skills acquired during stay
16.02.2019 / 20.02.2019	Institute Ruđer Bošković, Zagreb, Croatia	Boris Kovačević, David Smith	Exchange with experts in computational chemistry and modelling of radical reactions in related systems

3.3.2 Summer schools

Paras Kumar

From / to	Name of summer school	Location
09.06.2019 / 11.06.2019	IGF 25 Summer School on Fracture Mechanics	Catania, Italy

Tarakeshwar Lakshmipathy

From / to	Name of summer school	Location
13.09.2019 / 15.09.2019	6th Summer school on Fracture Mechanics	Cracow, Poland

Tobias Müller

From / to	Name of summer school	Location
17.07.2019 / 19.07.2019	ICICP Summer School	Erlangen, Germany

Dhananjay Phansalkar

From / to	Name of summer school	Location
13.09.2019 / 15.09.2019	6th Summer school on Fracture Mechanics	Cracow, Poland

Sukhminder Singh

From / to	Name of summer school	Location
09.06.2019 / 11.06.2019	IGF 25 Summer School on Fracture Mechanics	Catania, Italy

Florian Wullschläger

From / to	Name of summer school	Location
08.07.2019 / 18.07.2019	CCP5 Summer School	Durham, United Kingdom

4 Selected Highlights

4.1 Long Night of Sciences

On 19 October 2019 from 6 pm to 1 am numerous institutes in the Erlangen, Fuerth and Nuremberg region participated in the Long Night of Sciences (Lange Nacht der Wissenschaften, LNdW). The Research Training Group GRK 2423 FRASCAL also presented the interested public its research topics in a vivid way.

FRASCAL was involved in the Science Night with five stations.

The first booth was located right at the entrance to the showroom inviting visitors to learn about the different modes of fracture demonstrated by using simple everyday materials such as paper, Styrofoam and PU foam. It was also exciting to observe how differently cracks propagate in the various materials. Finally, the idea and the fracture behaviour of composite materials could also be demonstrated with plastic straws and ice-cream sticks.

At a different stand, young and old were able to learn how different materials break with the example of sweets. Thus, lollipops exhibit a brittle behaviour, comparable e.g. with glass. Some caramel-filled chocolate bars, however, deform only before they break and behave like a metal. Even the breaking behaviour of particle composites or layer composites could be shown very clearly with chocolate bars spiked with puffed grain (even with predetermined breaking points!) or chocolate bars with alternately arranged waffle and chocolate layers. Of course, the visitors could convince themselves of the different behaviour and take the demonstration material with them.

At another station, not only the female scientific members of GRK 2423 FRASCAL were presented in a photo gallery, but visitors could also test their knowledge of (further) famous female researchers in the form of a quiz and - if successful - were rewarded with a small sweet prize.

At the same booth, the audience could learn about the history of fracture mechanics, got to know or remember historic, spectacular accidents of means of transport due to material failure and what role fracture mechanics plays in avalanche release. Likewise, important scientists were presented, who made substantial contributions in the areas of fracture theory and mechanics, material fatigue and computational methods in mechanics.

To show that our RTG is developing simulation methods to better understand the multi-scale nature of fracture behaviour, visitors were given the opportunity to use virtual-reality glasses to virtually explore the world of a crack in three-dimensional space with atomic resolution and experience "virtual destruction" in this way. An impressive experience!

The presentation of the GRK 2423 FRASCAL attracted a lot of attention throughout the whole night and it was amazing how the doctoral researchers of FRASCAL, with their diverse, creative ideas and fresh presentations made the topic “fracture” and “fracture behaviour of various materials” accessible to the general public.

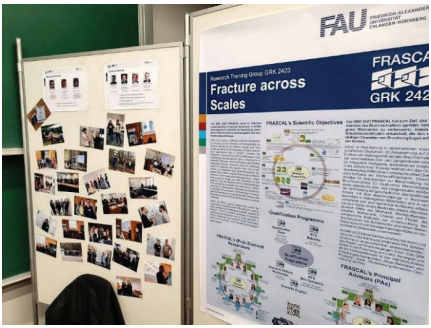

Figure 49: Impressions of the Long Night of Sciences.

4.2 Social events

BBQ

Immediately after the soft skills seminar “Gender Diversity in Research”, the doctoral researchers organized a barbecue afternoon on July 19. In the best summer weather, not only could the grilled food be enjoyed, but there was also the opportunity for intensive and lively discussions on the subject of the seminar.

Figure 50: Impressions of the BBQ in July.

Year-end event

After the 2nd RTG seminar on December 13, RTG spokesperson Prof. Paul Steinmann warmly greeted all FRASCAL members and thanked everyone for their commitment to the Research Training Group last year, which was also its first year. He sent his words of thanks in a video message from sunny Cape Town, where Paul Steinmann spends a sabbatical.

Afterwards, Prof. Erik Bitzek presented a review of the first year of FRASCAL in a Christmas atmosphere. It became clear how impressively many activities have already been carried out: a large number of mini lectures, several soft skills seminars, three software development workshops, regular English coaching units, RTG seminars, visitors workshop, building up a FRASCAL library from 28 books and much more ...

With an outlook of the planned activities for the coming, hopefully equally successful year, the day ended with a cosy get-together.

Figure 51: Impressions from FRASCAL's year-end event.

4.3 FRASCAL library

LIBRARY FRASCAL GRK 2423

At the beginning of the Research Training Group, a separate library was set up exclusively for FRASCAL members. Gradually, specialist books on FRASCAL-relevant topics are purchased.

28 new books have already been acquired in the first year of FRASCAL.

For a complete list, see Appendix 4.

5 Appendices

5.1 Appendix 1: Programme of the 1st RTG Seminar

Programme of the 1st RTG-Seminar			
Date	27 June 2019	Time	9:15 – 15:50
Venue	RRZE, Room 2.049, Martensstraße 1, 91058 Erlangen		

Lectures: 15 min + 5 min discussion

Time	Name	Title of Presentation
9:15 – 9:30	WELCOME & INTRODUCTION	
9:30 – 9:50	Tobias Müller (P1)	*Chemistry at the crack tip: First MD simulations*
9:50 – 10:10	Tarakeshwar Lakshmipathy (P2)	*Influence of crack tip radius on fracture behaviour: An atomistic study*
10:10 – 10:30	Julian Konrad (P3)	*Preparation of polymer composites for MD-simulations*
10:30 – 10:50	COFFEE BREAK	
10:50 – 11:10	Ali Mauricio Velasco Sabogal (P4)	*Multisphere fitting algorithm to represent arbitrary shaped grains*
11:10 – 11:30	Jonas Ritter (P5)	*Identification of a suitable framework for the micromechanical simulation of compressive failure in highly porous materials*
11:30 – 11:50	Christof Bauer (P6)	*Adaptivity of the Capriccio-Method: Particle-based regions moving within a continuum*
11:50 – 13:30	BOARD OF PAS / PHOTO SESSION / JOINT LUNCH	
13:30 – 13:50	Nosaibeh Esfandiary (P7)	*Modelling fracture in materials with hierarchical microstructures*
13:50 – 14:10	Paras Kumar (P8)	*Implementing viscoelasticity with deal.ii - Software development aspects*
14:10 – 14:30	Dhananjay Phansalkar (P9)	*Analytical and numerical solutions of 1D quasi static phase field problem*
14:30 – 14:50	COFFEE BREAK	
14:50 – 15:10	Elmira Birang (P10)	*On configurational forces in molecular statics*
15:10 – 15:30	Sukhminder Singh (P11)	*Uniqueness challenge in the solution of quasi-static crack problem*
15:30 – 15:50	Christian Wick (P12)	*Modelling chemical change in epoxy resins: Model chemistries and curing reactions*

5.2 Appendix 2: Programme of the 2nd RTG Seminar

Programme of the 2nd RTG-Seminar			
Date	13 December 2019	Time	9:50 – 15:50
Venue	LTM, Room 00.044, Egerlandstraße 5, 91058 Erlangen		

Lectures: 15 min + 5 min discussion

Time	Name	Title of Presentation
09:50 – 10:00	WELCOME & INTRODUCTION	
10:00 – 10:20	Christian Wick, P12	*Breaking Bonds in Epoxy Networks*
10:20 – 10:40	Sukhminder Singh, P11	*Gradient-Based Material Optimization for Fracture Control*
10:40 – 11:00	Elmira Birang, P10	*Atomistic Configurational Forces: An Analysis Tool for Crack Propagation in Molecular Dynamics*
11:00 – 11:20	COFFEE BREAK	
11:20 – 11:40	Ina Schmidt, P10	*Computational Bone Remodeling Dependent on Biological Availability*
11:40 – 12:00	Dimosthenis Floros, P10	*On Configurational Forces for Gradient-Enhanced Inelasticity*
12:00 – 12:20	Julian Konrad, P3	*Development of a Dissociative Force Field for Fracture Mechanics of Epoxy Resins*
12:20 – 13:20	LUNCH BREAK	
13:20 – 13:40	Achraf Atila, P2	*Atomistic Study of Mechanical and Structural Anisotropy of Metaphosphate Glasses*
13:40 – 14:00	Tarakeshwar Lakshmipathy, P2	*Influence of Crack Tip Radius on Fracture Behaviour: An Atomistic Study*
14:00 – 14:20	Tobias Müller, P1	*Chemistry at the Crack Tip*
14:20 – 14:40	Florian Wullschläger, P1	*Mechanical and Chemical Properties of 2D Materials*
15:00 – 20:00	One Year GRK 2423 FRASCAL – A Review	

5.3 Appendix 3: Programme of the Kick-Off Meeting

Programme of the Kick-Off Meeting (1st Visitors Workshop)			
Date	2 April 2020	Time	14:00 – 19:30
Venue	Hans-Georg-Waeber-Saal, Schottkystraße 10, 91058 Erlangen		

Lectures: 45 min + 15 min discussion

Time	Name	Title of Presentation
14:00 – 14:30	OPENING & WELCOME Prof. Paul Steinmann (spokesperson) Prof. Erik Bitzek (co-spokesperson)	
14:30 – 15:30	**Prof. Michael Ortiz** California Institute of Technology, Pasadena, CA, USA	*Multiscale analysis of fracture under geostatic conditions*
15:30 – 16:00	COFFEE BREAK	
16:00 – 17:00	**Prof. Elias Aifantis** Aristotle University of Thessaloniki, Thessaloniki, Greece	*Gradient fractional/fractal models for deformation and fracture*
17:00 – 18:00	**Dr. Laurent Ponson** Institut Jean le Rond d'Alembert Université Pierre et Marie Curie, Paris, France	*Deciphering the roughness of cracks: what fracture surfaces teach us about the dissipative mechanisms controlling the toughness of materials*
18:00 – 18:30	WELCOME RECEPTION WITH SNACKS	
18:30 – 19:30 (cancelled due to illness)	**Dr. Bernd Flessner** Zentralinstitut für Wissenschaftsreflexion und Schlüsselqualifikationen ZiWiS, FAU Erlangen, Erlangen, Germany	*Fiktive Materialien - Vom Cavorit zum Dilithium* *„New materials" from a quite different angle - materials that express the visions and dreams of scientists and researchers.*

5.4 Appendix 4: List of book inventory

1. Computational methods in elasticity and plasticity solids and porous media
   Anandarajah, Annalingam, 2010

2. Nonlinear problems of elasticity
   Antman, Stuart S., 2005

3. Nonlinear continuum mechanics of solids fundamental mathematical and physical concepts
   Başar, Yavuz, 2010

4. Elasticity and plasticity of large deformations an introduction
   Bertram, Albrecht, 2012

5. Solid mechanics theory, modeling, and problems
   Bertram, Albrecht, 2015

6. The theory of linear viscoelasticity
   Bland, David Russell, 2016

7. Nonlinear continuum mechanics for finite element analysis
   Bonet, Javier; Wood Richard D., 2008

8. Plasticity modeling & computation
   Borja, Ronaldo I., 2013

9. Gamma-convergence for beginners
   Braides, Andrea, 2002

10. Atomistic computer simulations a practical guide
    Brázdová, Veronika, 2013

11. Continuum mechanics concise theory and problems
    Chadwick, Peter, 1999

12. Theory of plasticity
    Chakrabarty, Jagabanduhu, 2006

13. Plasticity for structural engineers
    Chen, Wai-Fah, 2007

14. Handbook of differential equations; Stationary partial differential equations; Vol 3
    Chipot, Michel; Quittner Pavol (eds.), 2006

15. Viscoelasticity of polymers Theory and numerical algorithms
    Cho, Kwang Soo, 2016

16. Theory of viscoelasticity
    Christensen, Richard M., 2003

17. Mechanics and physics of porous solids
Coussy, Olivier, 2010

18. Dynamic fracture mechanics
Freund, Lambert B., 1990

19. Fracture Mechanics With an Introduction to Micromechanics (copy 1)
Gross, Dietmar, 2018

20. Fracture Mechanics With an Introduction to Micromechanics (copy 2)
Gross, Dietmar, 2018

21. Statistical models for the fracture of disordered media
Herrmann, Hans. J.; Roux, Stéphane (eds.), 1990

22. Nonlinear solid mechanics a continuum approach for engineering
Holzapfel, Gerhard A., 2001

23. A course on nonlinear fracture mechanics
Hutchinson, John W., 1980

24. Advanced fracture mechanics
Kanninen, Melvin F., 1985

25. Molecular modelling principles and applications
Leach, Andrew R., 2001

26. Tribology on the small scale a modern textbook on friction, lubrication, and wear
Mate, C. Mathew, 2019

27. Modern quantum chemistry introduction to advanced electronic structure theory
Szabó, Attila, 1996

28. Computational Homogenization of Heterogeneous Materials with Finite Elements
Yvonnet, Julien, 2019