Friedrich-Alexander-Universität
Erlangen-Nürnberg

Annual Report 2021

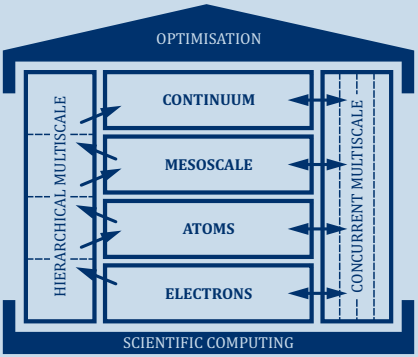
of the Research Training Group GRK 2423

FRASCAL

GRK 2423

Fracture across Scales:

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



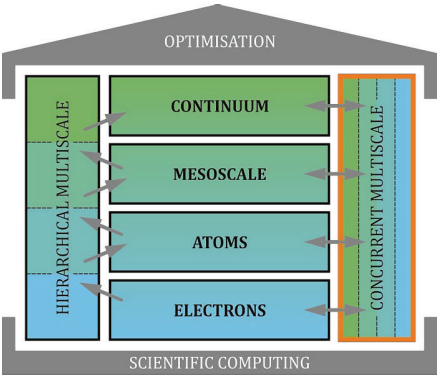
Annual Report
of the Research Training Group GRK 2423

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, until August 2021)
Prof. Dr. rer. nat. Michael Stingl (co-spokesperson, since September 2021)



2021

www.frascal.fau.de

Impressum

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Preface

Already the third year of our Research Training Group GRK 2423 FRASCAL has past!

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

FRASCAL started in January 2019 with its first cohort of doctoral researchers. Fortunately, we were able to shape and use the first year largely as planned, i.e. onboarding the new doctoral researchers – preparing, scheduling and pursuing the qualification programme, in particular the multiple FRASCAL mini lectures – and developing initial success steps in the various research projects P1-P12. The second and third year of FRASCAL, i.e. 2020 and 2021, however, were overshadowed by the Corona pandemic. Nevertheless, all FRASCAL members demonstrated great resilience and endurance in view of the past and unfortunately still ongoing hardships.

As a tribute to the pandemic, most FRASCAL activities since 2020 took place only online, e.g. FRASCAL seminars and symposia by guest researchers, FRASCAL mini lectures, and, noteworthy, the weekly FRASCAL online meetings. There, we in particular conducted FRASCAL TOPZ (Topical Overview Presentation Zoomposia) which, jointly with the ensuing and engaging discussions, helped review the amazing progress made in the various research projects P1-P12.

At the end of the year 2021, we are still pursuing our research mostly at home, however hope dies last. FRASCAL's first cohort of doctoral researchers mostly finished their third year, approaching the home stretch by finishing their doctoral theses, which are based on the fantastic research work done. Their accomplished scientific and qualification achievements are stunningly impressive, thus there are no obstacles, neither formal nor regarding content, for successful doctoral theses.

The second cohort of doctoral students is already in the starting block and looking forward to the continuation of exciting research.

This annual report is testimony of FRASCAL's great progress during the year 2021.

I am looking forward to see FRASCAL flourishing further.

Erlangen, December 2021

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

Spokesperson:

Prof. Dr.-Ing. Paul Steinmann

Co-spokesperson:

Prof. Dr.-Ing. Erik Bitzek (until August 2021)
Prof. Dr. rer. nat. Michael Stingl (since September 2021)

Doctoral researchers' spokesperson:

Jonas Ritter (until March 2021)
Paras Kumar (since April 2021)

Doctoral researchers' gender representative:

Christof Bauer (until March 2021)
Nosaibeh Esfandiary (since April 2021)

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, Prof. 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, PD Dr.-Ing. habil.	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: Postdoctoral researcher

Post Doc	Chair, Department, Work Address	Contact Data (Tel / Fax, Email, Web)	Research Area
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 3: 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	Competence Unit for Scientific Computing, CSC 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
Laurien, Marie	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-64 407/ -413, marie.laurien@fau.de www.ltm.tf.fau.eu	Continuum-kinematics-inspired peridynamic modelling of fracture
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 at the Crack Tip

		chemistry.nat.fau.eu/ccc/groups	
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 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
Hiemer, Stefan	Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65 062 / -066, stefan.hiemer@fau.de, matsim.techfak.uni-erlangen.de	Machine Learning of Failure of Disordered Materials
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
Marzulli, Valentina	Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraße 3, 91058 Erlangen	+49 9131 85-70 498 / -518, valentina.marzulli@fau.de, mss.cbi.fau.de	Mechanical characterization of granular 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	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, wuyang.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)
Albert, Jacob	P6, S. Pfaller	Mechanical Engineering	May 2021 – Aug 2021
Dhamo, Kevin	P1, B. Meyer	Chemistry	Jan 2021 – Sep 2021
Gossler, Mattis	P1, B. Meyer	Chemistry	Jan 2021 – Mar 2021
Hsu, Lan-Tien	P2, E. Bitzek	Advanced Materials and Processes	Jan 2021 – Aug 2021
Kashiri, Mani	P10, P. Steinmann	Mechanical Engineering	Jan 2021 – May 2021
Kirsan, Azad	P1, B. Meyer	Chemistry	Jan 2021 – Mar 2021
Laubert, Lukas	P6, S. Pfaller	Mechanical Engineering	15 Jun 2021– 14 Sep 2021
Müller, Valentin	P3, D. Zahn	Molecular Science	Mar 2021 – Dec 2021
Müller-Hillebrand, Johannes	P3, D. Zahn	Chemistry	Jan 2021 – 15 May 2021 Jul 2021 – Dec 2021
Pahi, Sampanna	P12, A.-S. Smith	Physics	Feb 2021 – Dec 2021
Pyka, Leon	P2, E. Bitzek	Materials Science and Engineering	Jan 2021 – Sep 2021
Ritthaler, Marina	P6, S. Pfaller	Mechanical Engineering	May 2021 – Sep 2021
Rohracker, Maurice	P8, J. Mergheim, P. Kumar	Computational Engineering	Mar 2021 – Dec 2021
Topraksal, Ece	P12, A.-S. Smith	Advanced Materials and Processes	Apr 2021 – Dec 2021

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 Energy 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

Figure 1: Members of FRASCAL at the 6th RTG-Seminar in Neuhof an der Zenn on 15 October 2021. (Image: private)

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.	Competence Unit for Scientific Computing, CSC, Martensstraße 5a, 91058 Erlangen	+49 9131 85-20782 / -20785, andrea.dakkouri@fau.de, www.frascal.fau.eu	FRASCAL Coordination
Güthlein, Nicole	Competence Unit for Scientific Computing, CSC, Martensstraße 5a, 91058 Erlangen	+49 9131 85 20780 / -20785, guethlein@math.fau.de, www.zisc.fau.de	CSC Administration
Pflug, Lukas, Dr. rer. nat.	Department of Mathematics Chair of Applied Mathematics, Cauerstraße 11, 91058 Erlangen	+49 9131 85 67139 / -67134, lukas.pflug@fau.de, www.zisc.fau.de	CSC Managing Director

1.4 Reporting period

01 January 2021 to 31 December 2021

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, P12), 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).

P1: Chemistry at the Crack Tip

Tobias Müller and Bernd Meyer

In last year's report, I showed that a multitude of different crack tip structures and relaxation patterns of the inner crack surfaces exist as local energy minima. This makes the search for the reaction path for crack opening (i.e. how to break the next bond) a challenge. Furthermore, along the reaction path the outer boundary conditions have to be adjusted (i.e. the positions of the outer fixed atoms as given by the far-field solution of linear elastic continuum theory). This outer boundary is determined uniquely by the position α of the centre of the linear elastic strain field ("pacman structure"). Figure 2 shows that when the pacman structure is relaxed without adjusting the boundary (α = 0, i.e. using fixed boundary conditions), a large artificial strain field is introduced in the finite cut-out. It disappears when the position of the strain field center is corrected, i.e. when using a flexible boundary approach. Adjusting the boundary is in particular important for achieving size consistency.

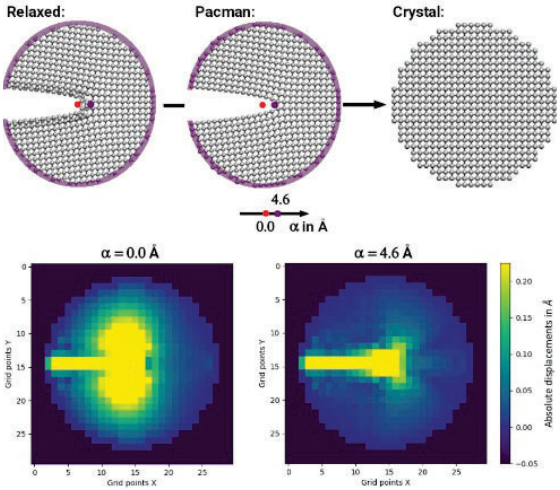

Figure 2: Illustration of the atomic displacements when a pacman structure is relaxed. Upper row: The purple ring indicates the fixed outer Si atoms. The amplitude of the displacement of each atom with respect to the reference pacman is color coded and is mapped onto the bulk crystal structure. The result is shown in the lower row. The calculation was done for an initial strain field centre at α = 0, (i.e. the last intact bond at the crack tip in the pacman structure is in the centre of the cut-out) and for the adjusted centre at α = 4.6 Å (as shown in the upper row).

Initially, the corrected position of the strain field centre was determined by a matching of displacement fields. In the last year, I developed a second method, which is based on the energy of the cut-out. With a practical method for adjusting the strain field centre (i.e. the boundary conditions for the finite cut-out) at hand, it is now possible to address the question how a crack advances under constant load. I started from the global energy minimum structure, in which the last intact bond is located at position b1, see Figure 3. It is now important to realize that after breaking bond b1, the crack tip structure at b2 will be different. The crack tip structure b1 cannot be transferred to b2 because it would require that the alternating up and down relaxation pattern of the Si atoms is flipped along the whole crack surface. Thus, the crack has to advance via an intermediate structure at b2 before the initial global energy minimum crack tip structure can be formed at b3.

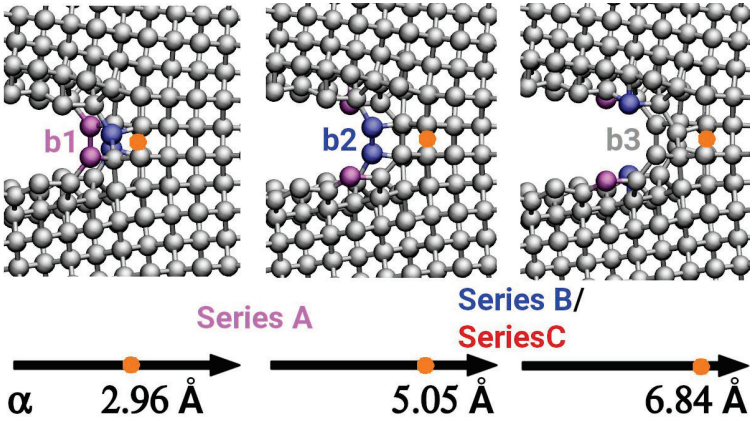

Figure 3: Schematic illustration of crack tip advancement from bond b1 to b3 via a local energy minimum structure at b2. The position of the strain field centre is shown by an orange dot.

A first attempt was made to calculate a full energy profile for the advancement of the crack from position b1 to b3. The challenging part is the adjustment of the boundary conditions along the path, making it difficult to use well-established methods like nudged elastic band (NEB). Thus, I first tested a simpler procedure in which the length of bond b1 is used as reaction coordinate. The bond length is increased in several steps until bond b1 is broken and structure b2 is formed, see Figure 3. At each step, the two atoms defining bond b1 are fixed, all other atoms are relaxed, and the outer boundary region is aligned by adjusting α. The energy along this path is shown in Figure 4 (Series A). The same procedure is then repeated for bond b2, see Figure 4 (Series B). Unfortunately, the final result was not structure b3, i.e. the identical structure as b1 but shifted by two bonds. Instead, an additional bond was broken. In Series C this bond was closed to yield finally structure b3. An important constituency check is that the energies at the beginning and end of the path are the same as shown in Figure 4. Along the configurations of Series B, a huge energy barrier is encountered. This indicates that the simple procedure to break bonds by just elongating them is not suitable for finding the minimum energy pathway for crack propagation. The aim for the future is therefore to develop a more sophisticated method, which allows to follow the minimum energy pathway while simultaneously adjusting the outer boundary conditions.

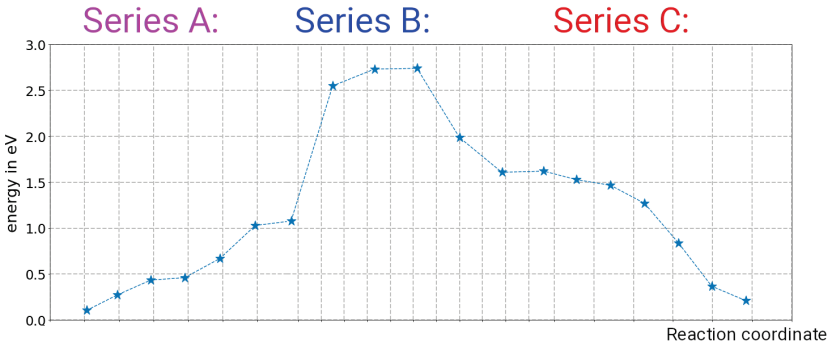

Figure 4: Energy profile for crack tip advancement from bond b1 to b3. Series A and B represent the cleavage of b1 and b2, respectively, and Series C shows an additional bond closing step.

P1: Probing the Conformational Flexibility of Norbornadiene (NBD) / Quadricyclane (QC) – Fullerene Hybrids by Molecular Dynamics Simulations

Florian Wullschläger and Bernd Meyer

The norbornadiene (NBD) / quadricyclane (QC) interconversion couple is a promising concept for the efficient realization of molecular solar thermal energy storage systems. After light induced intramolecular cycloaddition of NBD, the highly strained metastable QC isomer is formed. The energy stored as strain energy in chemical bonds can be released as thermal energy. In a collaboration with the Hirsch group from Organic Chemistry we studied the light-only-controlled interconversion of NBD/QC–fullerene hybrids with three different linker units, which has the opportunity of selective photoswitching in both directions. The aim was to show that the distance between fullerene and QC moiety plays a key role in the back-reaction to the respective NBD hybrid.

With the help of molecular dynamics simulations using the LAMMPS software package and the generalized Amber force field (GAFF) I was able to generate QC–fullerene distance frequency distributions of the different hybrids. The distance between the centers of mass of the QC moieties and the respective fullerene cores was derived every 100 fs from 5 ns trajectories, see Figure 5. The resulting distance distribution explains the decreasing rates of the back-reactions estimated from 1H-NMR and indicates an intramolecular interaction between fullerene and QC as main driving force.

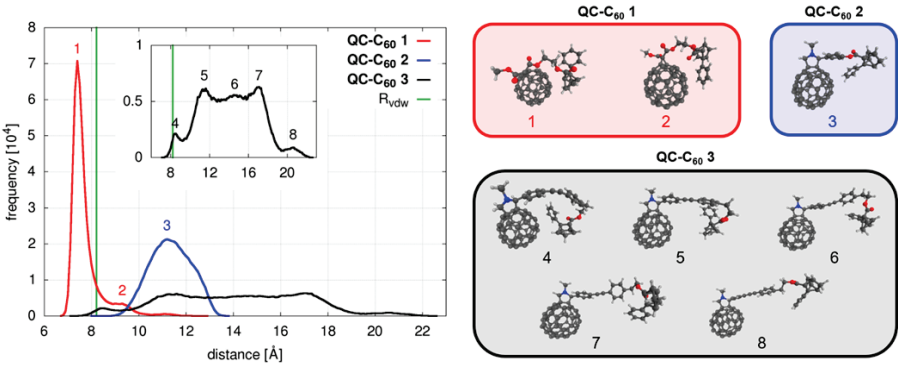

*Figure 5: Left side: Histogram of the distance between the centres of mass of the QC moiety and the fullerene for the three QC– fullerene hybrids **QC-C60 1-3** with different spacer unit, derived from the MD simulations. The numbers indicate the distances where representative structures were picked. Right side: Representative structures of **QC-C60 1-3** hybrids during the MD simulation at the indicated distances.*

To shine more light into this proposed mechanism, I calculated frontier molecular orbitals of the QC–fullerene hybrids using the ORCA program package at the B3LYP/def2-TZVP level of theory. These calculations show that the LUMO is always exclusively located on the fullerene core, which is in line with its strong electron accepting property, see Figure 6. I also see for all different hybrids two to three orbitals within the range of a few tenths of an eV of the HOMO with exclusive localization on the QC moiety or the linker unit, which in combination with the fact that QC is one of the easiest to oxidize saturated hydrocarbons also confirms the proposed intramolecular mechanism.

The distance dependency of the recombination rate of light-only-controlled interconversion of NBD/QC–fullerene hybrids was proofed and the proposed intramolecular mechanism for the back-reaction from QC to NBD was further verified. The results of the molecular dynamics simulations explain the change in the lifetimes of the hybrids for different QC-fullerene distances and provide more insights into the mechanism of the back-reaction [1]. In the future, I will investigate the influence of solvents by performing molecular dynamics simulations in dichloromethane.

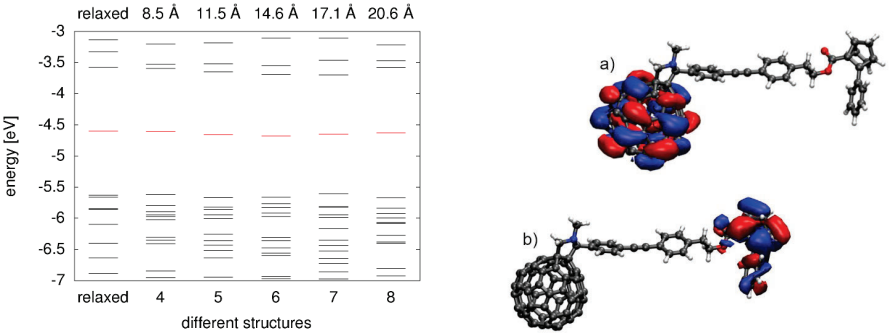

*Figure 6: Left side: Energies of the molecular orbitals of the different structures of **QC-C60 3**. The red lines are the mid-points between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). Right side: Representative frontier molecular orbital of **QC-C60** 3, a) LUMO and b) HOMO (isovalue 0.0128 au).*

Reference

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P2: Scale-Bridging in Fracture Mechanics: Ab Initio Simulations, Atomistics and Continuum Models

Tarakeshwar Lakshmipathy and Erik Bitzek

Objectives and status

Density functional theory (DFT) is an ab initio method that due to its computationally expensive nature has been seldom used in fracture simulations. Classical atomistic simulations (where millions of atoms can be simulated) on the other hand, have been widely used to study fracture at the atomic scale. However, the classical interatomic interactions (potentials) used in atomistic simulations, especially for bcc metals, can lead to artefacts [1]. Hence, it is necessary to benchmark these potentials using DFT. In collaboration with FRASCAL project P1, fracture simulations were performed on blunted cracks in Tungsten using DFT and compared to various embedded atom method (EAM) potentials, as well as a modified-EAM (MEAM) potential. It was found that the EAM potentials were unable to qualitatively match the results from DFT. The MEAM potential reproduced the DFT results in only one of the crack systems studied, whereas significant deviations were present in the other crack system (see Figure 7).

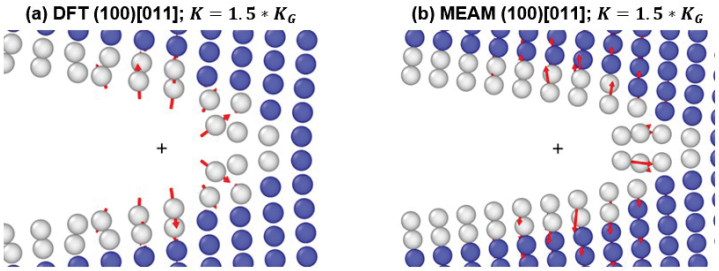

Figure 7: Displacement of atoms during relaxation in the crack system with (100) crack plane and crack front along the [011] direction. The red arrows show displacements due to relaxation with 2x magnification. In the case of DFT (a), the bond at the crack tip atoms undergoes cleavage at 1.5 time the theoretical Griffith load (K_G). However, with the MEAM potential (b) at an equivalent load, the crack tip atoms move inwards without cleavage.

In atomistic simulations, deviations from the continuum theory of linear elastic fracture mechanics (LEFM) due to the nonlinear response of materials are widely acknowledged [2]. However, deviations due to geometrical nonlinearities and time-history dependence have not received much attention. To showcase the influence of geometrical nonlinearities arising from the discrete (i.e., atomic) nature of matter, simulations with nearest neighbour harmonic potentials (analogous to a networks of springs) with varying cut-offs were performed. Cracks were inserted into the atomic lattice using the linear elastic anisotropic displacement field. In addition, the role of history dependence on the deviations were also explored by performing quasistatic calculations. It was found that the geometrical nonlinearities manifested as displacement of atoms away from the LEFM-prescribed positions during relaxation (see Figure 8(a)). These displacements led to deviations in the separation distances of crack tip atoms, which further resulted in significant deviations in fracture toughness in the quasistatic loading scenario.

The harmonic potentials were also used to study the influence of blunting radius (ρ) of a pre-existing crack on fracture reinitiation toughness (K_{IC}). The Creager-Paris equations based on linear elasticity [3] were used with the mean stress criterion to develop a scaling relation of fracture toughness as a function of blunting radius. An earlier work [4] had shown that this approach could predict the fracture reinitiation toughness in cases of macroscopic notches. However, in this work, a factor that accounts for stress amplification at surface steps as well as the aforementioned geometrical nonlinearities had to be introduced (see Figure 8(b)). Furthermore, a lower limit for the maximum crack tip radius for this model was found (~950 nm), above which the original model by [4] can be used.

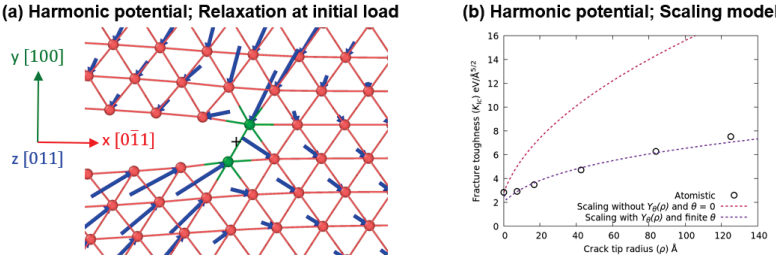

Figure 8: (a) Displacements during relaxation in the sharp crack configuration at K_{in}. The blue arrows indicate displacements due to relaxation magnified 50 times (b) The scaling model with the correction factor ($Y_\theta(\rho)$) (purple line) compared to the original model without the factor (red line).

Propagating cracks were simulated with the harmonic potentials using various crack systems to investigate dynamical instabilities. Some crack systems showed branching and kinking which are being further investigated to study the influence of the simulation setup on instabilities. Ramped viscous damping boundaries were used and calibrated to prevent the reflection of sound waves from the boundaries of the simulation box.

Conclusions, main achievements and outlook

The results using Tungsten show that the studied, widely used classical interatomic potentials are unable to qualitatively reproduce the results from DFT. It is hypothesized that the deviations are due to surface relaxation not being considered in the creation of such potentials, and possibly since covalent bonding present in bcc metals is not well described by the EAM formalism. It is planned to compare the DFT results with simulations using a more sophisticated analytical bond order potential (BOP) [5] and an atomic cluster expansion (ACE) potential [6].

The simulations with harmonic potentials show that deviations from LEFM due to the nonlinear response of materials are in addition to the deviations caused by geometrical nonlinearities and history-dependence. Additionally, the fracture toughness cannot be predicted using separation distances of crack tip atoms in the case of quasistatic loading. Moreover, in the case of blunted cracks, stress amplification at surface steps also contributes towards the deviations from LEFM.

In the case of propagating cracks, a crack system where the crack was found to propagate even at high velocities on the cleavage plane is being considered for use in more advanced simulations with e.g., precipitates, disorders etc. Furthermore, it is also planned to investigate the branching and kinking phenomena by comparing them to continuum simulations (collaboration with FRASCAL project P9).

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P2: Topology-Controlled Deformation Behaviour of Oxide Glasses

Achraf Atila and Erik Bitzek

Introduction and status

Oxide glasses are used in many applications, such as screens for mobile devices and optical fibres [1]. However, their application range is limited by their brittleness and low resistance to damage [2]. Hence, in recent years, gaining a mechanistic understanding of the deformation and fracture behaviour of oxide glasses has become the focus of many studies [3]. The strength of oxide glasses is strongly affected by flaws at the nano-scale [4]. The disordered structure of the glasses makes it, however, non-trivial to analyse how these flaws lead to macroscopic fracture and how flaws are formed and evolve under mechanical loads. To understand the deformation behaviour and fracture of oxide glasses, it is, therefore, crucial to comprehend the atomic-scale mechanisms by which defects are affecting glass strength; in particular, how plastic deformation (e.g., under compression or shear) leads to flaw and how the nucleation of flaws depends on the local chemical composition, as well as how they influence the mechanical behaviour of glasses?

We performed a series of molecular dynamics simulations of binary sodium silicate glasses with varying sodium content to address these questions using an empirical force field. First, pristine glasses were produced through the conventional melt-quenching technique. Then, we deformed them either by tension, compression, or shear and subsequently unloaded them to 0 MPa from different maximum strain values. We then calculated the local elastic bulk and shear moduli before and after deformation, following the procedure described in Ref. [5]. In Figure 9, we use the atomic density to show the spatial distribution after unloading of atoms with high remaining shear strain and high shear modulus and the atoms that have switched bonds. All samples are pre-deformed and unloaded from different strain levels depending on the deformation mode. The plasticity of the glass can be directly attributed to the bond switching events, as highlighted for the pre-compressed and pre-sheared samples.

On the contrary, few bond switching events are present during tension, indicating the brittle nature of the glass. Although the samples pre-deformed in compression and shear have a high percentage of switched bonds, they showed different mechanical behaviour when reloaded in tension. In the tensile reloading, more plasticity was observed in the samples pre-deformed in compression than in shear.

Conclusion and outlook

Our results highlight that bond switching events are responsible for the plastic deformation of glasses. Depending on the loading mode, the plastically deforming areas can self-organize, e.g. in a shear band shown in the bottom row. For compression and shear, the local deformation also correlates somewhat with an increase in local shear modulus. I.e., atoms with higher shear strain also have higher shear modulus and are the atoms that switched bonds (see Figure 9). The presented results highlight the importance of local analysis of the glass structure in order to get a clear understanding of its deformation behaviour. It is planned to compare the results obtained for silica glass with the results for sodium silicate glasses to understand the effect of sodium as a network modifier on the deformation behaviour of silicate glasses.

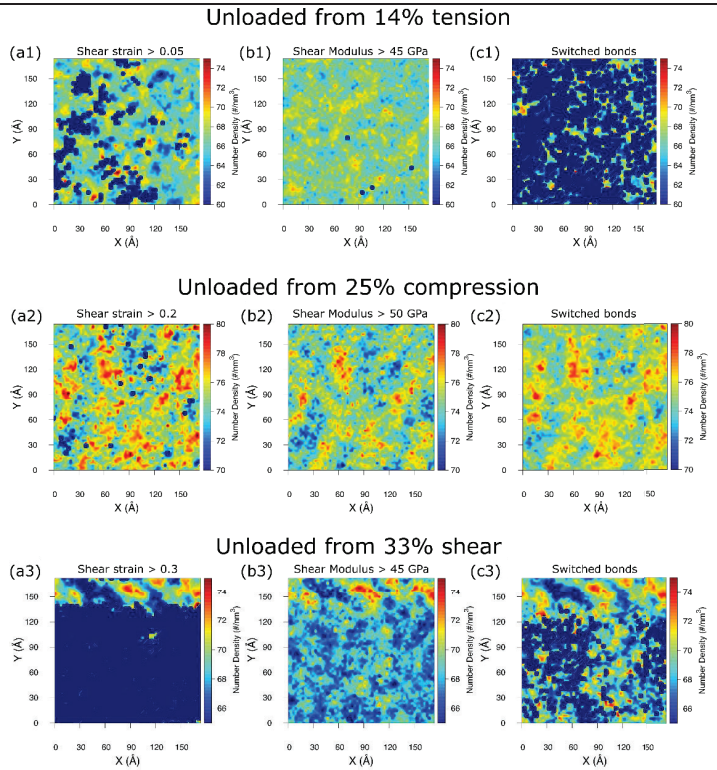

Figure 9: Spatial distributions of the number density of atoms in pre-deformed and unloaded glasses experiencing (a) large shear strain; (b) large shear modulus; and that have switched bonds (c) for different modes of deformation. The shear strain was calculated compared to the pristine glass. We used a threshold value for each deformation mode to select the atoms with a shear strain higher than 0.05 for tension along the x-axis, 0.2 for compression along the x-axis, and 0.3 for shear in the x-direction along the xy-plane. For the shear modulus, the selected atoms have a shear modulus higher than 45 GPa in tension and shear and 50 GPa in compression. All simulations were performed at T=300 K and strain rates of 10^8 1/s.

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P3: Fracture Mechanics of Epoxy Resin with Dissociative Force Field

Julian Konrad and Dirk Zahn

Bulk

We successfully developed a reactive Force Field for curing and deformation until fracture of epoxy resins. The parametrization was based on quantum mechanics calculations for the curing reaction, which we state as the most important reaction in this system in relation to bond forming and dissociation.

Bulk properties were compared to a reference system [Meißner, 2020] and experimental data. Cross-linking degrees of 98% were foremost achieved in an atomistic model, moreover the determination of density, glass transition temperature, $Q_{formation}$ and the elastic constants young's, shear und bulk modulus was in accordance with other studies.

After verification of those properties, we performed tensile deformation runs for different strain rates to explore the material behaviour under uniaxial stress.

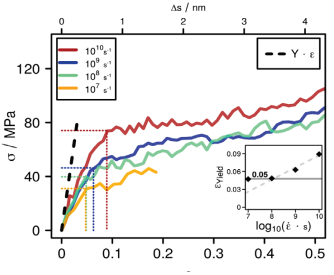

Figure 10: Close-up of the stress-strain diagram for different strain rates.

Our first goal determining the yield point is shown in a close-up of the stress-strain profiles (Figure 10) highlighting the transition from (non-linearly) elastic to plastic deformation. The yield point identification is based on the kinks in the curves as indicated by the dotted lines. The resulting ε_{yield} is also plotted as a function of the strain rate using a logarithmic scale and gets confirmed by experimental work [Littell, 2008].

Furthermore, we tackled the ultimate stress with uniaxial tensile deformation at different pulling rates (Figure 11: left to right: $\Delta\dot{s}$ = 84, 8.4 and 0.84 ms). The upper panel shows the stress profiles upon model elongation (red curve) and after additional relaxation whilst keeping Δs constant (grey), respectively. The elastic and plastic regimes in the stress-strain diagram are indicated by grey and blue bars, whilst void nucleation and fracture is indicated in red, respectively. During quasi-static relaxation, we monitor the absolute change in epoxy cross-linking (percentages denoted in blue) and the fraction of re-organized links (shown as flags). Along the constant strain relaxation runs we extrapolated the stresses to $t \rightarrow \infty$ which corresponds to a vanishing strain rate according to: $\sigma_t = \sigma_{visco} \cdot \exp\left(-\frac{t}{\tau_{visco}}\right) + \sigma_{t\rightarrow\infty}$

The resulting $\sigma_{ultimate}$ of about 84 MPa is in reasonably good agreement to the experiment (70 MPa) [Little, 2008] in comparison to other models which miss this quantity by a factor of 10 [Barr, 2016].

The lower panel illustrates the mechanical work (red curve) and the potential energy of the epoxy model (black) during tensile testing. Moreover, for a series of snapshots we reversed the pulling using the same rate as during the tensile tests. This leads to (partial) restoring of the cross-linking (numbers next to blue arrows) and the potential energy. The profile (grey) of the resulting minimum energy configurations indicates the damage energy stemming from plastic deformation and void formation. The zero point of the potential energy profiles is chosen as that of the pristine simulation model prior to tensile testing.

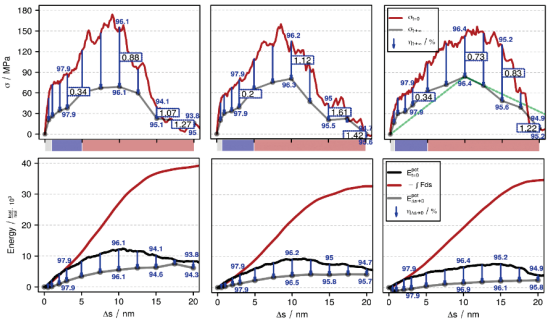

Figure 11: Stress-elongation diagram (upper panel) and energy-elongation diagram (lower panel) of tensile deformation until fracture including investigations on reorganization processes, vanishing strain rates and damage.

By bilinear approximation (green lines Figure 11) we can access the quantities work of separation = 1.1 J/m^2, Δs_{crit} = 10 nm with $\sigma_{ultimate}$ = 84 MPa and $\Delta s_{final\ separation}$ = 25.7 nm as input for continuum models like cohesive zone models.

Forms & Interfaces

Investigating interfaces of cured epoxy resins demands curing in present of the desired interface, unlike for metals which can be simply cut out from bulk. Interactions of the resin with the interface as well as geometrical boundaries of the interface lead to structuring even before curing, but especially during the curing process. Therefore, we applied the boundaries to the unreacted thermoset as follows: we induced i) cylindrical geometry (8, 9 and 10 nm diameter) (Figure 12), placed ii) spherical particles in the form of hard spheres (3, 4 and 5 nm diameter), inserted a iii) a silica nano-particle (5 nm) and set up a iv) flat interfaces (vacuum, silica, magnetite, aramid and cellulose). Before accessing mechanical properties, we studied the network on atomic level after curing considering the coordination number of DETDA molecules (Figure 13 right) and the spatial orientation of epon molecules with respect to the distance to the interface (Figure 13 left).

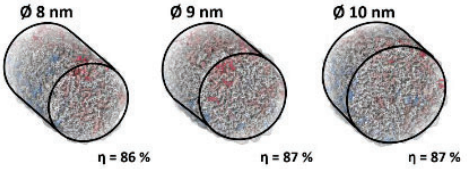

Figure 12: Rod-like systems for different diameter and crosslinking degree η, respectively and cross-linking convergence depicted in red (epon) and blue (DETDA) demonstrating the influence of the geometry of the interface to the crosslinking.

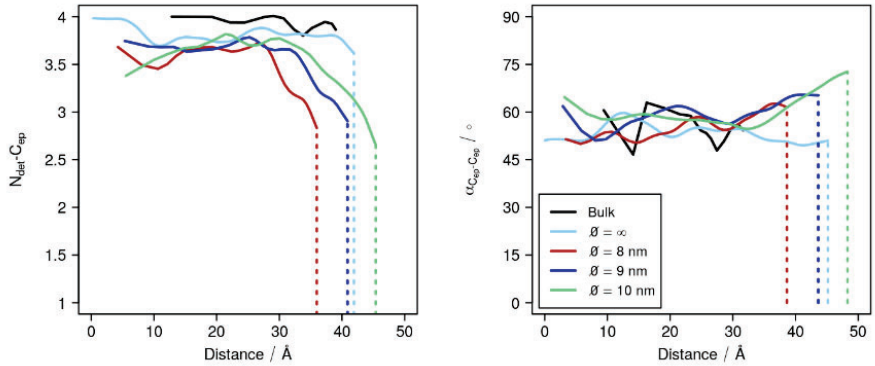

Figure 13: Geometrical and chemical structuring of rod-like epoxy systems showing influence of the interface.

P4: Multiscale Fractures in Large Scale DEM Simulations

Ali Mauricio Velasco Sabogal and Thorsten Pöschel

The present project aims at the construction of a realistic and fast method to simulate the fracture grains on granular material simulations. The grain and fragment shape can be irregular and the interparticle contacts are computed via the multi-sphere representation method. This method has been implemented on MercuryDPM [1], an open-source software for the simulation of granular materials.

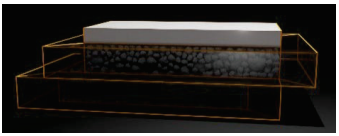

Figure 14: Shear test: the yellow upper cavity has been displaced respect to the lower one.

With this new tool in hand, some benchmark simulations have been performed. The first interesting system is the so-called shear test: a set of two cavities in contact that is filled by a granular material. A heavy lid is placed on top of the material and then the upper cavity is displaced in one axis. This movement generate a shear stress on the granular material at the height of the boundary between the two cavities (Figure 14).

Three different shapes have been considered fill the cavity for the shear test (Figure 15) the results shown that, angular particles impose a higher resistance to the shear cavity displacement in early stages of the tests. (Figure 16), later, the presence of voids in materials with more angular particles decreases the measured tangential force.

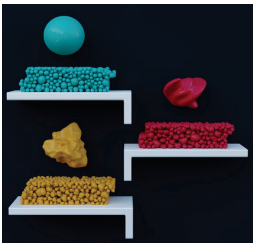

Figure 15: Direct shear test on granular materials with different grain shapes.

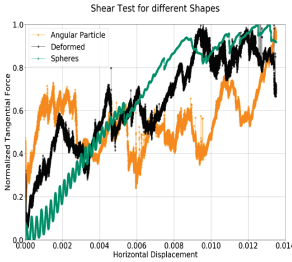

Figure 16: Normalized Tangential Force as a function of the horizontal displacement on shear test simulations for three different particles.

The last part of the project has been focused on how to model the fractures of material grains. To this aim, we define a grain fracture criterion as follows: when the stress on a particle overcomes a certain threshold ϵ, the particle will break. To break a particle, we compute a degradation plane that is oriented in the direction of maximum shear stress, as proposed by P. Iliev *et. al*. [3]. The shape of the particle is then subdivided by this plane and a new multi-sphere representation is computed for each fragment. The computation of the stress on each particle is, nevertheless, computed from the mean stress tensor by considering each contact force.

One accurate and simple way to define the fracture threshold ϵ is suggested by J. Yiang *et. al*. [2], in this work, J. Yiang *et. al*. start by finding a scalar quantity related with the stress state of the particle that can also give account for the grain fracture. Let us start by considering the strain energy W_e defined by:

$$W_e = \frac{1}{2}\boldsymbol{\sigma} : \boldsymbol{e} \quad W_e := \frac{1}{2E}\left[\frac{2}{3}(1+\nu)\,\sigma_\nu^2 + 3\,(1-2\nu)\,\sigma_h^2\right] = \frac{\psi^2}{2E}$$

Where σ is the stress tensor, e is the strain tensor, E and ν are the Young Modulus and Poisson ratio respectively and, σ_h and σ_ν are the hydrostatic and von Misses stresses. The quantity ψ is called Strain Energy field (SEF), and it is given by:

$$\psi^2(\boldsymbol{\sigma},\nu) = \sigma_\nu\left[\frac{2}{3}(1+\nu) + 3(1-2\nu)\left(\frac{\sigma_h}{\sigma_\nu}\right)^2\right]^{1/2}$$

The research work done by of J. Yiang *et. al*, show that SEF is an appropriate quantity to be used as a fracture threshold criterion.

The computation of the SEF and the simulation of the grain fractures have been included

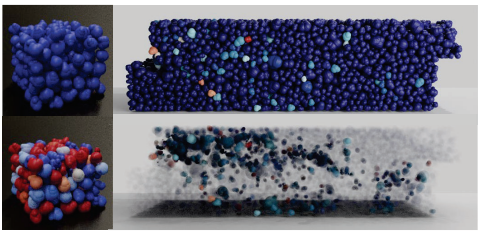

Figure 17: Left: Uniaxial compression on a granular material. Uncompressed material (top) compressed material (bottom). Right: Shear test with strain energy computation and fractures.

in our model in MercuryDPM and some results for uniaxial compression and shear tests are shown in Figure 17. The colour of the particles represents the intensity of the SEF. Note that our model allows us to identify the breakage of grains during a shear test and to visualize its effect on the macroscopic behaviour of the granular sample. Further implementations in different systems and the collection of statistics through parametric analysis is the following and final step for this project. This is left for a subsequent report.

Finally, as an additional related project, we describe here the work done in collaboration with Prof. José Daniel Muñoz from the national university of Colombia. The idea proposed by Prof. Muñoz is to extend our already developed tool for the simulation of breakable irregular discrete elements and study the fracture in solid brittle materials, instead of granular materials.

To this aim, a block of a continuous solid material is discretized into Votonoï cells, each cell is, in turn, represented as a multi-sphere discrete material element (Figure 18). The multi-sphere representation is useful to compute the contact between the faces of the Voronoï cells. However, to ensure a stable solid brick, the contact model between the multi-sphere elements should be modified with respect to the one used for granular materials. In this case, the multi-sphere elements should be linked by an elastic force such that a solid material can be resembled.

Figure 18: Solid block material discretized as a set of multi-sphere cells.

This problem has been successfully solved by defining a beam-like force between two overlapping spheres, i. e. an elastic cylindrical beam is defined to be between the centres of the spheres, the radius of the beam is equal to the overlapping radius (Figure 19). The force and bending moment at each end of the beam Q as a function of the linear and rotational displacements at each end U can be found through the stiffness matrix k and the linear relation $Q = kU$. [4]

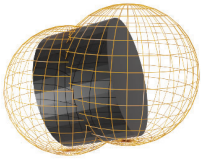

Figure 19: Modelled beam interaction between two spheres.

A common simulation procedure is the following: Once the initial array is defined and the interactions are modelled as beams an external load can be applied to the solid brick. The effect of any load will generate stress states on the elements. This stress states can be, again, quantified by computing the SEF on each cell. The computations of SEF on the discrete elements of the block will indicate the regions with a higher stress, and therefore the regions through which an eventual fracture will occur. The next step is, therefore, to subdivide (refine) the element whose SEF overcomes a certain threshold ε, but without breaking it, instead, we repeat the refinement process until a representation of the fracture path is accurately described by the refined elements. With this model, we are able to use MercuryDPM to track with a high accuracy the fracture surfaces inside solid brittle materials at a low computational cost. The model is still in construction and test phases, Figure 20 show some preliminary results.

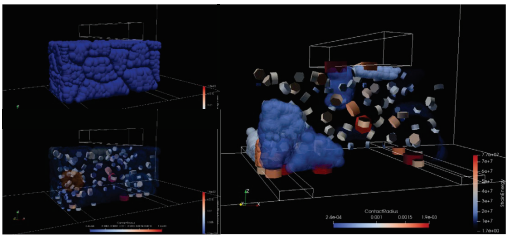

Figure 20: Preliminary simulations of fracture in solid materials by multi-sphere DEM model with a beam-like interaction force.

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P4: Experiment to Study the Stress Regime within a Layer of Granular Material During a Quasi-Static Penetration Process at Different Gravity Levels

Valentina Marzulli and Thorsten Pöschel

Designing in situ resource utilisation applications for space exploration requires accurate description of the mechanical behaviour of the soil. Therefore, it is of great importance to understand the effect of the in-situ conditions on the mechanical response of the soil. Over the past decades, several regolith simulants have been manufactured and tested to study the mechanical response of Lunar or Martian soils and, thus, to support the development of upcoming lander missions. For instance, quasi-static and dynamic penetration tests have been performed to study the interaction between the InSight HP3 Mole with a Martian regolith simulant (Marshall et al. 2017). Unfortunately, during the NASA InSight mission the Mole was not able to hammer itself into the Martian surface for more than about 30 centimetres, while it was expected to penetrate at least for 3 meters. Despite the challenging efforts made by the mission team to fix the problem scraping soil on top of the Mole to provide added friction, the experiment did not succeed. This event teaches us that the human and robotic exploration of planetary surfaces still requires a great effort by the scientific community to gain more knowledge on the mechanical response of extra-terrestrial soils with respect to penetration processes. New missions are supposed to develop new technologies on the Moon and Mars in order to extract resources beneath the surface of these celestial bodies. As previously published, we have already deeply characterized the multiscale mechanical properties of the Lunar regolith simulant DNA-1A (Marzulli and Cafaro 2019; Sandeep et al. 2019; Marzulli et al. 2020). In the past year we have also designed a novel setup (Figure 21) to measure the stress regime within a column of Lunar regolith during a penetration process under hyper-gravity conditions. We tested different granular materials in this experiment, such as the above-mentioned Lunar simulant DNA-1A as well as the Lunar simulant EAC-1, Ottawa sand and glass beads, both used as benchmark materials due to the high consistency of their surface morphological features. To perform this experiment, we successfully submitted a proposal for using the Large Diameter Centrifuge (LDC) of the ESA-CORA-GBF. The main objectives that led us to design and perform this experiment are mainly to understand the physics behind a penetration process in granular materials under different gravity conditions and to develop a reliable mechanical model capable of numerically simulating a wide range of processes that will take place on the Moon (e.g. hammering, drilling and excavation on the Lunar surface, in-situ tests, modelling of wheel-soil interaction for rovers operating on the Lunar surface, and so on). Unfortunately, we could not directly carry out this experiment under Moon gravity conditions. In fact, a parabolic flight would allow to maintain Moon gravity conditions for just few seconds, while this experiment needs few minutes. Moreover, in parabolic flights the g-value is not stable enough due to drifts. Therefore, to overcome this problem we decided to perform such experiment under hyper-gravity conditions (up to 20g) and to extrapolate the results to the low gravity conditions. This experimental investigation is still in progress but we have already achieved very promising results testing our apparatus under earth-gravity conditions (Marzulli et al., in preparation). Once the hyper-gravity tests will be done, we will use the experimental results to calibrate the numerical mechanical model of the Lunar soil by extrapolation.

The main objectives of my project can be divided in two different parts: a) understanding the physics behind a quasi-static penetration process in granular materials under different gravitational conditions and b) develop a reliable mechanical model capable of simulating a wide range of processes that will take place on the Moon (e.g. building of lunar structures, in-situ tests, modelling of wheel-soil interaction for rovers operating on the lunar surface, and so on). Unfortunately, it is not possible to directly carry out this experiment under Moon gravity conditions. In fact, in a parabolic flight it is possible to maintain Moon gravity conditions for just few seconds, while this experiment takes place in few minutes. Therefore, to overcome this problem we decided to perform such experiment under hyper-gravity conditions (up to 20g) and to extrapolate the results to the low gravity conditions. For this purpose, we first needed to design and build the experimental setup. In the last year, I have been involved in the design of this innovative setup (Figure 21) and on the modelling via DEM simulations of the penetration process. In parallel, I have also carried out preliminary tests to calibrate each component (i.e. piezoresistive sensors, electric piston, force sensor). The setup has been designed considering all the restrictions and requirements provided by the LDC user's guidelines.

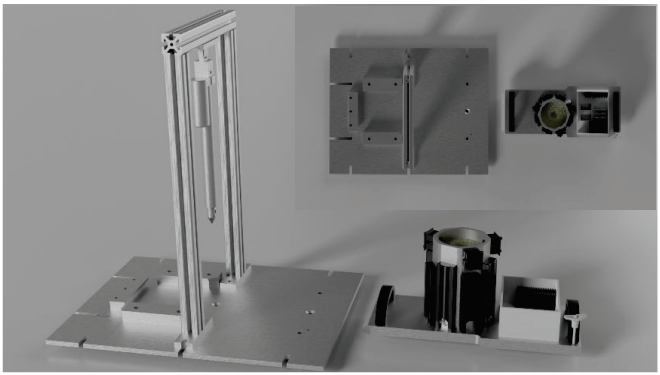

Figure 21: 3D model of the improved experimental setup.

The setup can be divided into two different parts: the aluminium frame supporting the electric piston and laser system and the detachable aluminium cylinder. The aluminium frame is directly attached to the aluminium plate, in turn fastened to the gondola through underlying layers of rubber and wood needed for reducing vibration. The aluminium cylinder is instead placed on a detachable plate. The cylinder is equipped with 45 piezoresistive sensors placed along the lateral wall and at the base and capable to measure the pressure exerted by the granulate in interaction with the walls during the penetration process. Three polycarbonate windows are located at the top of the cylinder to monitor via cameras possible variations of the granular surface. With this purpose, a laser diode with line projection head to monitor the heap profile in a cross section of the granular surface is also provided. LEDs will be placed at the top of the cylinder to ensure good illumination.

In the first months of the current year, the setup has been built at the Laboratory of the Institute for Multiscale Simulation (Figure 22).

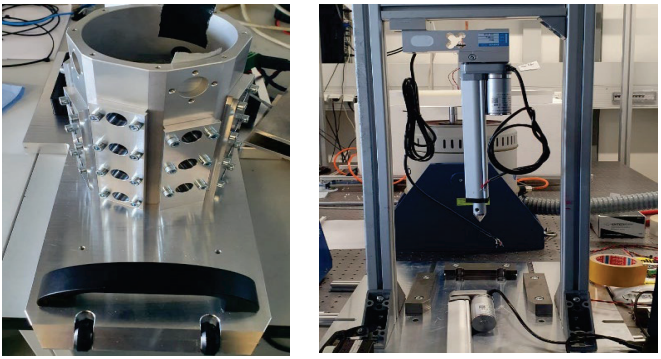

Figure 22: Aluminium cylinder and aluminium frame.

P5: High Strain Rate Compression of Porous Brittle Snow Structures

Jonas Ritter and Michael Zaiser

We investigated the fracture of porous snow structures subjected to uniaxial compression by simulations and experiments. For simulations we use the non-local peridynamic theory that allows to treat the discontinuous displacement field of fracture in a unified manner [1,2,3]. Porous snow structure geometries are obtained from micro computed tomography images [4]. The segmented voxel data are trimmed in a cuboid specimen shape. External load is applied through flat plates on top and below the specimen by controlling their external enforced time-varying displacement. As material model for the structures matrix we utilize a Linear Peridynamic Solid (LPS) which behaves similar to an isotropic linear elastic material in classical continuum mechanics. Progressive damage is captured by a critical stretch model which is related to the fracture properties of the simulated matrix material. Two different dimensions of the porous structure are simulated. One that represents the real size of the cubical specimen of 2 mm edge length and the other with a length of 60 mm. Both specimen sizes are in the simulation subjected to the same strain rates of 5 s^{-1}, 10 s^{-1} and 20 s^{-1} with respect to the cubic dimensions. In addition, the larger dimension is 3d printed by selective laser sintering of PA12 polymer by our cooperation partners of FRASCAL's project 4. Those specimens are tested experimentally under quasi-static compression where primarily the axis of load is varied to analyse the structural anisotropy. A direct comparison to the simulation results is therefore not feasible. In the simulations, the smaller dimensioned specimen is simulated with the material properties of ice with a bulk modulus $K = 8.9\ GPa$, a shear modulus G=3.5 GPa and a plain strain fracture toughness of $K_{Ic} = 120\ kPa\sqrt{m}$ whereas the larger one with the properties of PA12 with a Young's modulus $E = 1.6\ GPa$, a Poisson's ratio $\upsilon = 0.4$ and a critical energy release rate of $G_c = 6.5\ kJ/m^2$. For the smaller specimen with the material properties of ice the simulations show a minor influence of the strain rate on the results. With increasing external strain rate the peak load is slightly higher and the failing process slightly delayed (Figure 23).

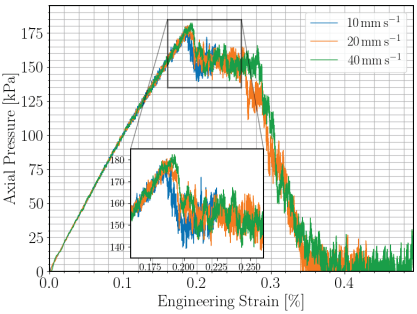

Figure 23: Influence of the strain rate on the compression for the small specimen and the ice matrix material. The blue line corresponds to the slowest rate of 5 s⁻¹ and the orange and green one to 10 s⁻¹ and 20 s⁻¹, respectively.

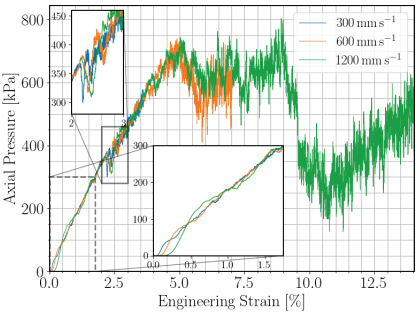

Figure 24: Strain rate dependence for the large specimen with an edge length of 60 mm. Blue shows the slowest rate and green the fastest applied displacement rate. The lower inset shows the inertia effects at the simulation beginning in more detail.

For the larger specimen with the material properties of PA12 the influence of the strain rate is more significant, as can be seen from Figure 24. For small strains an inertia influence is dominant that results in a delayed reaction of the specimen on the external applied constant displacement rate. However, for the failure process a similar effect as for the smaller specimen can be observed, namely a more and more delayed failure with increasing applied strain rate. Simulations for different loading directions exhibit a transversal isotropy for the simulated porous snow structure. The axis of snow deposition is weaker compared to the axes located in the snowpack plane. Those two show a nearly similar mechanical response, see Figure 25. The simulations of the larger specimen exhibit the same trend as well as the experiments under quasi-static load conditions. At 0.4 % strain, the failure is localized in the small specimen simulated with the properties of ice, as shown in Figure 26. This localization of the fracture events separates the structure into two parts. Such a clear localization is not be found for the same structure but with a larger dimension and the material properties of PA12.

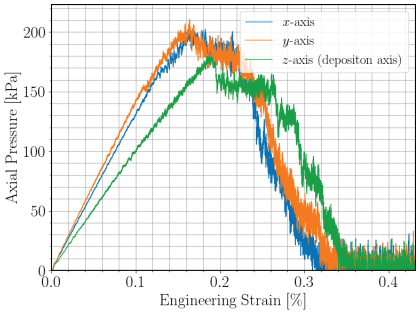

Figure 25: Stress-strain relation for the different spatial axis of the small specimen. The green line shows the result for the significant weaker deposition axis, whereas the results shown by the orange and blue line are almost identical.

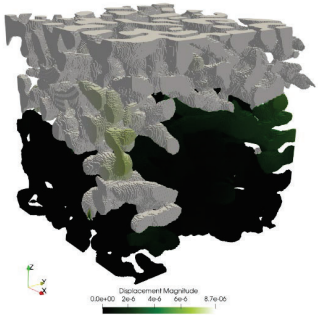

Figure 26: Localized deformation of the small specimen with an edge length of 2 mm which indicates the separation of the specimen into an upper and lower part.

Overall successful dynamic simulations for different displacement rates were done for two different dimensions of the same snow microstructure. For the smaller one the properties of ice have been used whereas for the larger specimen properties of sintered PA12 powder. The simulations capture the transversal anisotropic behaviour of the microstructure which was also confirmed by quasi-static experiments on the 3d printed structure. The simulations of the smaller dimensioned specimen exhibit a localization of the failure within the structure which ends up in a total separation of the specimen into two parts. In future, further simulations are carried out to get a better understanding of the structural failure process. To this end, simulation parameters are varied such as specimen size and dimensions, material properties and model, and the structure itself. Finally, structural properties should be linked to the simulated mechanical response to understand how the structure influences the compressive failure of porous brittle solids such as snow.

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P5: Exploiting Artificial Intelligence for Predicting Subcritical Failure of Microstructurally Disordered Materials

Stefan Hiemer and Michael Zaiser

Objectives and status

In this project we study subcritical failure in disordered systems by identifying the governing variables/patterns by machine learning. Our simulations methods are molecular dynamics of glasses, random fuse networks and a finite element creep model. Fuse networks and finite elements serve as proxies for the mesoscale and comparison to experiments. Atomistic models are used to identify precursors and beginning of plasticity as their time limitation renders creep simulations impossible.

For the prediction of the time to failure in the finite element creep model in pure shear we can build on already published work on which we have improved increasing stability of the prediction as well as the absolute accuracy. Investigations with random forests reveal that for samples with low disorder the cumulative damage within the entire damage is most important for the machine learning model to make a successful prediction. Damage localized within a small horizontal/vertical window also shows some minor importance while e. g. time is not relevant. For high disorder the cumulative damage, the damage localized within said window as well as the time have similar relevance. The importance of the localized within a small window can be explained with shear bands which form for pure shear loading in horizontal/vertical direction. This should be taken with a grain of salt as the predictions in the low disorder case are inaccurate, but still better than using simple intuitive baselines. As random forests make a deterministic prediction for the time to failure and the finite element model is governed by a stochastic process, we constructed an analytical model to derive the proper distribution for the prediction with the stress state of the individual elements as internal variables. The goal of this approach is to construct a Bayesian model with the right functional form for the posterior distribution. To verify the analytical model and to investigate the generality of our previous findings, we have created a new creep random fuse network model as well as a creep fibre bundle model.

In the atomistic part of this project, we resorted to create a 2D silica glass (Figure 27) dataset in uniaxial tension to test new machine learning approaches without having to worry about the computational scaling problems encountered in the 3D case. We manage to predict the location of the first bond rupture via a simple image recognition approach as well as a local approach. In the local approach the neighbourhood of an atom is encoded via a set of rotation and translation invariant symmetry functions and the prediction is made for each atom whether it is involved in the plastic event. As in mechanics the orientation of the atomic configuration with respect to the load is vital, we include this by affine transforming the system according to the loading. Both approaches yield good results despite being completely different in nature. The first has no information about the important symmetry of the problem but has information of the entire system. The image recognition approach manages to predict the rupture strain reasonably and locates the bond breakage within a standard deviation calculated across geometrically (but result-invariant) transformations of the sample. The local approach successfully identifies a subset which contains ~ 97 % of the particles involved in a plastic event while labelling ~ 96 % correctly as non-bond breaking (Figure 28).

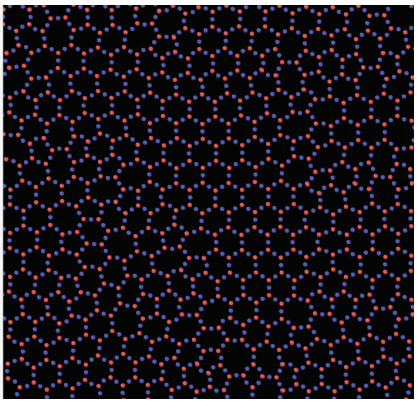

Figure 27: Snapshot of two-dimensional silica glass. Our molecular dynamics model manages to capture the double layer structure where the atoms are aligned perfectly on top of each other. This enables our image recognition approach since a snapshot does not miss any information due to the alignment. Silicon atoms are displayed red while oxygen is marked blue.

Conclusions, achievements, and outlook

To investigate the generality of our previous findings for the prediction of the sample lifetime in the finite element creep model, we are going to investigate a novel fuse network creep model. To verify

an analytical model of the lifetime distribution with the element stresses as internal variables, we are going use an equal load sharing fibre bundle model where the stress is straight forward. For the prediction of plasticity on the atomistic level we aim to combine the merits of our image recognition approach with the local approach to combine global information of the entire atomistic system while still preserving all relevant symmetries.

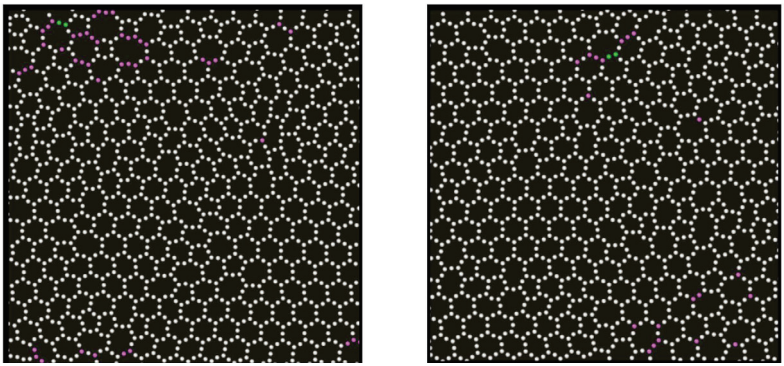

Figure 28: Predictions of the local approach. Green atoms are correctly predicted as involved in a plastic event while violet ones are falsely labelled to undergo plastic deformation. Grey indicates no bond breaking correctly predicted by the estimator.

P5 Modelling Failure and Flaw Tolerance of Hierarchically Structured Materials

Seyyed Ahmad Hosseini and Michael Zaiser

Objectives and status

We developed a Beam Lattice Model (BLM) in 2D and 3D to be used for investigating the mechanical properties, fracture, and flaw tolerance of hierarchically structured materials and randomized variants thereof (see Figure 29).

BLM explicitly preserves fundamental features of continuum mechanics, allowing it to reproduce macroscopic elastic properties of any type of material. We then used our model to analyse the process of damage accumulation (characterized by the locations and timings of beam breakage avalanches prior to global failure) and of global failure.

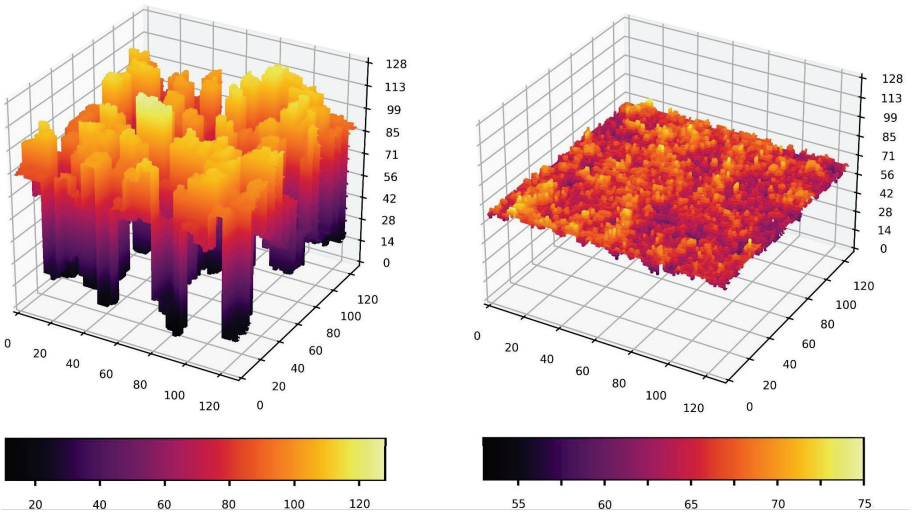

Figure 29: Typical fracture surface of 3D lattice variants; left: hierarchical, right: random.

Conclusions, main achievements, and outlook

We demonstrated that irrespective of the degree of material disorder, hierarchical materials never fail by crack nucleation and propagation. Instead, the load redistribution becomes more 'diffuse' among broken and many intact beam elements in the neighbourhood of an emergent cluster, thus causing large jumps in growth of clusters that grow in a 'stop-and-go' manner to the point that the material is not 'crack-sensitive' and brittle and the unloading as damage progresses is more gradual.

As a result, the material has much higher toughness than under eventual crack instability and catastrophic brittle crack growth. The hierarchical modular organization thus proves efficient in containing damage which hardly ever propagates across modular boundaries: crack-tip stress concentrations, which ultimately lead to failure by supercritical crack propagation, are thus efficiently mitigated.

P6: Preliminaries for Adaptively Switching Between FE and MD Resolution

Christof Bauer and Sebastian Pfaller

Embedded in our long-term research focusing on multiscale fracture simulations of polymers, the present project aims at introducing adaptivity to the partitioned-domain multiscale Capriccio method [1]. Specifically, for a crack propagating trough the material, only the vicinity of the crack tip is resolved at fine scale particle resolution, whereas the remaining region is treated by a coarser continuum scale. An essential prerequisite to follow the moving crack tip is to adaptively switch between FE and MD descriptions depending on the local load level in arbitrary sub-domains. This, in turn, implies that the change of description is necessary at a certain deformation state and thus requires an appropriately pre-deformed MD domain.

On the one hand, we generate a specific deformation state of the molecular system without time-consuming recalculations using a hybrid molecular dynamics-continuum mechanical (MD-CM) method [2], cf. Figure 30a. Our specific focus is on the appropriate choice of boundary conditions used for the MD system: In case of non-affine deformations, classical periodic boundary conditions (PBC) cannot be used to pre-deform the MD region. Instead, non-periodic boundary conditions, as for instance the stochastic boundary conditions (SBC) employed in the Capriccio method, have to be chosen. On the other hand, concerning switching back from fine scale particle resolution to coarser continuum description, we apply deformations from MD to FE by using local space averaging of microscopic quantities. In particular, we use the Murdoch-Hardy [3] procedure to derive displacement fields from MD deformation simulations, cf. Figure 30b. We consider polystyrene at coarse-grained (CG) resolution and use the Capriccio method to study the system behaviour of the coupled MD-FE system under uniaxial loading.

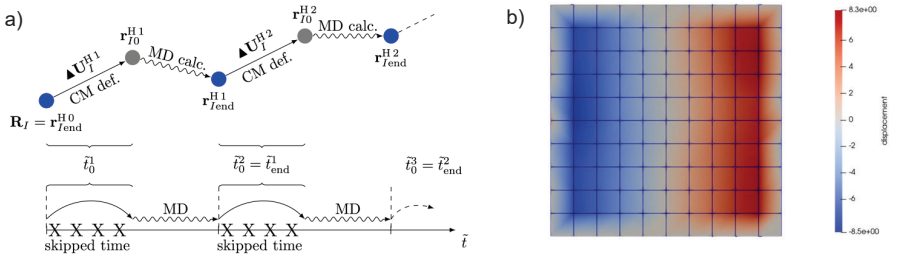

Figure 30: a) The hybrid MD-CM method: Load application (prescribed displacement ▲ $U_I^{H\,I\,s}$ according to affine deformation) and intermediate MD equilibration. based on [2] b) Displacement field of a sample MD system under uniaxial tension calculated using the Murdoch-Hardy procedure.

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P6: Extended Boundary Conditions for MD-FE Coupling of Amorphous Polymers

Maximilian Ries[1], Yash Jain[2], Paul Steinmann[1] and Sebastian Pfaller[1]

[1] Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg

[2] Department of Chemistry, Technische Universität Darmstadt

Polymer nanocomposites exhibit enhanced mechanical, thermal, and optical properties compared to the neat polymer, which are mainly attributed to the interactions between the filler and the polymer matrix. A multi-scale modelling approach has to account for this modification of the macroscopic properties due to microscopic interactions. For this purpose, the Capriccio method [1] has been explicitly developed for amorphous polymer composites and embeds a molecular dynamics domain (small scale) into a larger finite element region (coarse scale).

The finite molecular dynamics domain requires switching from the periodic boundary conditions commonly used in molecular dynamics (MD) to nonperiodic stochastic boundary conditions [2]. The necessary trimming of the polymer chains causes missing nonbonded interaction partners, which leads to a free surface from the MD particles' point of view and thus to undesirable surface effects. To compensate for this, we re-establish the missing interactions by introducing so-called fur atoms. These particles follow the continuum deformation and thus act as an external potential for the inner MD particles, which mimics the continuation of the material.

The necessary amount of fur atoms can be derived by matching the periodic reference density under zero-load conditions. With this system at hand, we can reproduce the stress-strain curve of a pure MD reference system for uniaxial tension. Furthermore, we are able to apply non-affine deformation, such as bending, which is not possible by conventional MD. Figure 31 shows that both the applied deformation and the measured stress distribution in the inner MD region match the expectations [3].

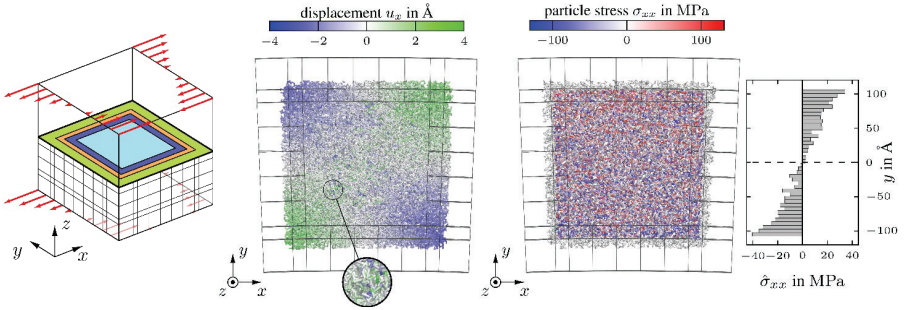

Figure 31: Pure bending: Deformation setup (left), particle displacement (mid left), particle stress (mid right), and mean stress averaged over x- and z-direction (right) at maximum load.

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P6: Extension of the Inelastic Capriccio Method for Fracture Simulations of Amorphous Polymers

Wuyang Zhao, Paul Steinmann and Sebastian Pfaller

The Capriccio method in [1] has been designed for coupled MD-FE simulations of amorphous polymers and recently extended to inelasticity [2]. We further develop it for fracture simulations of polymers [3].

As shown in Figure 32(a), a cubic MD domain is embedded into a cubic FE domain. To implement Mode-I deformation in x-direction, a pre-crack is generated by deleting the corresponding atoms in the MD domain and elements in the FE domain. In addition, non-periodic boundary conditions are employed in x- and y-direction, while periodic boundary conditions are used in z-direction in the MD domain. The coupled system is loaded by deforming the outer surfaces of the FE domain normal to the x-direction with a constant elongation rate of 1 %/ns. The deformed system at the elongation of 20 % is shown in Figure 1(b), which demonstrates the capability of the extended Capriccio method for fracture simulations of amorphous polymers.

Nevertheless, there are still several aspects to be improved. Firstly, the crack propagation is not observed yet at the elongation ratio of 20 % depicted in Figure 32(b), but is expected at larger deformations. In addition, bond breakage is not considered yet in our simulations. These issues are to be considered the subsequent works.

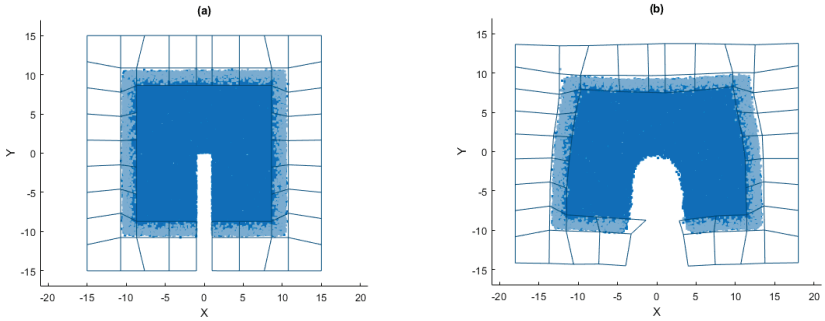

Figure 32: Cross-section of coupled MD-FE system for polystyrene with pre-crack: (a) initial configuration; (b) deformed state under Mode-I deformation at an elongation ratio of 20 % with constant elongation rate.

References

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P7: Crack morphology and Adhesion Properties of Hierarchical Materials

Nosaibeh Esfandiary and Paolo Moretti

Our research in the third year of the Project funding period has focused on the extension of our modelling approach to the case of a more realistic failure criterion within our model for hierarchical structure detachment, and to the analysis of the resulting fracture surfaces, by means of statistical analysis and graph theory.

In our previous work, we considered a simplified failure criterion for our detachment geometry, allowing for failure only at the interface. While this approach produces compelling results in the prediction of hierarchical material detachment, it also constrains fracture patterns to two-dimensional flat surfaces, as it works under the assumption that fracture away from the interface is negligible.

For the current research period, we thus introduced the parameter t, which indicates the ratio between the average load threshold away from the interface (i.e. in the bulk) and the average load threshold at the interface. While the case $t \gg 1$ corresponds to our assumptions in the previous phase of our project, here we have focused on choices of $t \approx 1$, where cohesive and adhesive forces gradually become comparable. While t controls the averages of threshold distributions, the distributions themselves follow the familiar Weibull functional forms with shape parameter β, in analogy with our previous work.

Under the new assumptions, our simulations now produce three-dimensional fracture patterns, which we can analyse by quantifying the prevalence of failure events near the interface. The motivation behind this choice resides in the observation of "ideal" fracture behaviour in problems of hierarchical biomaterial adhesion, such as for the paradigmatic example of the gecko pad [1,2]. In cases like that of the gecko, ideal behaviour refers to the ability of localizing fracture at the interface, resulting in an ideal reusable adhesive material. While the actual mechanics of gecko pad adhesion include a number of phenomena and active response mechanisms [3], which our model evidently does not include, here we focus on the role of the hierarchical organization in shaping the detachment profiles. As we did previously in this project, we compare our results to reference non-hierarchical systems.

Figure 33 shows typical results from our simulations, where the fraction of broken links/elements is plotted as a function of the distance from the interface. It appears that the damage centres in hierarchical systems are mostly localized at the interface and not strongly dependent on the value of t. This behaviour is significantly different from what we observe in reference systems, where approaching $t = 1$, we observe, as expected, uniform detachment profiles. In order to investigate the origin of the localization phenomenon in hierarchical systems, we investigate the Laplacian spectrum of the network structure after failure, in search for signals of spectral localization.

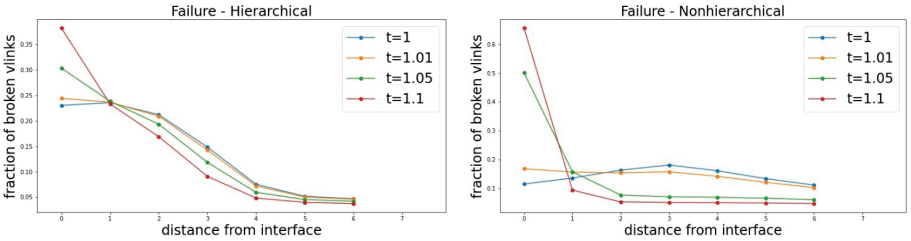

Figure 33: Damage profiles in hierarchical and non-hierarchical models of adhesion. We quantify damage by looking at the fraction of removed links in the vertical (or load carrying direction). Distance from the interface is measured in units of interplane spacing.

Simulation data are for systems of linear size L = 64. Heterogeneity in element response is given by threshold distributions with shape parameter β = 4. Data are collected at failure.

Figure 34 shows the eigenvalue density (or density of states) in the lower spectral edge of the graph Laplacian matrices. Excess low eigenvalues point to excess soft vibrational modes, slow relaxation and spatial localization. We observe that such excess modes are indeed prevalent in the hierarchical case. In spite of the simplicity of our approach, which forgoes several mechanical and chemical aspects of biomaterial adhesion, our results show that the hierarchical structure alone is responsible for robust fracture patterns, which prevalently occur at the interface.

For the reminder of the funding period, we will focus on the thesis writing activities and the preparation of two publications containing our more recent results. At the same time, we will continue with our graph-theoretical analysis approach to the study of three-dimensional fracture patterns, using the methods previously developed within the associate project P7, especially with the aim of identifying localized predictors of failure in our hierarchical systems.

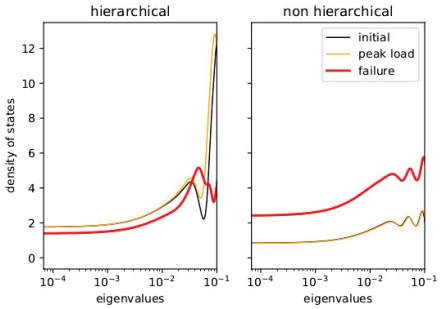

Figure 34: Density of low eigenvalues of the Laplacian matrix L of hierarchical and non-hierarchical systems at failure. The generic element of L is given by $L_{ij} = \delta_{ij} \sum_{l=1}^{N} A_{jl} - A_{ij}$, *where N is the number of nodes in the network, indices indicate individual nodes, and* A_{ij} *is the adjacency matrix of the network.*

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P7: Spectral Signatures of Fault Tolerant Neural Architectures

Samaneh Esfandiary and Paolo Moretti

This associate project focuses on the impact of hierarchical network organization in the robustness of biological systems, with special emphasis on human brain networks. In analogy with the main project P7, where the problem of fracture and detachment mechanics is considered, and hierarchical organization is found to promote distributed failure patterns, the associate project P7 studies the effects of hierarchical microstructural organization of brain connectivity in the way neural activity is distributed across brain regions [1,2]. More importantly, the associate project P7 provides spectral graph theory tools, which are subsequently used to analyse fracture patterns in the main project [3]. The confluence of the two research projects is happening at this stage, when several concepts are being exchanged between the two lines of investigation.

In its current stage, the associate project P7 has turned its attention to the analysis of real neural data obtained by our collaborators at the BioCruces Health Center (Spain) and the Harvard Medical School (USA). In our previous work (published last year in Physical Review Research) we hypothesized that the spectra of networks of neural connectivity exhibit excess low eigenvalues, pointing to their ability to avoid pathological states of global activation. During the current funding period we were able to verify this hypothesis in the experimental data provided by our collaborators. Figure 35 shows the density of eigenvalues of the Laplacian matrices for 49 subjects, compared to reference data that was obtained by randomizing the corresponding networks, and thus removing the hierarchical organization. The real data exhibits excess eigenvalues in the lower spectral edge (Lifshitz tails), which our previous studies have connected to the dynamic fingerprints of "normal" brain activity.

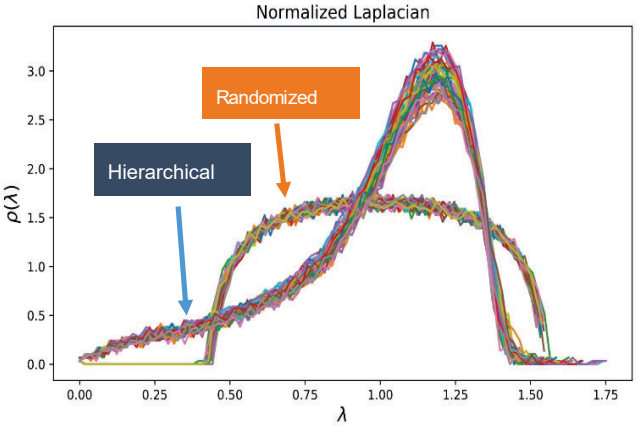

Figure 35: Density of eigenvalues of the Random Walk Laplacian matrices, for brain networks recorded for 49 patients of ages in the 20-35 range. The reference curves (indicated as Randomized) are obtained by switch-randomizations of the initial network structures, which implies a random rewiring of the network links, but preserves the degree sequences.

Eigenvalues are computed from the Random Walk Laplacian matrices, as introduced in the previous stages of our work [4]. Density of eigenvalues (density of states, as from the condensed matter problem that we share the formalism of) are defined as

$$\rho(\lambda) = \sum_{m=1}^{N} \delta(\lambda - \lambda_m)$$

where N is the number of nodes in the network and λ_m denotes the m-th eigenvalue of the Random Walk Laplacian matrix.

Our result also provides significant clues to the problem of fracture in hierarchical materials that main project P7 addresses. In particular, we were able to identify the same excess low Laplacian eigenvalues in the network models that P7 uses to simulate hierarchical material fracture, showing that similarly patterned hierarchical microstructures produce the same phenomena of distributed activity and/or damage, in a seemingly different biosystem model.

Our current work focuses on the introduction of the concept of local density of states, in order to spatially resolve the spectral properties of our networks and their associated dynamic signatures. This can be seen in Figure 36, where we show the local density of states for a choice of eigenvalues in the "low" range, computed at every node and plotted as a function of the nodes' degrees, that is their number of neighbors. Our result obviously shows that the local density of states is globally higher in the hierarchical case, but that interestingly nodes of lower degree contribute more heavily to this property. Back to the fracture problem of P7, this analysis method may allow us to identify regions in our hierarchical microstructures, which exhibit lesser stiffness (lower eigenvalues) and thus would be more prone to failure. In the light of these results, the projected work for the next months will include application of our novel formalism both to the main Project P7 and to the epoxy networks generated within Project P3. Further work will concentrate on the PhD thesis and the completion of a new publication.

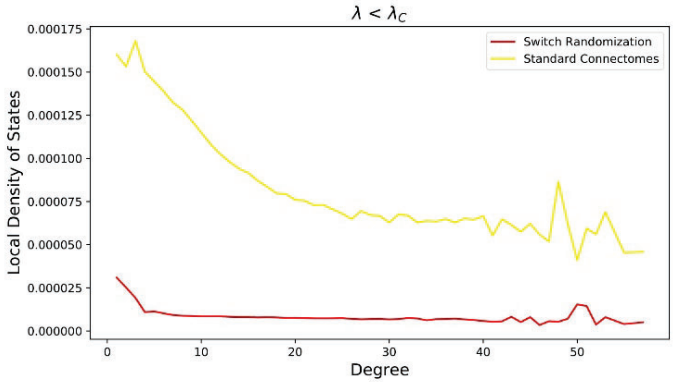

Figure 36: Local density of states for eigenvalues in the "low" range ($\lambda < \lambda_c$, where $\lambda_c \approx 0.4$ indicates the point where the density of states crosses in Figure 35).

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P8: Finite Deformation Phase-Field Fracture Models

Paras Kumar and Julia Mergheim

Crack propagation in heterogeneous materials, such as polymer nano-composites, involves complex crack topologies including branching and coalescence of multiple cracks. Traditionally, discrete crack approaches such as the XFEM have been employed for modeling cracks within the Finite Element framework. In the recent years however, the diffuse modeling approaches, also referred to as phase-field fracture models [1,2], have arisen as the preferred alternative for the aforementioned use case. This is primarily due to their ability to efficiently capture complex crack topologies. The phase-field approach involves approximation of the discrete crack by means of a continuous crack phase-field z, yielding a coupled nonlinear problem, which in the minimization form reads: Find $z \in [0,1]$, $\boldsymbol{\varphi}: \Omega \to \mathbb{R}^{\dim}$, s.t.

$$\left\{ \underbrace{\int_{\mathcal{B}_0} \Psi_d(\mathbf{F}, z)\,\mathrm{d}V}_{=:\mathcal{U}} + \underbrace{\int_{\mathcal{B}_0} \frac{G_c}{c_\omega}\left[\frac{\omega(z)}{l_c} + l_c\,|\mathrm{Grad}\,z|^2\right]\mathrm{d}V}_{=:\mathcal{G}} \underbrace{- \int_{\mathcal{B}_0} \mathbf{b}_0 \cdot \boldsymbol{\varphi}\,\mathrm{d}V - \int_{\partial\mathcal{B}_0} \mathbf{t}_0 \cdot \boldsymbol{\varphi}\,\mathrm{d}A}_{=:-\mathcal{W}^{\mathrm{ext}}} \right\} \to \inf$$

where, the terms $\mathcal{U}$, $\mathcal{G}$ and $\mathcal{W}^{\mathrm{ext}}$ denote the total elastic energy, the diffuse approximation to the fracture energy, and the external work respectively. Here, $z = 1$, denotes intact material while failure is denoted by the condition $z = 0$.

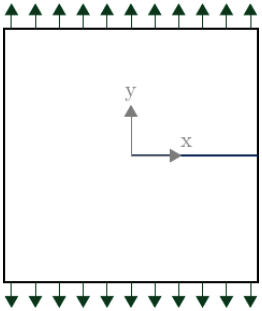

Figure 37: Setup for the SENT benchmark test [3].

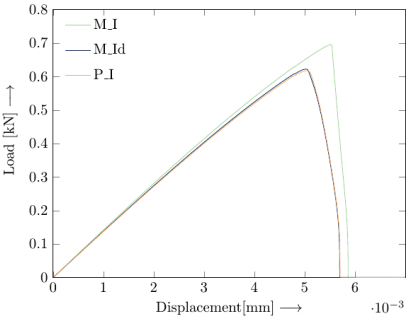

Figure 38: Influence of initial crack modelling strategy on the force-displacement curve for the SENT test.

Modeling of existing cracks is one of the open questions concerning this approach [4]. An intuitive choice is the *phase-field induced* crack (P_I), wherein, all of the crack phase-field degrees of freedom (DOFs) corresponding to the element layer containing the initial crack is set to the damaged value, i.e. $z = 0.0$. Another possibility involves a *mesh induced crack* (M_I) wherein the initial crack is modeled as a slit in the domain. Optionally, Dirichlet boundary conditions corresponding to $z = 0.0$, could be applied on the slit (M_Id). Figure 38 depicts the influence of the two approaches on the load-displacement curve for the single-edge-notched-tension (SENT) benchmark problem, cf. Figure 37. It is evident that the M_I approach, owing to higher initial overall stiffness, leads to a higher peak load.

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P9: Dynamic Phase-Field Model for the Brittle Fracture

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The fracture mechanics describe the state mechanical system during crack initiation, nucleation, and propagation. Typically, based on material behaviour, the modelling of fracture can be distinguished into brittle and ductile fractures. We observe brittle fracture in materials such as glass, ceramics, cast iron and graphite, etc., ductile fracture in aluminium, steel, copper, etc. These fractures can be modelled as a discrete crack (leading to numerical difficulties) or a diffused crack (resulting in a decrease in accuracy) [1]. However, in this project, we are interested in simulating diffused cracks with improved accuracy and lowered computational cost. The approach we took in a quasi-static regime to progress along this direction can be explored in our submitted paper [2]. Nonetheless, when we observe complex cracks in our daily lives, these crack paths occur in a dynamic setting in which inertial effects and rate-dependent rapid loading must be taken into account.

We investigate these dynamic effects in crack propagation under the framework of the phase-field model. The action for such a system is given by the standard dynamic phase-field model [3]

$$\begin{aligned} E(\mathbf{u},\dot{\mathbf{u}},c) &= \int_0^T \int_\Omega \left[\frac{1}{2}\rho\dot{\mathbf{u}}\cdot\dot{\mathbf{u}} - [1-c]^2\psi(\boldsymbol{\varepsilon}) - \mathcal{G}_c\left[\frac{c^2}{2\epsilon}+\frac{\epsilon}{2}|\nabla c|^2\right]\right] d\mathbf{x}\, dt \\ \psi(\boldsymbol{\varepsilon}) &= \frac{1}{2}\boldsymbol{\varepsilon}(\mathbf{u}):[\mathbb{C}\boldsymbol{\varepsilon}(\mathbf{u})] = \frac{1}{2}\lambda[\mathrm{tr}(\boldsymbol{\varepsilon})]^2 + \mu[\boldsymbol{\varepsilon}:\boldsymbol{\varepsilon}] \end{aligned} \tag{1}$$

where T, $\mathbf{u}, \dot{\mathbf{u}}, c$ and $\boldsymbol{\varepsilon}$ are the end time, displacement field, velocity field, phase field and strain tensor respectively. ϵ is a constant regularization parameter, and ρ, $\mathcal{G}_c$, λ and μ are material parameters. Stationary point of the action (1) with respect to $\mathbf{u}$ and c yields the following Euler-Lagrange equations

$$\begin{aligned} \nabla\cdot\boldsymbol{\sigma} &= \rho\ddot{\mathbf{u}} \qquad \text{in} \quad \Omega\times(0,T] \\ \frac{c\mathcal{G}_c}{\epsilon} - 2[1-c]\psi(\boldsymbol{\varepsilon}) - \mathcal{G}_c\nabla\cdot[\epsilon\nabla c] &= 0 \qquad \text{in} \quad \Omega\times(0,T]. \end{aligned} \tag{2}$$

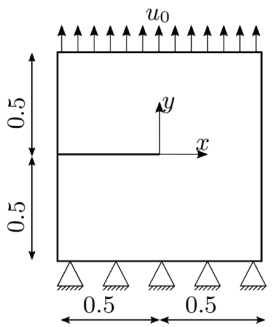

Figure 39: 2D problem set-up.

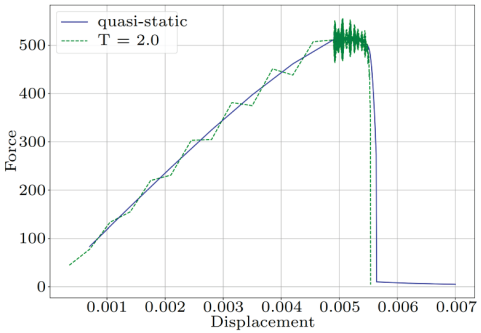

Figure 40: Force vs. displacement plot.

In addition to these equations of motion (2), the typical initial and boundary conditions for phase-field problems are $\mathbf{u}(\mathbf{x},0) = \mathbf{g}_0(\mathbf{x}) = 0$ for $\mathbf{x}\in\overline{\Omega}, \dot{\mathbf{u}}(\mathbf{x},0) = \mathbf{v}_0(\mathbf{x}) = 0$ for $\mathbf{x}\in\overline{\Omega}$ and $\mathbf{u} = \mathbf{u}_0$ on $\partial\Omega_\mathrm{d}\times(0,T], \mathbf{c} = \mathbf{c}_0$ on $\partial\Omega_\mathrm{p}\times(0,T], \nabla c\cdot\mathbf{n} = 0$ on $\partial\Omega\backslash\partial\Omega_\mathrm{p}\times(0,T]$ respectively. The domain is discretized with finite elements and the problem is solved using a staggered approach for robustness. Furthermore, we validated the dynamic phase-field implementation comparing the force vs. displacement curve between the dynamic and the quasi-static scenario Figure 40 for a Single Edge Notch Tension (SENT) specimen as seen in Figure 39.

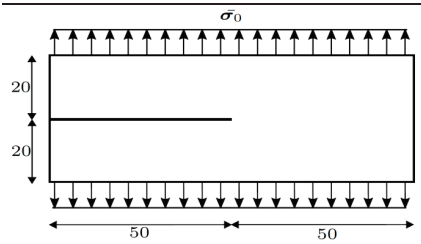

Figure 41: 2D problem for crack branching.

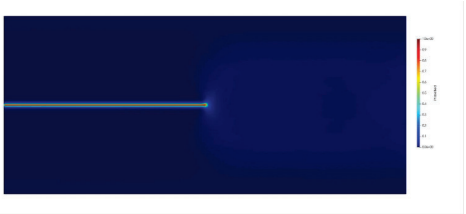

Figure 42: Initial crack with phase field.

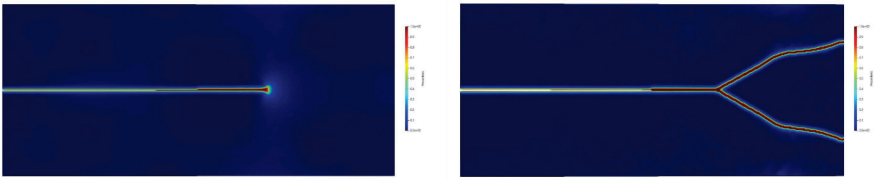

Figure 43: Evolution of phase field showing to crack branch.

With the valid implementation, we simulated a problem with traction on the boundary Figure 41. The initial phase field can be seen in Figure 42, and the evolution of the phase-field, showing crack branching, is depicted in Figure 43. The future steps in our project are to extend our model, the spatially adaptive phase-field model in the dynamic case.

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P10: Peridynamic Analysis of Nonlocal Wrinkling Instabilities in Bilayered Systems

Marie Laurien, Ali Javili and Paul Steinmann

Peridynamics (PD) is a nonlocal continuum formulation that was introduced by Silling [1] in 2000. The method was designed to cope with modeling damage where the use of partial differential equations, following classical continuum mechanics, would lead to singularities. To this end, motivated by molecular dynamics, spatial derivatives in the governing equations are replaced by integrals over the neighborhood of a continuum point. The integral terms comprise the interaction forces acting across a finite distance and are accountable for the nonlocal character of the method. This aspect carries the potential to model nonlocal material behavior in a variety of applications.

The basic version of PD is called bond-based PD and relies on the assumption of pairwise interactions. In our first study [2], bond-based PD is applied to add a nonlocal perspective to the analysis of surface wrinkles that are observed in a variety of biological tissues, e.g. the human brain [3]. The underlying mechanism is based on a film that is attached to a compliant substrate and buckles when it is compressed. Since the film is not freestanding but bonded to the substrate, it is hindered from buckling into a single wave. Instead, short-wavelength buckling is the energetically favored equilibrium state of the system, which appears in form of sinusoidal surface wrinkles. In the past, the wrinkling of bilayers has been analyzed at length through local models based on classical continuum mechanics. However, the influence of nonlocal effects remains mostly unknown. We have developed a computational model that is capable of predicting the main characteristics of the wrinkling pattern using peridynamics. The numerical procedure includes an accompanying eigenvalue analysis that allows to precisely capture the critical conditions of the instability since the formation of wrinkles mathematically translates into a bifurcation problem. The results of several parameter studies suggest that the level of nonlocality of a material model has quantitative influence on the main wrinkling characteristics, while most trends qualitatively coincide with predictions from the local analytical solution. However, a relation between the film thickness and the critical compression is revealed that is not existent in the local theory. Moreover, the wrinkling patterns in Figure 44 illustrate that PD is able to capture boundary effects that are not accessible for local models.

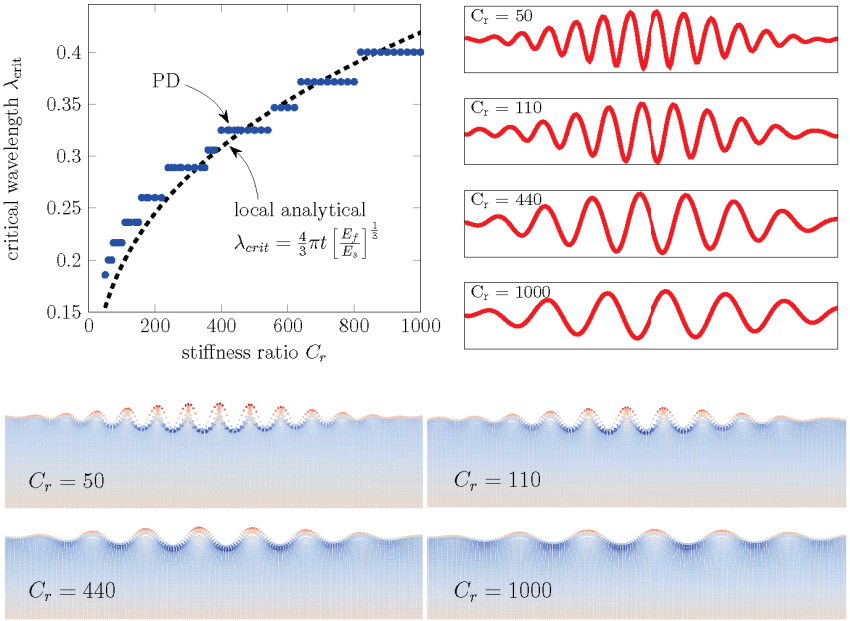

Figure 44: Top left: critical wavelength λ_{crit} versus stiffness ratio C_r. Top right: wrinkling patterns for an exemplary selection of stiffness ratios C_r. Bottom: corresponding deformed configurations.

Since bond-based PD is restricted to a fixed Poisson's ratio, Javili et al. [4] have recently presented the theory of continuum-kinematics-inspired peridynamics (CPD). CPD accounts for the change in area and volume by considering also two- and three-neighbor interactions. In order to extend the analysis of a bilayer to incompressible materials, an approach to cope with material interfaces using CPD is introduced. The nonlocal interface is realized via a purely geometrical contact of the two materials within an overlap region. As the size of the overlap is determined by the horizon size, a sharp interface is recovered with decreasing nonlocality (cf. Figure 45).

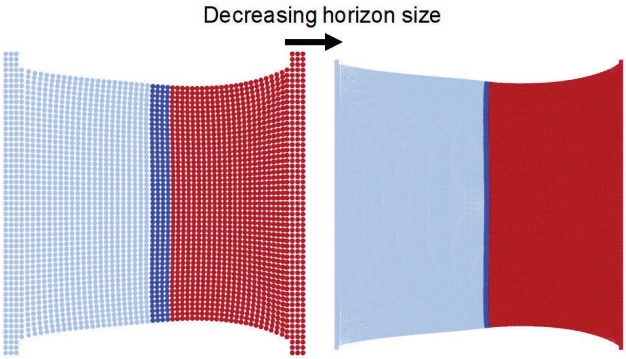

Figure 45: Peridynamic composite with a nonlocal interface (dark blue) for two different horizon sizes.

The aim of future work within FRASCAL will be to develop a CPD framework associated with configurational mechanics to model fracture.

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P10: Bone Fracture Healing

Ina Schmidt, Areti Papastavrou and Paul Steinmann

Motivation

Bone fracture healing is quite a complex process which can be subdivided into an inflammatory phase including haematoma formation, a reparative phase separated into soft and hard callus formation and finally followed by the remodelling phase, which takes much longer than the first two phases and in which the rapidly formed secondary bone realigns in the direction of principal loading. There is already a numerous amount of research working on the simulation of bone fracture healing, however, most of them only focussing on secondary healing at the shaft of long bones (Geris et al. 2010), (Ghiasi et al. 2019), (Lacroix et al. 2002).

One major goal of the project was to create an appropriate bone fracture healing model. To differentiate from previous work, the focus was set on modelling primary healing at the end of long bones and therefore not studying callus formation. Additionally, the model is required to be efficient and easily extendable to further aspects like age-dependency as well as adaptable to patient specific characteristics.

Project status

A model calculating the evolution of bone density due to mechanical loading as well as under consideration of fracture healing was created. For further details see (Schmidt et al. 2021b). For the sake of efficiency and to easily adapt the model to other common problems, the continuum bone remodelling framework as described in (Kuhl and Steinmann. 2003) was chosen. Therein the biological homeostasis is in principle based on mechanical stimulation. To involve the healing process, the evolution equation describing the temporal change in nominal density is altered by an additional healing stimulus and according time controlled prefactor functions. A fracture is therefore modelled time-dependent as well as locally by setting the nominal density at each integration point which belongs to the fracture area to almost zero, as depicted in Figure 46 (first picture). To represent the highly dynamic biological process, different healing prefactor functions can be applied. The example in Figure 46 shows the results with an adaptive healing function starting with a rapid healing process soon after the fracture occurred and which subsequently smoothly slows down.

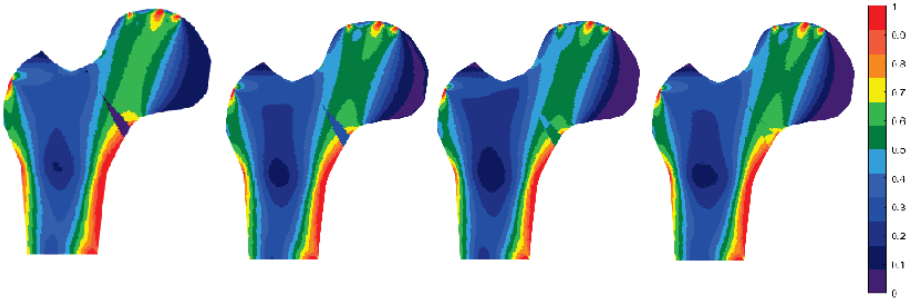

Figure 46: Fracture Healing: Evolution of nominal density at different times.

Observe, that at first, the density in the fracture area increases steadily, while the surrounding area slightly experiences bone loss, because of the lack of mechanical stimulation resulting from immobilisation (second picture). In the last two pictures, the remodelling phase of the healing process is illustrated. Quickly built bone there orients itself to the principal loading and thus, the fracture zone adapts to the surrounding density distribution again.

Conclusion & Outlook

The implemented algorithm not only proves to be particularly efficient, but can also be easily adapted to different fracture patterns, patient-specific bone geometries and different loading therapies. Furthermore, it can be easily extended by other aspects such as age dependency or the availability of nutrients, see also (Papastavrou et al. 2020a), (Papastavrou et al. 2020b) and (Schmidt et al. 2021a).

Note that the model is based on a rather phenomenological approach. For quantitative validation, huge clinical data sets are essential, which are difficult to access due to ethical and medical concerns regarding too frequent radiation exposure.

Additionally, a mesoscopic model was developed to better understand and study the anisotropic behaviour of cancellous (spongy) bone. For this purpose, different initial grids were generated based on the theory of an ideal truss and subsequently investigated under different loading conditions. Nevertheless, further research is needed in this topic along with an appropriate coupling between the mesoscopic and the macroscopic model.

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P11: Material Optimization for Fracture Control

Sukhminder Singh, Lukas Pflug and Michael Stingl

The aim of the present work is to optimize heterogeneous structures to enhance their resistance to delamination, when subjected to quasi-static, externally applied boundary displacement. Linear elastic behaviour is assumed for the materially homogeneous spatial subdomains, while the interfaces between them are governed by a softening adhesive model. The objective of the optimization problem is to find optimal shapes of inclusions embedded in a matrix so that the mechanical work of the applied boundary displacement is maximized. This in turn should increase the delamination resistance of the structure. For simplicity, inclusions are assumed to be elliptical, parameterized by major and minor radii along with their orientations within the structure. The interfaces are modelled using the eXtended Finite Element Method (XFEM), which allows automated meshing of the structural domain for different configurations of the inclusion shapes. The optimization problem formulation has the following characteristics:

1. Derivatives of the objective function cannot be computed due to the presence of unstable crack growth, as the global stiffness matrix becomes singular at the critical points of instability.
2. There exists switching of crack patterns (bifurcation) with small perturbations of the design parameters. This renders the objective function discontinuous.
3. High sensitivity of the observed fracture response w.r.t. pseudo-time discretization and finite element remeshing of the structure adds noise to the objective function.

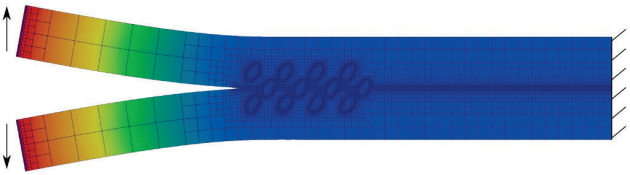

Figure 47: Structural setup and finite element discretization.

These properties necessitate reformulation of the optimization problem as a stochastic optimization problem. In this approach, we minimize or maximize the expected value of the structural response, resulting in a robust design against small perturbations and uncertainties in the design parameters. The optimization problem is stated as

$$\min_x F(x) = \mathrm{E}_{x,\sigma}\left[f(Y)\right] = \int_{R^d} f(y)p(y;x,\sigma)\,\mathrm{d}y$$

where $x \in R^d$ is design vector, $f: R^d \to R$ is the structural response function and $p: R^d \to R$ is multivariate normal probability density function. To approximate the above d-dimensional integral within an optimization framework, two methods have been tried:

1. The simplest one is the Monte-Carlo integration method and the samples generated over the past optimization iterations are used with importance weights [1] to guarantee convergence w.r.t. the number of samples (N). This method does not assume anything about the degree of smoothness of the integrand and in theory, the order of convergence is independent of the dimension d. A major drawback of using this method is its slow convergence rate w.r.t. the number of function evaluations and the integration error decreases at $O(N^{-1/2})$.
2. Stochastic expansion - Here, with a few initial samples, a meta-model (surrogate) is fitted globally to the original response function. In every optimization iteration, the surrogate model is refined as more and more samples are added to it and a local or global extremum is obtained by solving a stochastic optimization sub-problem on the surrogate function. Currently, we use Voronoi-piecewise surrogate [2] as an approximation to the original response function, which can handle noise and adapt to discontinuities. Nevertheless, the convergence rate w.r.t. problem dimension needs to be determined by numerical experiments and compared with the Monte Carlo approach in the context of stochastic optimization.

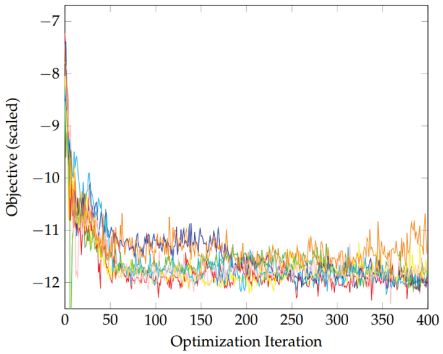

Figure 48: Objective value w.r.t. optimization iteration for a 12 degrees of freedom design problem, determined over 7 repetitions. The objective value is estimated by Monte-Carlo method with 12 response function evaluations per optimization iteration. Even after after 400 × 12 = 4800 function evaluations, the objective value is oscillatory w.r.t. optimization iteration due to the slow convergence rate of Monte-Carlo integration.

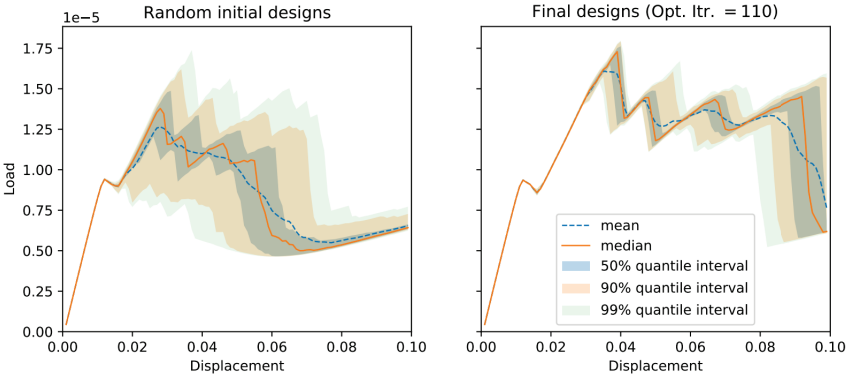

Figure 49: Load-displacement curves for random initial and final designs for 7 optimization runs with 12 samples each.

Conclusions, main achievements, and outlook

The optimization problem involving delamination can be solved using stochastic and surrogate-based optimization methods. However, the maximum dimension for which the optimization problem can be solved with good integration accuracy and a limited number of expensive function evaluations is small (≈10). Further research is needed in the direction of modelling of surrogates which can better approximate the response function in the region close to a local optimum employing a small number of function evaluations and incorporate discontinuities.

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P12: Modelling Molecular Bond Rupture by Density Functional Theory Calculations

Christian R. Wick, Mattia Livraghi, Sampanna Pahi, Ece Topraksal and Ana-Sunčana Smith

In the first funding period, the aim of the 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.

In the last period, we concentrated our studies on the validation of density functional theory (DFT) for the investigation of molecular bond breaking under force and obtained a detailed understanding of the behavior of molecular bonds in simple (epoxy and non-epoxy) model systems utilizing 1D and 2D COGEF (COnstrained Geometries simulate External Force[1]) calculations. To investigate the performance of DFT for bond breaking calculations in our epoxy systems, we computed Bond Dissociation Energy Profiles (BDEPs) for 17 different molecular bonds of 4 different bond types including C-C, C-O, C-S and C-N bonds at the reference RI-NEVPT2-F12[2] / cc-pVTZ-F12 // B3LYP/def2-TZVPP level of theory. We justified the accuracy of our reference calculations by comparing the estimated BDE from our scans to experimental and G4MP2-6x[3] computed values (not shown). Finally, based on our reference BDPEs, we evaluated the performance of 35 different functionals available in Gaussian16 performing Single Point (SP) calculations on the B3LYP/def2-TZVPP optimized structures. We chose the cc-pVDZ basis set for the DFT SP calculations in order to allow for fast calculations in our larger EPOXY systems. A part of the results is summarized in Figure 50. Our data shows that the pure functionals BP86 and PBEPBE perform best for all systems except C-S bonds are involved. Surprisingly, M06-L or the hybrid M06-D3 are showing the best compromise if all bond types are of interest. In both cases, the overall Mean Unsigned Error is well below 15 kJ mol^{-1}, which is very close to the desired chemical accuracy.

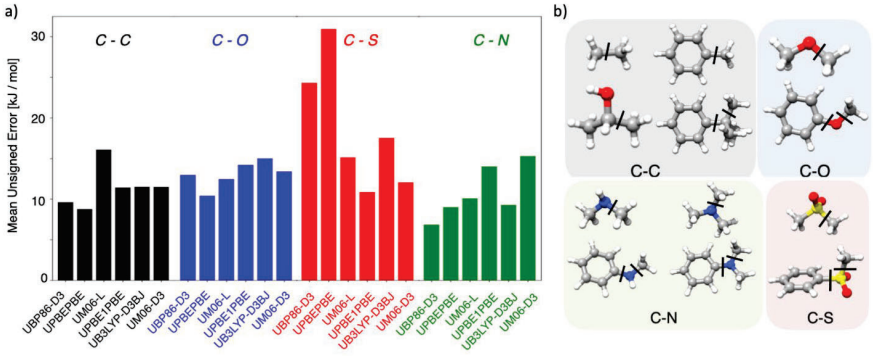

Figure 50: Performance of different DFT functionals with respect to computing bond dissociation energy profiles. a) Mean Unsigned Error computed for the different bond types observed in a DGEBA/DDS epoxy resin using RI-NEVPT2-F12 / cc-pVTZ-F12 // B3LYP/def2-TZVPP as reference. Only the best 6 functionals out of 35 tested functionals are shown. b) the model systems used to compute a total of 17 bond dissociation energy profiles. The bonds investigated are marked by a black line.

In parallel to our efforts to find a suitable level of theory for our envisaged hybrid calculations, we extended the COGEF procedure in several ways. In order to allow for more sophisticated COGEF calculation, we developed an inhouse COGEF package (written in python) interfacing to Gaussian16, which offers several advanced functionalities: the standard operational mode includes an iterative COGEF procedure monitoring stability analysis and geometry convergence at every cycle. This is necessary to ensure stability of the computed wave functions and reliability of the results. Nevertheless, the classic COGEF procedure will not allow to break a specific bond of the model system. Indeed, the outcome of the COGEF procedure depends strongly on the initial structure and not only the bond with the lowest BDE might be broken. We therefore introduced the targeted COGEF procedure, which allows to break any bond of the system by modifying the guess structure at every

iteration. Instead of moving only a single atom at each iteration of the COGEF procedure, the fragments of the molecule left and right to the bond of interest will be moved. An example of such a calculation is shown in Figure 51 a). The targeted procedure allows to investigate the individual bond strength of all the bonds in the model complex and shows that bonds b3 and b4 are very similar in terms of the characteristic measures F_{max} and BDE. We further extended the functionality to a 2D procedure[4], depicted in Figure 51 b). Here, we computed the full energy profile as a function of d and the bond length b of bond b4. The classic COGEF procedure misses the low energy open shell singlet structure for larger d values and stays on the high energy closed shell surface. The targeted procedure overcomes the barrier between the closed shell and open shell structures for larger d values. Recently, we extended the COGEF procedure also to ONIOM type calculations, developing a hybrid Mechanical Embedding / Electrostatic Embedding optimization scheme for COGEF calculations of larger systems to investigate size effects of the COGEF method. We are currently investigating the potential of such calculations to identify bonds in epoxy models, which are likely to break and to define a measure to deem a bond broken based on DFT calculations. This measure will be utilized in our hybrid Molecular Dynamics simulations for accurate modelling of epoxy resins in the next period.

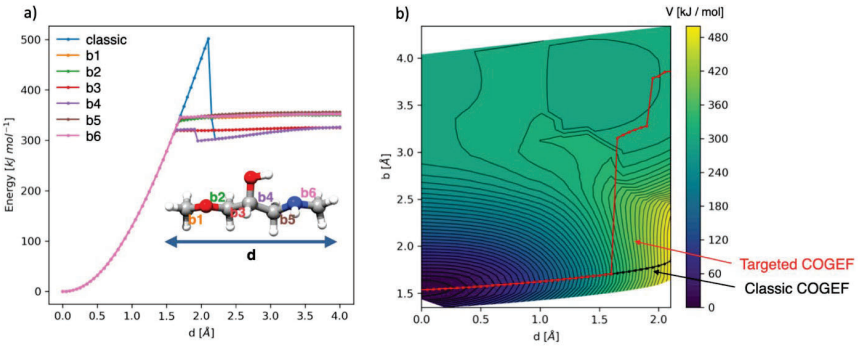

Figure 51: COGEF energy profiles for an aliphatic amine cured epoxy model system. A) Computed 1D COGEF profiles for the classic and targeted COGEF procedures. The model system is shown as inset. d corresponds to the distance between the outer-most H atoms (arrow). In the classic procedure, bond number 4 will rupture, however, the classic curve overshoots the dissociation energy by more than 140 kJ mol-1. The targeted COGEF procedure allows to break any particular bond of the model system. (Little) overshooting is avoided by moving backwards after spin contamination is observed (i.e. <S^2> >= 0.5) B) 2D COGEF profile computed for bond number 4 (b4) in a). The classical and targeted COGEF profiles are indicated by black and red lines, respectively. The 2D profile reveals the problem observed in the classic procedure – the system remains on a closed shell surface and is not able to overcome the barrier to reach the open shell singlet state with one of the bonds broken.

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P10: Generalized Interface Laws for Nonlinear Kinematics

Lucie Spannraft, Julia Mergheim and Paul Steinmann

Interface (in-) elasticity and cohesive zone models are two main concepts to describe interfaces in the continuum mechanics framework. Interface (in-) elasticity, permitting a traction jump $[\![\bar{\boldsymbol{T}}]\!] \neq \boldsymbol{0}$, introduces energetic quantities as a response to tangential loading. In contrast, cohesive zone models can respond to tension and shear loading by a displacement jump $[\![\boldsymbol{\varphi}]\!] \neq \boldsymbol{0}$. Variationally consistent anisotropic cohesive zone models include a dependence on structural tensors to comply with physical constraints.

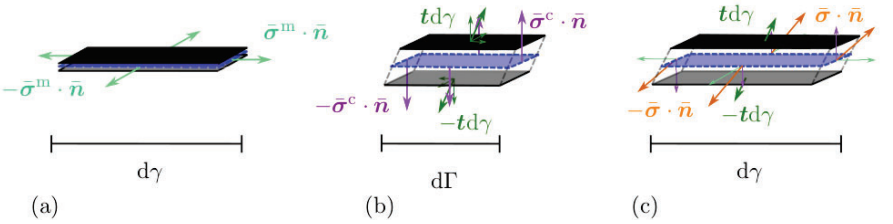

Figure 52: Coherent energetic (a), anisotropic cohesive (b), generalized interface (c).

Our generalized mechanical interface model for nonlinear kinematics is derived from the interfacial strain energy density $\bar{\Psi}$, which is composed of a membrane part $\bar{\Psi}^{\mathrm{m}}$ and a cohesive part $\bar{\Psi}^{\mathrm{c}}$. Thus, the model allows for both, traction and displacement jumps, cf. Figure 52. For thermodynamical consistency, the dependence of the cohesive strain energy density on the spatial interface normal vector $\bar{\boldsymbol{m}}$ is expressed by means of the interface deformation gradient $\bar{\boldsymbol{F}}$.

$$\bar{\Psi} = \bar{\Psi}(\bar{\boldsymbol{F}}, [\![\boldsymbol{\varphi}]\!]) = \bar{\Psi}^{\mathrm{m}}(\bar{\boldsymbol{F}}) + \bar{\Psi}^{\mathrm{c}}(\bar{\boldsymbol{F}}, [\![\boldsymbol{\varphi}]\!])$$

For a hyperelastic model accounting for irreversible damage, we couple the cohesive and membrane contributions providing an interaction among the normal, tangential and in-plane degradation. The model is implemented in a user subroutine in Abaqus and solved for zero-thickness user elements at the interface. Numerical results show a dependence of the cohesive tractions, the interface Piola stresses, the fracture length, the damage initiation and progression on the damage coupling, see Figure 53.

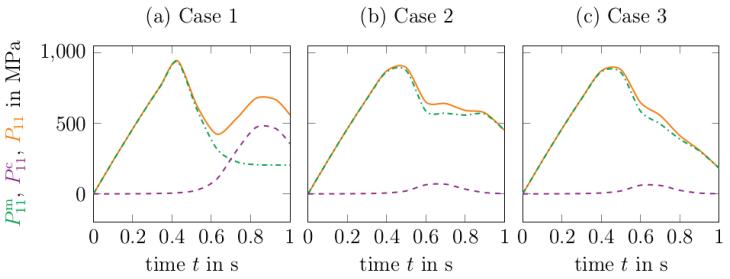

Figure 53: Interface Piola stress entry $\bar{P}_{11}$ with membrane and cohesive contributions $\bar{P}_{11}^{m}$, $\bar{P}_{11}^{c}$ plotted over time t for different types of damage coupling in a peel-test.

2.2 Publications

(in alphabetical order)

Journal Articles

[1] **S. Elmira Birang O., Harold S. Park, Ana-Sunčana Smith, Paul Steinmann**
Atomistic configurational forces in crystalline fracture
Forces in Mechanics 4 (2021) 100044
DOI: 10.1016/j.finmec.2021.100044

[2] **S. Elmira Birang O., Ana-Sunčana Smith, Paul Steinmann**
Phonon-based thermal configurational forces: Definitions and applications in rupture of semiconductors
Engineering Fracture Mechanics, Volume 257 (2021) 108014
DOI: 10.1016/j.engfracmech.2021.108014

[3] **S. Elmira Birang O., Paul Steinmann**
Discrete Configurational Mechanics for the Computational Study of Atomistic Fracture Mechanics
Journal of Forces in Mechanics, 2 (2021) 100009
DOI: 10.1016/j.finmec.2020.100009

[4] **Stefan Hiemer, Stefano Zapperi**
From mechanism-based to data-driven approaches in materials science
Materials Theory 5 (2021) 4
DOI: 10.1186/s41313-021-00027-3

[5] **Seyyed Ahmad Hosseini, Paolo Moretti, Avraam Konstantinidis, Michael Zaiser**
Beam network model for fracture of materials with hierarchical microstructure
International Journal of Fracture, 227(2) (2021) 243-257
DOI: 10.1007/s10704-020-00511-w

[6] **Julian Konrad, Robert Meißner, Erik Bitzek, Dirk Zahn**
A molecular simulation analysis of bond reorganization in epoxy resins: from curing to deformation and fracture
ACS Polymers Au 1(3) (2021) 165-174
DOI: 10.1021/acspolymersau.1c00016

[7] **Julian Konrad, Dirk Zahn**
Accessing the mechanical properties of molecular materials from atomic simulation
AIMS Materials Science, 8(6) (2021) 867-880
DOI: 10.3934/matersci.2021053

[8] **Paras Kumar, Paul Steinmann, Julia Mergheim**
Enhanced Computational Homogenization Techniques for Modelling Size Effects in Polymer Composite
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DOI: 10.1007/s00466-021-02037-x

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An Exact Algorithm to Detect the Percolation Transition in Molecular Dynamics Simulations of Cross-Linking Polymer Networks
J. Chem. Theory Comput. 17, 10, (2021) 6449–6457
DOI: 10.1021/acs.jctc.1c00423

[10] **Patrick Lorenz, Florian Wullschläger, Antonia Rüter, Bernd Meyer, Andreas Hirsch**
Tunable Photoswitching in Norbornadiene (NBD)/Quadricyclane (QC) - Fullerene Hybrids
Chemistry-A European Journal, 27, (2021) 14501 –14507
DOI: 10.1002/chem.202102109

[11] **Maximilian Ries, Gunnar Possart, Paul Steinmann, Sebastian Pfaller**
A coupled MD-FE methodology to characterize mechanical interphases in polymeric nanocomposites
International Journal of Mechanical Sciences, 204 (2021) 106564
DOI: 10.1016/j.ijmecsci.2021.106564

[12] **Ina Schmidt, Jacob Albert, Marina Ritthaler, Areti Papastavrou, Paul Steinmann**
Bone fracture healing within continuum bone remodeling
Computer methods in Biomechanics and Biomedical Engineering (2021)
DOI: 10.1080/10255842.2021.1998465

[13] **Ina Schmidt, Areti Papastavrou, Paul Steinmann**
Concurrent consideration of cortical and cancellous bone within continuum bone remodelling
Computer Methods in Biomechanics and Biomedical Engineering, ISSN: 1025-5842
DOI: 10.1080/10255842.2021.1880573

[14] **Sukhminder Singh, Lukas Pflug, Michael Stingl**
Material optimization to enhance delamination resistance of composite structures using viscous regularization
Computer Methods in Applied Mechanics and Engineering, 382 (2021) 113881
DOI: 10.1016/j.cma.2021.113881

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Phys. Rev. B 104 (2021) 125412
DOI: 10.1103/PhysRevB.104.125412

[17] **Wuyang Zhao, Maximilian Ries, Paul Steinmann, Sebastian Pfaller**
A viscoelastic-viscoplastic constitutive model for glassy polymers informed by molecular dynamics simulations

International Journal of Solids and Structures, 226-227, 111071
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A particle-continuum coupling method for multiscale simulations of viscoelastic – viscoplastic amorphous glassy polymers
International Journal for Numerical Methods in Engineering (2021).
DOI:10.1002/nme.6836

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[1] **Christof Bauer, Sebastian Pfaller**
Combined continuum mechanics and molecular dynamics approach for uniaxial deformation of a thermoplastic polymer
Proceedings in Applied Mathematics and Mechanics 20(1), Wiley-VCH GmbH, 2021
DOI: 10.1002/pamm.202000149

[2] **Paras Kumar, Julia Mergheim**
Size Effects in Computational Homogenization of Polymer Nano-Composites
Proceedings in Applied Mathematics and Mechanics 20(1), Wiley-VCH GmbH, 2021
DOI: 10.1002/pamm.202000047

[3] **Maximilian Ries, Yash Jain, Florian Müller-Plathe, Sebastian Pfaller**
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8th ECCOMAS Thematic Conference on the Mechanical Response of Composite, 2021
DOI: 10.23967/composites.2021.014

[4] **Maximilian Ries, Paul Steinmann, Sebastian Pfaller**
The Hybrid Capriccio Method: A 1D Study for Further Advancement
Proceedings of 14th WCCM-ECCOMAS Congress, January 2021
DOI: 10.23967/wccm-eccomas.2020.335

[5] **Maximilian Ries, Felix Weber, Maximilian Striegel, Paul Steinmann, Sebastian Pfaller**
Multiscale FE-MD Coupling: Influence of the Chain Length on the Mechanical Behavior of Coarse-Grained Polystyrene
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Material optimization for controlling interfacial damage in composite structures
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DOI: 10.1002/pamm.202000344

[7] **Wuyang Zhao, Sebastian Pfaller**
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Proceedings in Applied Mathematics and Mechanics 20(1), Wiley-VCH GmbH, 2021
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Atomistic configurational forces in crystalline fracture

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ARTICLE INFO

Keywords:
Atomistic configurational mechanics
Configurational forces
Many-body potentials
Fracture mechanics

ABSTRACT

Configurational atomistic forces contribute to the configurational mechanics (i.e. non-equilibrium) problem that determines the release of total potential energy of an atomistic system upon variation of the atomistic positions relative to the initial atomic configuration. These forces drive energetically favorable irreversible re-organizations of the material body, and thus characterize the tendency of crystalline defects to propagate. In this work, we provide new expressions for the atomistic configurational forces for two realistic interatomic potentials, i.e. the embedded atom potential (EAM) for metals, and second generation reactive bond order (REBO-II) potential for hydrocarbons. We present a range of numerical examples involving quasistatic fracture for both FCC metals and mono and bi-layer graphene at zero Kelvin that demonstrate the ability to predict defect nucleation and evolution using the proposed atomistic configurational mechanics approach. Furthermore, we provide the contributions for each potential including two-body stretching, three-body mixed-mode stretching-bending, and four-body mixed-mode stretching-bending-twisting terms that make towards defect nucleation and propagation.

1. Introduction

We use the concept of spatial and material atomistic forces derived for various many-body potentials. In a quasi-static setting considered here, spatial atomistic forces contribute to the classical *deformational* (equilibrium) problem seeking to minimise the total potential energy of an atomistic system when varying the spatial atomistic positions. By contrast, material atomistic forces contribute to the *configurational* (non-equilibrium) problem that determines the release of total potential energy of an atomistic system when varying the material (initial) atomistic positions. Thereby, material atomistic forces characterise the tendency of generic atomistic defects to propagate, i.e., they drive energetically favourable re-organisations of the material atomistic configuration. Atomistic configurational forces provide a tool to study configurational changes which inherently occur during a fracture and failure process. Configurational forces are associated with *any* lattice defect irrespective of its type, i.e., point, line and planar defects which can be for example, vacancies, interstitials, substitutionals, Stone-Wales, 5-8-5, cracks, dislocations, twinning, stacking faults, surfaces, grain or twining boundaries. Taken together, every lattice irregularity results in configurational force driving its evolution relative to the material configuration.

In our prior works [1,2], we established the first principles of atomistic configurational mechanics. Therein, the concept of deformational and configurational atomistic pair, triplet and tetrad forces are introduced. Configurational pair force accounts for the changes in total energy due to the changes in the pair length. Variations in the area formed by a triplet of atoms is captured using the notion of configurational triplet force. In a similar fashion, the energetic variations associated with the variations in the tetrad volume defines configurational tetrad force. Notably, the proposed theoretical framework in [2] compares well to the energy-momentum structure of the Eshelby stress in the continuum configurational mechanics [3]. The continuum setting of configurational mechanics are presented for example in [4–10] as well as our own contributions to configurational mechanics in [11–16]. However, to a large extent we have not yet studied computational examples from the realm of atomistic fracture- and configurational-mechanics.

In this work, we initially elaborate on deformational and configurational formulations applicable on substantive materials. Next, we present a number of diverse numerical examples to demonstrate the applicability of the approach to crystalline fracture. We investigate in the derivation of energy release during the fracture of crystalline

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Phonon-based thermal configurational forces: Definitions and applications in rupture of semiconductors

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Effective empirical potential
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Spatial and material settings

ABSTRACT

A general framework encompassing spatial and material settings of atomistic crystalline systems is presented. Theoretical and computational analysis of configurational forces in the context of atomistic thermomechanics constitutes the central topic of the presented paper. We distinguish between atomistic configurational forces stemming from the changes in static energy density and the changes in vibrational energy density. To this end, we first propose a novel *atomistic phonon-based thermal configurational forces* rendering infinitesimal changes in vibrational energy density under configurational variations. Next, we employ pair and triplet configurational forces resulting from the changes in static energy density due to two-body stretch and three-body stretch-bending. Using thermal configurational forces, we study numerically the problem of temperature rise, bond stretching and bending occurring at the crack tip induced by brittle crack propagation in crystalline lattices. Energy release caused by large harmonic vibrations and deformations is estimated by the magnitude of configurational forces at the crack tip. The atomistic temperature is shown to be governed by atom-wise frequency through local entropy. Finally, we demonstrate suitability and versatility of atomistic configurational forces in analyzing fracture of silicon diamond lattice subjected to mode-I loading at different finite temperatures.

1. Introduction

Configurational forces acting on defects is very well proved to be a powerful analysis tool to study continuum defect mechanics including fracture. Thereby, defect evolution relative to the material occurs through variations of the material configuration. Energetically, configurational forces relate to variations in the material configuration, thus configurational forces are energetically conjugate to continuum defect evolution. The notion of *continuum thermal configurational forces* in terms of entropy density and temperature gradient applicable to finite-strain thermoelastic materials under quasi-static process is originally introduced by Epstein [1] and Epstein and Maugin [2]. Furthermore, Dascalu and Maugin [3] elaborated thermal configurational forces using the notion of thermal displacement introduced by Green and Naghdi [4] for thermoelasticity without energy dissipation. The realm of configurational thermomechanics is extended over the decades, Maugin and Berezovski [5] presented the applications of thermal configurational forces, e.g., thermal forces appearing at the crack tip or at the surface of a propagating phase transition front. In our own contributions [6–9], deformational and configurational thermomechanical settings are extended for various constitutive models capturing bulk, surface and interface of a continuum body. Considering the applicability of thermal configurational forces in assessing fracture of a continuum body, here we initiate the principles for *atomistic configurational thermomechanics* and present

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Discrete configurational mechanics for the computational study of atomistic fracture mechanics

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ABSTRACT

We formulate discrete configurational mechanics in an atomistic setting, discuss the corresponding computational details, and demonstrate its utility via computational analyses of atomistic fracture mechanics problems. To this end, we first propose a novel *Configurational-Force-Criterion* (CFC) to predict crack propagation into an atomic crystalline lattice. Thereby, specifically, the CFC relies on comparing discrete configurational forces with a corresponding *Crack-Propagation-Threshold* (CPT) in the quasi-static approximation of atomistic systems at zero Kelvin. Next, based on the CFC, we introduce a quasi-static computational atomistic crack propagation algorithm. Therein, whenever an atomic pair meets the CFC, we modify the lattice connectivity by deleting the corresponding interatomic bond, thus resulting in true irreversibility, i.e. dissipation upon crack extension. Finally, based on different choices for the magnitude of the CPT employed in the CFC, we demonstrate suitability and versatility of discrete configurational mechanics in analyzing atomistic fracture mechanics.

1. Introduction

Eshelby and Mott [1] introduced the concept of (configurational) forces acting on elastic singularities or, likewise, on inhomogeneities in an elastic medium, whereby, arguably, the idea traces back to Burton [2]. According to Eshelby [3], a descriptive definition of configurational forces is as follows: "*... the configuration of a defect can be specified by a parameter. Following the terminology of analytical mechanics and thermodynamics we can call the rate of decrease of total energy of the system with respect to the parameter the generalized force acting on that parameter, in simple cases, on the defect itself*". Mathematically, Eshelby [4] cast the essence of configurational continuum mechanics into the energy-momentum or rather Eshelby stress tensor. The corresponding Eshelby traction relates to the total energy variation of a continuum body as its material placement varies.

The importance of the Eshelby stress remained initially underappreciated until it appeared as integrand in the path-independent J-integral as proposed by Cherepanov [5] and Rice [6] in continuum fracture mechanics. According to the Eshelby-type interpretation, a crack tip singularity behaves like a defect, whereby the singular Eshelby traction at the crack tip is analogous to the crack driving force as expressed by the J-integral or, similarly, as embedded into the notion of energy release rate, see Irwin [7].

The milestone work of Maugin [8] (who denoted configurational mechanics/forces as material mechanics/forces) advocated further implications, extensions and applications of configurational continuum mechanics. Maugin and Trimarco [9] proposed the (un)balance of configurational momentum that differs from the common balance of deformational momentum. The latter serves to determine the deformation of a system, whether continuous or discrete, under initial and boundary-value conditions. It is worth underlining that, even if straightforward manipulations allow deducing configurational momentum from its deformational counterpart, these operations are, however, not without relevance since the (un)balance of configurational momentum is instrumental when studying continuum defect mechanics. Relations between deformational and configurational continuum mechanics extend to various constitutive material classes, see, e.g., hyperelastostatics [10], elastoplasticity [11], hyperelastodynamics [12], thermo-hyperelastodynamics [13].

Taken together, the concept of configurational forces acting on defects proves a powerful analysis tool to study continuum defect mechanics including fracture. Thereby, continuum defect evolution relative to the material occurs through variations of the material configuration. Energetically, configurational forces relate to variations in the material configuration, thus configurational forces are energetically conjugate to continuum defect evolution.

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ORIGINAL PAPER

Beam network model for fracture of materials with hierarchical microstructure

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Abstract We introduce a beam network model for hierarchically patterned materials. In these materials, load-parallel gaps intercept stress transmission in the load perpendicular direction in such a manner that damage is confined within hierarchically nested, load-carrying 'modules'. We describe the morphological characteristics of such materials in terms of deterministically constructed, hierarchical beam network (DHBN) models and randomized variants thereof. We then use these models to analyse the process of damage accumulation (characterized by the locations and timings of beam breakages prior to global failures, and the concomitant avalanche statistics) and of global failure. We demonstrate that, irrespective of the degree of local disorder, failure of hierarchically (micro)structured materials is characterized by diffuse local damage nucleation which ultimately percolates on the network, but never by stress-driven propagation of a critical crack. Failure of non hierarchical reference networks, on the other hand, is characterized by the sequence of damage nucleation, crack formation and crack propagation. These differences are apparent at low and intermediate degrees of material disorder but disappear in very strongly disordered materials where the local failure strengths exhibit extreme scatter. We furthermore demonstrate that, independent of material disorder, the different modes of failure lead to significant differences in fracture surface morphology.

Keywords Fracture · Beam lattice model · Hierarchical microstructure · Avalanche precursors · Crack roughness

1 Introduction

Hierarchical materials consist of microstructural features which have themselves internal (micro)structures, forming self-similar repeating patterns at different scales. Such microstructures are ubiquitous in biological materials (Fratzl and Weinkamer 2007). Collagen, for instance, exhibits a hierarchical modular organization ranging from molecules over microfibrils and fibers to hierarchical fiber bundles. Other examples include the hierarchical structure of bone (Launey et al. 2010) and wood (Fratzl and Weinkamer 2007).

Hierarchical modular organization can serve multiple, even conflicting goals simultaneously: in addition to higher material strength, it ensures enhanced toughness over that of an assembly of isolated collagen molecules (Gautieri et al. 2011), and helps to efficiently distribute loads which improves structural resilience. Despite their hierarchical structure, all natural mate-

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Materials Theory

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From mechanism-based to data-driven approaches in materials science

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Abstract

A time-honored approach in theoretical materials science revolves around the search for basic mechanisms that should incorporate key feature of the phenomenon under investigation. Recent years have witnessed an explosion across areas of science of a data-driven approach fueled by recent advances in machine learning. Here we provide a brief perspective on the strengths and weaknesses of mechanism based and data-driven approaches in the context of the mechanics of materials. We discuss recent literature on dislocation dynamics, atomistic plast city in glasses focusing on the empirical discovery of governing equations through artificial intelligence. We conclude highlighting the main open issues and suggesting possible improvements and future trajectories in the fields.

Keywords: Machine learning, Perspective, Dislocation dynamics, Plasticity in glasses, Equation discovery

Introduction

The common goal of continuum mechanics is to establish the macroscopic response to a stimulus in a given geometry for a certain material. This response can be a simple scalar quantity like a force acting on a cantilever or a fully fledged tensorial constitutive model. Ideally, to develop such macroscopic relationships, one would like to derive the governing equations from first principles starting from a microscopic description under a set of approximations. A well established example is the theory of linear elasticity (Landau and Lifshitz 1986), which can be derived based on general symmetry consideration or even as a large-scale limit of an atomic scale description of a crystal. As soon as one considers applications outside the linear regime like in plasticity, a rigorous approach becomes impossible as the approximation from first principles is neither analytically obvious nor computationally feasible. To deal with this issue, traditionally scientists have attempted to derive models from simple underlying material mechanisms, physical analogies or (semi-)empirical considerations which are then corroborated by fitting the usually limited data that were available. Examples of this general approach are provided by dislocation-based theories (Bulatov and Cai 2006; Bertin et al. 2020), spring-damper visco-elastic models (Macosko 1994; Bird et al. 1987) and the different yield hypothesis' in engineering.

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Article

A Molecular Simulation Approach to Bond Reorganization in Epoxy Resins: From Curing to Deformation and Fracture

Julian Konrad, Robert H. Meißner, Erik Bitzek, and Dirk Zahn*

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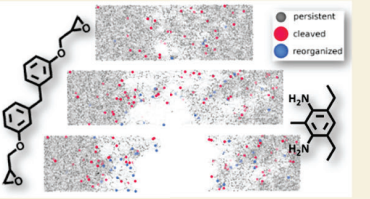
ABSTRACT: We model bond formation and dissociation processes in thermosetting polymer networks from molecular dynamics simulations. For this, a coarsened molecular mechanics model is derived from quantum calculations to provide effective interaction potentials that enable million-atoms scale simulations. The importance of bond (re)organization is demonstrated for (i) simulating epoxy resin formation—for which our approach leads to realistic network models which can now account for degrees of curing up to 98%. Moreover, (ii) we elucidate the competition of bond dissociation and bond reformation during plastic deformation and fracture. On this basis, we rationalize the molecular mechanisms that account for the irreversible nature of damaging epoxy polymers by mechanical load.



KEYWORDS: *epoxy resin, reactive force-field, molecular dynamics, curing fracture, tensile testing*

1. INTRODUCTION

Epoxy resins are widely used polymer materials featuring covalently bonded networks of at least two types of constituents.[1] The enormous industrial relevance of this class of compounds motivated an abundance of experimental studies of curing behavior and mechanical properties.[2−6] On the other hand, only a comparatively smaller number of molecular simulation studies have been performed for a deeper understanding of the underlying mechanisms.[7−16] A key hurdle to the atomic scale modeling of epoxy resins is given by the complexity of its network structure and thus the large and potentially multimillion atom systems required.[17] While practically no ordering is observed beyond the nanometer scale, local (atomic scale) arrangements are far from random and allow for almost 100% matching of bonding partners (experiments[18] indicate curing up to 99%). In the absence of full detail structure identification from crystallography, molecular simulation studies must either rely on "guessed" network structures or elucidate the curing process itself before addressing any characterization of mechanical properties.[14,16,19] The formation of epoxy networks is based on a cascade of linking events each based on bimolecular reactions of the epoxy compound (such as bisphenol A-diglycidylether) and amines used as multinary linker species. While individual linking reactions are thermally induced and in principle reversible, the overall binding network of the thermosetting polymer, however, forms in an irreversible manner. Indeed, with increasing degree of cross-linking, the initially mobile precursors are locked into a permanent network and the system evolves to a stiff epoxy resin. As a consequence, only the onset of thermoset curing is accessible to direct molecular dynamics (MD) or Monte Carlo (MC) simulation, and efficient protocols for assigning suitable binding partners are needed at later stages of network formation.[7,8,16,20,21] Despite ongoing progress, so far molecular simulation models still fall short of achieving the almost 100% degree of cross-linking that is reached in epoxy resins used in industrial applications.[18] The current benchmark of 93% cross-linking was obtained from a combined quantum mechanical/molecular mechanics approach that used smooth topology transfers[7,8] to facilitate network relaxation in the course of linking candidate pairs of reactants.[16] In that study, we focused the computationally demanding quantum calculations on individual linking reactions, while a Monte Carlo simulation type procedure is used to build an energetically favorable polymer network in a stepwise fashion. To this end, detailed balance, that is, the account of possible unlinking steps, could only be implemented for the explicit linking attempt under consideration. This ignores possible bond dissociation and reorganization at later stages of network formation. However, it is intuitive to expect that local corrections of the forming

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Mini review

Assessing the mechanical properties of molecular materials from atomic simulation

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Abstract: We review approaches to deriving mechanical properties from atomic simulations with a special emphasis on temperature-dependent characterization of polymer materials. The complex molecular network of such materials implies only partial, rather local ordering stemming from the entanglement of molecular moieties or covalent bonding of network nodes, whereas the polymer strands between the nodes may undergo nm-scale reorganization during thermal fluctuations. This not only leads to a strong temperature-dependence of the elastic moduli, but also gives rise to visco-elastic behavior that complicates characterization from molecular dynamics simulations. Indeed, tensile-testing approaches need rigorous evaluation of strain-rate dependences, provoking significant computational demands. Likewise, the use of fluctuations observed from unbiased constant-temperature, constant-pressure molecular dynamics simulation is not straight-forward. However, we suggest pre-processing from Fourier-filtering prior to taking Boltzmann-statistics to discriminate elastic-type vibrations of the simulation models for suitable application of linear-response theory.

Keywords: molecular materials; polymers; mechanical properties; molecular dynamics simulations

1. Introduction

For crystalline materials, the prediction of elastic properties became a routine task that usually relies on energy minimization to get equilibrium structures, followed by (numerical) assessment of the second derivatives of energy upon simulation cell deformation [1–3]. While this approach leads to elastic moduli of quite reasonable accuracy when characterizing metals and ionic crystals, molecular materials—in particular if they are not crystalline—show strong, and often non-linear,

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ORIGINAL PAPER

Enhanced computational homogenization techniques for modelling size effects in polymer composites

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Abstract
Several experimental investigations corroborate nanosized inclusions as being much more efficient reinforcements for strengthening polymers as compared to their microsized counterparts. The inadequacy of the standard first-order computational homogenization scheme, by virtue of lack of the requisite length scale to model such size effects, necessitates enhancements to the standard scheme. In this work, a thorough assessment of one such extension based on the idea of *interface energetics* is conducted. Systematic numerical experimentation and analysis demonstrate the limitation of the aforementioned approach in modeling mechanical behavior of composite materials where the filler material is much stiffer than the matrix. An alternative approach based on the idea of *continuously graded interphases* is introduced. Comprehensive evaluation of this technique by means of representative numerical examples reveals it to be the appropriate one for modeling nano-composite materials with different filler-matrix stiffness combinations.

Keywords Size Effect · Nano-Composite · Interface · Interphase · Computational Homogenization

1 Introduction

Incorporation of a secondary phase in the form of fibers or particles for the purpose of improving structural properties of polymers has been in practice for almost a century now. A daily life engineering application exemplifying this fact is the use of carbon black toughened rubbers in automobile tires. Glass-fiber-reinforced plastics, probably one of the most widely used polymer composites, present another classical instance. Furthermore, polymer composites, particulate composites in particular, find their usage in a variety of application fields ranging from aircraft structural components to biocompatible implants. See [31] and the references therein for a survey on applications of particulate composites.

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A crucial development in the domain of polymer composites has been the inclusion of nanosized filler particles instead of the commonly adopted microsized reinforcements. This has lead to the development of the very exciting and challenging field of nano-composites. One of the principal factors for the recent prevalence of nanosized inclusions over the conventional microsized ones, as demonstrated by experimental studies [5,6,9,11,43], is their better structural reinforcement capability. Nanosized filler particles when well dispersed within the polymer matrix, are much more effective at improving the mechanical performance of the base polymer. In [11], specimens based on alumina-particle-reinforced vinyl ester resin, over an exhaustive range of particles diameters, ranging from 70 μm down to 15 nm, where subjected to uni-axial tensile testing. The effective elastic modulus of the composite material was found to increase significantly as the size of the filler particles decreased from the μm range to the nm range. Similar observations w.r.t the macroscopic elastic and viscoelastic properties were made in [5,6], where nano-composites comprising of silica particles, with particle sizes ranging from 500 nm down to 15 nm, embedded in a poly methyl methacrylate matrix were tested. Some of the other morphological factors influencing the overall properties of a composite include the degree of interfacial adhesion between the particles and the matrix material, and the shape

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An Exact Algorithm to Detect the Percolation Transition in Molecular Dynamics Simulations of Cross-Linking Polymer Networks

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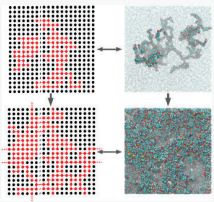
ABSTRACT: Periodic molecular dynamics simulations are developing to a routine tool for the investigation of complex, polymeric materials. A typical application is the simulation of the curing reaction of covalently cross-linked polymers, which provides detailed understanding of network formation at the molecular scale, with examples including gelation and glass transitions. In this article, we delineate the connection between percolation theory and gel-point detection in periodic polymeric networks. Specifically, we present an algorithm that can detect the onset of percolation during cross-linking of polymers in periodic molecular dynamic simulations. A sample implementation is provided at https://github.com/puls-group/percolation-analyzer. As an example, we apply the algorithm to simulations of an epoxy resin undergoing curing with an amine hardener. We also compare results with indirect gel point measurements obtained from monitoring the growth of the largest mass and the onset of secondary cycles.



INTRODUCTION

In recent years, the technological importance of cross-linked thermoset materials has been growing, with examples including low-cure-temperature composites for the aerospace industry,[1] molecularly imprinted polymers,[2] rubbery ion electronic components,[3] and drug delivery hydrogels.[4] The synthesis of a covalently cross-linked thermoset polymer affords the so-called curing reaction, which includes a very specific reaction extent known as the gel point. This is typically characterized by sharp changes in both soluble fraction and viscosity,[5−7] caused by the transition from a viscous liquid of single molecular entities to an insoluble covalently cross-linked solid. Recently, the available experimental methods to analyze this transition have been extensively reviewed.[8] The importance of gelation for several industrial processes is also well-known.[9] For example, many molding techniques for composite materials rely on the injection of liquid precursors; since the shape of the composite is irreversibly set after the occurrence of gelation, knowledge of the time window preceding the gel point is essential. Other manufacturing processes for which gelation is highly relevant include foaming, the design of self-repairing materials, and 3D printing. From a microscopic point of view, the Flory−Stockmayer[10,11] theory of polymer growth explains the gel transition by the appearance of a gel-like molecule of macroscopic extent, which spans the whole volume of the mixture and whose mass can be measured in macroscopic units, thus looking "infinite" from the monomer-weight scale.[5]

Lately, Molecular Dynamics (MD) simulations have proven to be an effective tool to investigate the curing reaction for thermoset polymers, paving the way for a more detailed understanding of the gelation process at the molecular level. In MD simulations, gelation is typically determined indirectly by seeking a sharp change in some physical or structural properties of the polymerizing system, which is supposed to signal the appearance of a volume-spanning, mass-dominant macromolecule. Thus, a common indirect mass-based measurement consists of determining the point at which the heaviest molecular group starts to significantly outweigh its runner-up. To this end, both a visual estimate[12] and the point of inflection of the largest-mass buildup[13] have been employed. A more analytical mass-based criterion is represented by the reduced molecular weight (RMW), which is defined as the molecular weight average of all the molecules in the system, except the largest one. The RMW rises until the largest group begins to predominate, after which it declines. On these grounds, its maximum point has been used to measure gelation.[14,15]

From a more structural point of view, the gel-like molecular group naturally englobes most of the still unreacted functionalities present in the system, thus marking the rise of intramolecular reactions (also known as secondary cycles). As a consequence, the inception of intramolecular polymerization is the other common indirect property employed for gel point detection.[16]

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Tunable Photoswitching in Norbornadiene (NBD)/Quadricyclane (QC) – Fullerene Hybrids

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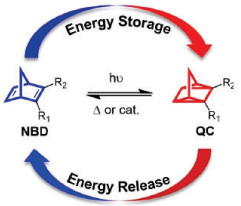
In memoriam of Prof. Michael Hanack.

Abstract: With respect to molecular switches, initializing the quadricyclane (QC) to norbornadiene (NBD) back-reaction by light is highly desirable. Our previous publication provided a unique solution for this purpose by utilizing covalently bound C_{60}. In this work, the fundamental processes within these hybrids has been investigated. Variation of the linker unit connecting the NBD/QC moiety with the fullerene core is used as a tool to tune the properties of the resulting hybrids. Utilizing the Prato reaction, two unprecedented NBD/QC – fullerene hybrids having a long-rigid and a short-rigid linker were synthesized. Molecular dynamics simulations revealed that this results in an average QC–C_{60} distance of up to 14.2 Å. By comparing the NBD–QC switching of these derivatives with the already established one having a flexible linker, valuable mechanistic insights were gained. Most importantly, spatial convergence of the QC moiety and the fullerene core is inevitable for an efficient back-reaction.

Introduction

The norbornadiene (NBD) – quadricyclane (QC) interconversion couple is a promising concept for the efficient realization of molecular solar thermal (MOST) energy storage systems.[1] In the course of the corresponding rearrangement, NBD undergoes a light-induced intramolecular cycloaddition to form its highly strained metastable isomer QC. During this process, energy is stored as strain energy in chemical bonds.[2] Upon demand this energy can be released as thermal energy (Scheme 1).[3]

Usually, this back-reaction from QC to NBD can be promoted thermally or catalytically. In addition, significant progress has been made lately in the electrochemically triggered energy release.[4] For a practical implementation of the NBD/QC system into a MOST device, a catalytic energy release is most suitable.[5] Therefore, considerable effort has been devoted to design efficient catalysts for this reaction.[6]



Scheme 1. The norbornadiene (NBD) – quadricyclane (QC) interconversion system. Introducing an electron donating group (EDG) and an electron withdrawing group (EWG) in the R_1/R_2 position gives push-pull substituted NBD/QC derivatives.

Next to these established methods there is another one that has not received much attention yet, but brings in the exciting opportunity of selective photoswitching in both directions.[7] In this particular case, the isomerization of QC to NBD is also induced by light. Such a light-only control is rather rare and in the recent literature only few examples have been reported.

For the application in MOST systems, this type of back-reaction may play a minor role, but it opens up completely new perspectives for the NBD/QC system in the field of molecular switches and information storage. Among these examples, our earlier publication on NBD/QC – fullerene hybrids stands out as the only example where light of a longer wavelength, than the one used for the isomerization of NBD to QC, can be used to promote the back-reaction (Scheme 2).[7a] This discovery encouraged us to investigate these hybrids as well as the underlying

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International Journal of Mechanical Sciences
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A coupled MD-FE methodology to characterize mechanical interphases in polymeric nanocomposites

Maximilian Ries, Gunnar Possart, Paul Steinmann, Sebastian Pfaller

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https://doi.org/10.1016/j.ijmecsci.2021.106564

Abstract

This contribution introduces an unconventional procedure to characterize spatial profiles of elastic and inelastic properties inside polymer interphases around nanoparticles. Interphases denote those regions in the polymer matrix whose mechanical properties are influenced by the filler surfaces and thus deviate from the bulk properties. They are of particular relevance in case of nano-sized filler particles with a comparatively large surface-to-volume ratio and hence can explain the frequent observation that the overall properties of polymer nanocomposites cannot be determined by classical mixing rules, which only consider the behavior of the individual constituents.

Interphase characterization for nanocomposites poses hardly solvable challenges to the experimenter and is still an unsolved problem in many cases. Instead of real experiments, we perform pseudo experiments using our recently developed Capriccio method, which is an MD-FE domain-decomposition tool specifically designed for amorphous polymers. These pseudo-experimental data then serve as input for a typical inverse parameter identification. With this procedure, spatially varying mechanical properties inside the polymer are, for the first time, translated into intuitively understandable profiles of continuum mechanical parameters.

As a model material, we employ silica-enforced polystyrene, for which our procedure reveals exponential saturation profiles for Young's modulus and the yield stress inside the interphase, where the former takes about seven times the bulk value at the particle surface and the latter roughly triples. Interestingly, hardening coefficient and Poisson's ratio of the polymer remain nearly constant inside the interphase. Besides gaining insight into the constitutive influence of filler particles, these unexpected and intriguing results also offer interesting explanatory options for the failure behavior of polymer nanocomposites.

Research Article

Bone fracture healing within a continuum bone remodelling framework

Ina Schmidt, Jacob Albert, Marina Ritthaler, Areti Papastavrou & Paul Steinmann

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Abstract

Bone fracture healing is a complex process which is still under research. Computer-aided patient-specific prediction of bone development, fracture risk, prevention and treatment approaches promises a significant milestone in clinical practice. With this long-term goal in mind, a novel model is presented and examined in this work in the context of continuum bone remodelling. Therein, a clear distinction is made between external mechanical stimulation and the biological healing process of an injured bone tissue. The model is implemented within a finite element framework and investigated for the example of a fractured proximal femur head. The results show promising perspectives for further application. Besides, the model offers the possibility of easily integrating other factors like age-dependency and the availability of nutrition. For the future, further studies with large clinical datasets are essential for validation.

Keywords: Bone remodelling | healing | bone fracture | femur head | finite element method

Concurrent consideration of cortical and cancellous bone within continuum bone remodelling

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ABSTRACT

Continuum bone remodelling is an important tool for predicting the effects of mechanical stimuli on bone density evolution. While the modelling of only cancellous bone is considered in many studies based on continuum bone remodelling, this work presents an approach of modelling also cortical bone and the interaction of both bone types. The distinction between bone types is made by introducing an initial volume fraction. A simple point-wise example is used to study the behaviour of novel model options, as well as a proximal femur example, where the interaction of both bone types is demonstrated using initial density distributions. The results of the proposed model options indicate that the consideration of cortical bone remarkably charges the density evolution of cancellous bone, and should therefore not be neglected.

KEYWORDS

bone remodelling; cortical bone; cancellous bone; density change; finite element method

1. Introduction

Tubular bone is characterised by cortical bone surrounding the bone marrow in the shaft and the cancellous bone at the proximal and distal ends. Due to its special microstructure composed of beams and plates (trabeculae), cancellous bone is also denoted as spongy bone. Depending on environmental changes, such as mechanical loading, bone can adapt its internal microstructure by altering the density and trabecular orientation. Remodelling of cancellous bone was first formulated by (Wolff 1892) and is referred to as Wolff's law of bone remodelling. Based on continuum mechanics and the finite element method, simulation approaches to bone remodelling were developed, see (Cowin and Hegedus 1976), (Huiskes et al. 1987), (Weinans et al. 1992), (Harrigan and Hamilton 1993), (Jacobs et al. 1995) and many more. Most of these studies address exclusively the adaptation of cancellous bone. Even if the focus is also on the adaptation of cortical bone, it is typically considered separately from spongy bone, see (Carter and Beaupré 2010). One of the few approaches involving the interaction of both bone types was investigated by (Hambli 2014) and (Barkaoui et al. 2019) based on the cellular activities of bone. Another proposal was developed by (Nutu 2018) based on the model of (Huiskes et al. 1987) for dental implants.

This work aims to simulate bone density changes of cancellous and cortical bone as

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Material optimization to enhance delamination resistance of composite structures using viscous regularization

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Abstract

Advances in the computational modeling of fracture of solids have opened up new possibilities for structural design optimization to enhance fracture properties. Here, we investigate material optimization and design to improve fracture behavior of composite structures under quasi-static conditions. The rate-independent structural problem considering cohesive fracture is ill-posed in its original form due to the non-unique nature of the solution. This renders the use of gradient-based optimization algorithms problematic. To overcome this issue, we introduce viscous regularization and a local approximation of the cohesive law into the governing state equations, and study the impact with the help of interfacial fracture of composite structures consisting of two or more materials. The fracture problem is then integrated into a material optimization framework. We study the effect of viscous regularization on the global landscape of the proposed objective function using a 2-dimensional delamination example with one design parameter and discuss difficulties resulting from the stabilization of inherently unstable crack states. In view of these issues, we finally propose considering multiple state problems, each limited to a single crack, with different predefined crack paths. In the end, we optimize the orientations of orthotropic inclusions embedded in a double-cantilever beam for the worst case of the potential crack paths.

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Atomistic two-, three- and four-body potentials. Spatial and material settings

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A B S T R A C T

In molecular dynamics or molecular statics (MD/MS) multi-body potentials empirically capture the energetic interactions in atomistic systems enabling the computation of the corresponding atomistic forces as energetic conjugates to the atomistic positions. We distinguish here between spatial and material atomistic positions and consequently between the corresponding spatial and material atomistic forces. In quasi-statics, i.e. MS, the former, also denoted as *deformational* atomistic forces, contribute to the classical deformational mechanics (i.e., equilibrium) problem that seeks to minimise the total potential energy of an atomistic system with respect to the atomistic positions relative to the ambient space. The latter, also denoted as *configurational* atomistic forces, contribute to the configurational mechanics (i.e., non-equilibrium) problem that determines the release of total potential energy of an atomistic system upon variation of the atomistic positions relative to the ambient material, i.e., due to perturbations of the material (initial) atomistic configuration. The importance of material atomistic forces is that they drive energetically favourable re-organisations of the material atomistic configuration, thereby characterising the tendency of generic atomistic defects to propagate. In this contribution we focus on two-, three-, and four-body potentials, whereby we distinguish between novel stretch- and classical angle-based potentials for the two latter cases. Taken together, as the main contribution, we derive expressions for the corresponding spatial and, for the first time, material atomistic forces and highlight their striking formal similarity. The derivations are detailed but the final expression compact and well-suited for numerical implementation.

1. Introduction

When modelling the energetic interactions in atomistic systems by molecular dynamics or molecular statics (MD/MS), multi-body potentials are a valid option to empirically approximate the complex energy landscape that is dictated by the underlying quantum mechanics. Most prominent of the numerous options for two-body potentials are the Buckingham and Lennard-Jones (1938) and the Lennard-Jones (1924a,b, 1925) potentials, which only account for the distance between atomistic *pairs*. Well-known among higher-order models is the Stillinger–Weber potential (Stillinger and Weber, 1985) which combines two- and three-body terms. A further typical example of a three-body potential is due to Tersoff (1988), which is a prominent member of the class of bond-order potentials that are motivated by the tight-binding approximation, see Albe et al. (2002). The Tersoff potential parameterises the atomistic energy by the distance between atomistic pairs and, in addition, includes atomistic *triplets* through the coefficients of a two-body term. Another common choice of a multi-body potential is the Embedded Atom potential (Daw and Baskes, 1984), which besides the distance between atomistic pairs accounts also for the embedding electron charge density of neighbouring atoms. Many approaches that rely on simple harmonic potentials to describe atomistic interactions are complemented by three-body terms parameterising the energetics of fluctuations around an average angle between atomistic triplets, typically based on a simple harmonic approximation. Furthermore, force fields, see e.g., Brooks et al. (1983) and Cornell et al. (1995) are complemented by four-body terms incorporating

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General relation between stacking order and Chern index: A topological map of minimally twisted bilayer graphene

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We derive a general relation between the stacking vector $\mathbf{u}$ describing the relative shift of two layers of bilayer graphene and the Chern index. We find $C = \nu(1 - \mathrm{sign}(|V_{\mathrm{AB}}| - |V_{\mathrm{BA}}|))$, where ν is a valley index and $|V_{\alpha\beta}|$ the absolute value of the $\mathbf{u}$ dependent stacking potentials that uniquely determine the interlayer interaction; AA stacking plays no role in the topological character. With this expression we show that while ideal and relaxed minimally twisted bilayer graphene appear so distinct as to be almost different materials, their Chern index maps are, remarkably, identical. The topological physics of this material is thus strongly robust to lattice relaxations.

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I. INTRODUCTION

Ideal and atomically relaxed twist bilayer graphene becomes, in the small angle regime, essentially different materials [1–5]. While the ideal lattice geometry is that of a moiré, for $\theta < 1°$ the material relaxes ("reconstructs" [3]) into domains of AB and BA stacking bounded by pure screw partial dislocations [6,7]. However, the remarkable electronic properties of the graphene twist bilayer have predominately been established for the ideal geometry [8–14], and a natural question is therefore how the rich electronic physics of the graphene moiré is impacted by the profound lattice relaxation that occurs at small angles [5,15–19].

AB and BA stacked bilayer graphene have different valley Chern numbers, generating a pair of topologically protected states with valley momentum locking at the domain walls of regions of AB and BA stacking. In the ordered network of AB and BA domains that constitute minimally twisted bilayer graphene these one-dimensional states lead to a "helical network" of valley-momentum locked states [20,21] and a remarkable electrically controllable and complete nesting of the Fermi surface [22], with a correspondingly rich magnetotransport that is only beginning to be explored [19,21]. In this paper we will ask the inverse question to that posed above: Can such a network of one-dimensional states be found in the moiré as well as the dislocation network?

Intuitively this may appear unlikely as while the partial dislocation network consists of a mosaic of well defined AB and BA tiles, the ideal moiré geometry does not possess such a bulk/boundary structure. However, as boundary states arise from the change in valley Chern number the possibility exists that, for sufficiently slow stacking modulation, such states exist in the ideal twist geometry through the dependence of the local valley Chern number on the local stacking vector. Remarkably, as we show here, the moiré and the partial dislocation network have essentially identical topological character, in the sense that the spatial dependence of the valley Chern number is indistinguishable between these two systems. This represents an example of a property of the twist bilayer fully robust to lattice relaxation and suggests (i) that the helical network will survive at twist angles when the relaxation to a dislocation network is incomplete and (ii) that in Dirac-Weyl materials for which the energetic balance of in-plane strain and interlayer stacking energy may not favor reconstruction to a dislocation network, the physics of the "helical network" may nevertheless be found.

Our approach will be to generalize the widely known fact that AB and BA stacked bilayer graphene have different valley Chern numbers to a statement concerning an arbitrary stacking vector and the corresponding Chern index. Employing the fact that, under quite general assumptions, the interlayer interaction in bilayer graphene can be represented by three unique "stacking potentials" (corresponding to the three high symmetry stacking types of AB, BA, and AA stacking), we demonstrate that the valley Chern index C depends only on the sign of the difference of the AB and BA potentials as

$$C = \nu - \nu\,\mathrm{sign}(|V_{\mathrm{AB}}| - |V_{\mathrm{BA}}|) \tag{1}$$

with $\nu = \pm 1$ an index labeling the conjugate K valleys. An intervening metallic state is required at a topological phase transition, and we show that the stacking phase diagram of bilayer graphene contains "permanent metal lines" at which the system remains metallic for arbitrary interlayer bias, and that these lines exactly correspond to the stacking vectors at which the valley Chern index changes (Sec. IV). We then numerically investigate the veracity of Eq. (1) through a

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A viscoelastic-viscoplastic constitutive model for glassy polymers informed by molecular dynamics simulations

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Highlights

- A novel VE-VP constitutive model for glassy polymers is calibrated by MD simulations.
- Different contributions to inelasticity in polymers are isolated in MD simulations.
- An interpretation of the physics behind the constitutive model is provided.
- The constitutive model is appropriate for the FE parts of MD-FE coupling simulations.

Abstract

This contribution presents a phenomenological viscoelastic-viscoplastic constitutive model informed by coarse-grained (CG) molecular dynamics (MD) simulations of pure glassy polystyrene (PS). In contrast to experiments, where viscoplasticity is caused by various effects simultaneously, these effects can be decomposed in MD simulations by adjusting the MD system. In the MD simulations considered here, neither bond breakage nor cross-links are introduced; instead, we focus on the intermolecular interaction of polymer chains. We employ a thermo-dynamically consistent generalized Maxwell framework parallelly comprising an elastic, a viscoelastic, and several elasto-viscoplastic modules with different yield stress to capture the viscoelastic and the viscoplastic mechanical behavior simultaneously. The yield stresses decrease with the maximum deformation the MD system has experienced. The constitutive model presented here is based on 10 material parameters, which can be identified by a few data sets and fits well the CG MD simulations of PS under uniaxial and biaxial deformation with time-proportional and cyclic loading conditions in a wide range of strain rates (0.1%/ns–20%/ns).

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RESEARCH ARTICLE

WILEY

A particle-continuum coupling method for multiscale simulations of viscoelastic–viscoplastic amorphous glassy polymers

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Abstract

In this contribution, we present a partitioned-domain method coupling a particle domain and a continuum domain for multiscale simulations of *inelastic amorphous* polymers under isothermal conditions. In the continuum domain, a viscoelastic–viscoplastic constitutive model calibrated from previous molecular dynamics (MD) simulations is employed to capture the inelastic properties of the polymer. Due to the material's rate-dependence, a temporal coupling scheme is introduced. The influence of the time-related parameters on the computational cost and accuracy is discussed. With appropriate parameters, multiscale simulations of glassy polystyrene under various loading conditions are implemented to showcase the method's capabilities to capture the mechanical behavior of polymers with different strain rates and with non-affine deformations of the MD domain.

KEYWORDS

inelasticity, multiscale simulation, particle-continuum coupling, partitioned-domain method, temporal coupling, thermoplastic polymers

1 | INTRODUCTION

Polymers show complex mechanical behavior due to their amorphous structure of long chains with entanglements or cross-links. To understand the mechanism behind it, treatments at the atomistic or molecular level are well-suited. In this regard, molecular dynamics (MD) simulations have become powerful tools for studying polymers, which are, for example, able to investigate the structural, dynamic, and geometric effects of the interphase in polymer nanocomposites (PNCs)[1-4] as well as the fracture of PNCs.[5,6] However, such fine-scale methods have two main restrictions: (i) the limitation of system sizes within the current computational capability and (ii) difficulties in applying macroscale boundary conditions to the MD systems. To overcome these, multiscale methods coupling MD simulations with continuum mechanics can play an important role.

Although various particle-continuum coupling approaches have been proposed in the past decades, few of them are appropriate for simulations of amorphous polymers, particularly for thermoplastics with viscoelastic or viscoplastic mechanical behavior. Following a classification of Tadmor and Miller,[7] these coupling methods can be subdivided into *hierarchical* and *partitioned-domain* methods. The former derives the current constitutive relation of the macroscale

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Combined continuum mechanics and molecular dynamics approach for uniaxial deformation of a thermoplastic polymer

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A hybrid molecular dynamics (MD)-continuum mechanics (CM) method for calculating a molecular system of an amorphous polymer under uniaxial tensile load was developed. In this contribution, the operating principle of this method is introduced and applied to a sample system. Furthermore, the practicability of the hybrid MD-CM approach is examined.

1 Introduction

Polymer materials are nowadays widely used in various fields of application, especially because of the ability of tuning the material properties to particular needs. As important mechanisms are inherent to the molecular scales that cannot be covered by continuum approaches whereas particle-based methods cannot approach engineering scales, multiscale methods offer great potential for investigating polymer behaviour across the scales. In [1], Pfaller et al. developed a novel partitioned-domain method adjusted to thermoplastic materials, coupling a continuum with a particle-based region. Our long-term research aims to investigate polymer fracture in multiscale fracture simulations. Thereto, the Capriccio method will be extended to adaptively moving particle-based regions within the continuum according to the ongoing deformation. A peculiarity arising is the correlation between the deformation of the continuum and the particle movements in the polymer bulk, which cannot be straightforwardly specified due to the amorphous structure of thermoplastics. As a first step, we introduce a hybrid method which combines the continuum mechanical with the particle-based deformation. There, we simulate the stress-strain behaviour of the polymer at the molecular level without using the total CPU time of a purely MD simulation.

2 Hybrid molecular dynamics-continuum mechanics method

To investigate the stress-strain behaviour of the polymer system, uniaxial tensile tests were performed using molecular dynamics. As the initial polymer system, atactic polystyrene (PS) in coarse grained resolution according to [2] was chosen to provide a sufficiently large number of polymer chains and relatively small CPU times. The molecular system considered consists of 300 PS chains with a chain length of 200 superatoms each. All calculations were carried out under periodic boundary conditions using the molecular dynamics code LAMMPS [3].

For the reference MD system, the deformation is applied by deforming the MD simulation box in tensile direction ii by a strain ε_{ii} with a constant strain rate $\dot{\varepsilon}_{ii} = \text{const}$ (Fig. 1a), whereby the particles are free to equilibrate according to the potentials employed here. As a measure of stress, the Cauchy stress is derived by $\boldsymbol{\sigma}(t) = -[\mathbf{p}(t) - p_{\text{atm}}\mathbf{1}]$ with the global pressure tensor $\mathbf{p}$ and unit tensor $\mathbf{1}$.

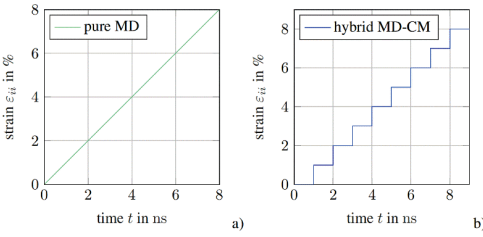

Fig. 1 **a** strain ε_{ii} applied to the reference MD system **b** stepwise applied strain in predefined load steps $\varepsilon_{ii}^{\text{ls}}$ in the hybrid MD-CM method

In the hybrid MD-CM method, the uniaxial tensile load is applied in load steps with a predefined load step size $\varepsilon_{ii}^{\text{ls}}$, cf. Fig. 1b. Each load step is triggered by displacing the superatoms according to a continuous displacement field $\mathbf{u}(\mathbf{R}_I, t) =$

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Size Effects in Computational Homogenization of Polymer Nano-Composites

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Nano-particles, as compared to micro-sized inclusions, result in a much better improvement to the mechanical properties of otherwise brittle polymers. Standard first-order computational homogenization lacks the length scale necessary to capture this size effect. In this work, a computational homogenization scheme enhanced with *interface energetics* is considered and its applicability to polymer nano-composites with different types of filler particles is assessed through systematic numerical experimentation. The study reveals that the method performs quantitatively much better in the case of softer inclusions as compared to the case where the inclusions are much stiffer than the matrix material, which happens in the case of silica nano-particles.

1 Introduction

Experimental evidence reveals nano-sized reinforcements to be more effective than micro-sized filler particles in terms of their ability to improve the mechanical behavior of otherwise brittle polymers [1]. The formation of an interphase layer around the filler particle, which is prominent in the case of nano-particles due to their much higher specific surface area (SSA), has drastic effects on the overall properties of the composite material [2]. Standard continuum-mechanics-based models, due to the absence of a necessary length scale, cannot capture this *size effect* and thus appropriate enhancements are needed.

In this work, we consider a modification of the standard first-order computational homogenization scheme, wherein the interface between the matrix and the filler materials is equipped with its own energetic structure. The next section summarizes the overall working principle of the approach. A detailed mathematical exposition on the topic of *interface energetics* and its application to homogenization can be found in [3, 4] and the references therein.

2 Interface-Energetics-Enhanced Computational Homogenization (IECH)

The fundamental idea of this approach is based on the concept of *lower dimensional energetics*. Herein, similar to the bulk, lower dimensional physical entities, such as interfaces between two materials, are equipped with their own specific strain energies [3]. Furthermore, the kinematic quantities (denoted as $\{\overline{\bullet}\}$) at any point on the interface are obtained through projection of their bulk counterparts (denoted as $\{\bullet\}$) by means of a second-order projection tensor given by $\overline{\mathbf{I}} = \mathbf{I} - \mathbf{N} \otimes \mathbf{N}$, where $\mathbf{N}$ denotes the unit normal to the interface in material configuration (see Figure 1) and $\mathbf{I}$ is the second-order unit tensor. Neglecting the body forces, the balances of linear momentum including contributions from the bulk $\mathcal{B}_0$ and the interface $\mathcal{I}_0$ are given as

$$\begin{aligned} \operatorname{Div} \mathbf{P} = \mathbf{0} \quad & \text{in } \mathcal{B}_0, \\ \overline{\operatorname{Div}}\, \overline{\mathbf{P}} + [\![\mathbf{P}]\!] \cdot \mathbf{N} = \mathbf{0} \quad & \text{on } \mathcal{I}_0, \end{aligned} \tag{1}$$

with the assumption that the interface is elastic, i.e. $[\![\varphi]\!] = \mathbf{0}, [\![\mathbf{P}]\!] \cdot \mathbf{N} \neq \mathbf{0}$. Here, $\mathbf{P}$ and $\overline{\mathbf{P}}$ represent the Piola stress for the bulk and the interface, respectively.

The inclusion of interface energetics in the computational homogenization scheme leads to an extended Hill-Mandel condition, and, consequently, the macroscopic Piola stress $\mathbf{P}^{\mathrm{M}}$ is computed as [4]

$$\mathbf{P}^{\mathrm{M}} = \frac{1}{|\mathcal{B}_0|} \left[\int_{\mathcal{B}_0} \mathbf{P}\, \mathrm{dV} + \int_{\mathcal{I}_0} \overline{\mathbf{P}}\, \mathrm{dA} \right] = \frac{1}{|\mathcal{B}_0|} \int_{\mathcal{B}_0} \mathbf{P}\, \mathrm{dV} + \underbrace{\frac{|\mathcal{I}_0|}{|\mathcal{B}_0|}}_{=:\frac{1}{S_l}} \frac{1}{|\mathcal{I}_0|} \int_{\mathcal{I}_0} \overline{\mathbf{P}}\, \mathrm{dA} = < \mathbf{P} >_{\mathcal{B}_0} + \frac{1}{S_l} < \overline{\mathbf{P}} >_{\mathcal{I}_0} \tag{2}$$

where $|\mathcal{B}_0|$ and $|\mathcal{I}_0|$ represent the volume of the RVE and the surface area of the interface, respectively. Thus, this approach includes the length scale S_l which allows us capture the size effect as explained below with the help of numerical examples.

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Recent advances and challenges in interfacial MD-FE coupling for amorphous polymers

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Keywords: atomistic-continuum coupling, amorphous polymer, concurrent multiscale simulation.

Summary: *Polymers are a highly versatile class of materials that can exhibit remarkable properties, especially in combination with nano-sized filler particles. However, the extremely small length scales pose major problems for the experimental investigation of the complex matrix-filler interactions. Instead, numerical methods can be used, of which multiscale approaches are particularly noteworthy since they, i.a., exploit the accuracy of particle-based methods while maintaining the efficiency of continuum mechanics. The complexity of these approaches lies in the design of the scale coupling that has to avoid coupling artifacts that might distort the results while being computationally efficient. In this contribution, we introduce an MD-FE coupling via an interface for amorphous polymers. The approach relies on padding atoms as particle representations of the continuum enabling interactions with the actual particles. We evaluate the new coupling scheme with a toy system of amorphous polystyrene and carefully discuss the system's behavior during an MD-FE equilibration run. We observe considerable oscillations of our sample system, which we attribute to a combination of the rigid coupling condition and insufficient force correction. Our results indicate that an interfacial coupling scheme cannot capture the dynamic behavior of amorphous polymers and emphasizes the need for an interphase-based coupling.*

14th World Congress on Computational Mechanics (WCCM)
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F. Chinesta, R. Abgrall, O. Allix and M. Kaliske (Eds)

THE HYBRID CAPRICCIO METHOD: A 1D STUDY FOR FURTHER ADVANCEMENT

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Key words: particle-continuum coupling, domain decomposition, multiscale-modeling

Abstract. Polymers and, in particular, polymer composites are known for the enormous adjustability of their mechanical, chemical, and thermal behavior. Multiscale methods are increasingly employed to unravel the polymer microstructure's impact on the material properties. These methods combine the accuracy of particle based techniques with the efficiency of continuum mechanical approaches. Amorphous polymers pose a special challenge since their microstructure does not continue periodically, and therefore special attention needs to be paid to the particle domain boundary.

In this study, we introduce a coupling via an interface between the continuum and the particle domain. Padding atoms as particle representations of the continuum, which serve as interaction partners for the atoms in the particle region, allow for the transfer of displacements and forces between the domains. We present a straightforward 1D example with simple interactions, evaluate the scheme's performance, discuss the resulting energy contributions, and identify an optimal set of coupling parameters. Eventually, this forms the basis for future 3D implementations.

1 INTRODUCTION

Polymers are an outstanding material since they are typically inexpensive, lightweight, and versatile. In particular, they can be adapted to numerous applications' requirements, e.g., by adding fillers. Particle-based numerical methods are often used to support the development of such composites. However, the enormous computational effort required to investigate sufficiently large samples limits their use substantially. Therefore, multiscale approaches are employed in many cases, using the accuracy of particle-based methods only where necessary and relying on a coarser description in the remaining regions. Recently, Zhao et al. [1] have introduced a continuum mechanical constitutive law that is capable of reproducing the mechanical behavior of polymers obtained from molecular dynamics simulations [2, 3].

A particle-continuum coupling has been realized for crystalline materials most prominently with the Quasicontinuum method [4, 5], the Arlequin method [6, 7] or the Bridging Domain method [8, 9]. Tad-

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MULTISCALE FE-MD COUPLING: INFLUENCE OF THE CHAIN LENGTH ON THE MECHANICAL BEHAVIOR OF COARSE-GRAINED POLYSTYRENE

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Key words: coarse graining, multiscale-modeling, mechanical behavior, molecular dynamics

Abstract. Polymers have become increasingly essential to cope with modern engineering challenges. To better understand their microstructure's influence, multi-scale approaches that couple molecular dynamics and continuum mechanics are emerging progressively. However, these simulation techniques require detailed knowledge of the material behavior, which is commonly derived from molecular dynamics simulations. Reducing the degrees of freedom by coarse graining enables the investigation of sufficiently large samples and thus we focus on coarse-grained (CG) polystyrene as a model material.

The goal of this contribution is two-fold: Firstly, we identify the minimum sample size necessary to analyze the mechanical properties. Secondly, we quantify the influence of chain length on the material behavior of polystyrene. To this end, we investigate density, end-to-end distance, stress-strain behavior, Young's modulus, and Poisson's ratio. In conclusion, we were able to verify that we can use significantly smaller samples for our investigations without affecting their structure or mechanical behavior. The chain length has a drastic influence on the mechanical properties, with a loss of stiffness in the range of 15 % for very short-chain specimens.

1 INTRODUCTION

Amorphous polymers, e.g., polystyrene, are used in various applications, but there are still aspects of their mechanical behavior that we do not understand well from an engineering perspective. Phenomena such as the fracture of polymers or polymer composites require a profound knowledge of the underly-

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Material optimization for controlling interfacial damage in composite structures

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Advances in the computational modeling of fracture in solid structures have opened up possibilities for structural design optimization. The rate-independent structural problem considering damage in its original form is ill-posed due to the non-unique nature of the solution, that poses difficulty in using gradient-based algorithms for material optimization. To overcome this issue, this work introduces a viscosity parameter in the governing state equations and, thus renders the structural problem well-posed. Material interfaces are modeled using an exponential, initially-elastic cohesive law and linear elasticity is assumed throughout the structural domain. The time-dependent fracture problem is solved via incremental variational approach with finite element discretization of the displacement field. Finally, the effectiveness of the method is illustrated by a material optimization example using a smooth gradient-based solver with first-order material sensitivities.

1 Cohesive zone model for interface damage

A solid, bounded Lipschitz domain $\Omega \subset \mathbb{R}^d, d \in \{2,3\}$, is considered with Dirichlet and Neumann boundaries Γ_{D} and Γ_{N}, respectively. The body is assumed to possess linear elasticity within a homogeneous material subdomain and the tractions $\boldsymbol{\tau} \in C^1(\mathbb{R}^d;\mathbb{R}^d)$ at the material interfaces, denoted by Γ_{C}, are given by an exponential cohesive law [4]. In the strong form, the governing equations are written as

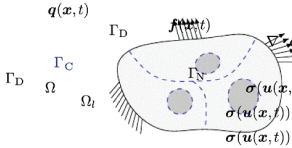

Fig. 1: A composite with material interfaces

$$
\begin{aligned}
\boldsymbol{\sigma}(\boldsymbol{u}(\boldsymbol{x},t)) &= \boldsymbol{0} && \boldsymbol{x} \in \Omega_l, l \in \mathcal{N}_\Omega,\ t \in [0,T], && \text{(1a)}\\
\boldsymbol{u}(\boldsymbol{x},t) &= \boldsymbol{q}(\boldsymbol{x},t) && \boldsymbol{x} \in \Gamma_{\mathrm{D}}, t \in [0,T], && \text{(1b)}\\
\boldsymbol{\sigma}(\boldsymbol{u}(\boldsymbol{x},t)) \cdot \boldsymbol{n}(\boldsymbol{x}) &= \boldsymbol{f}(\boldsymbol{x},t) && \boldsymbol{x} \in \Gamma_{\mathrm{N}},\ t \in [0,T], && \text{(1c)}\\
\boldsymbol{\sigma}(\boldsymbol{u}(\boldsymbol{x},t))^- \cdot \boldsymbol{n}(\boldsymbol{x})^- &= \boldsymbol{\tau}([\![\boldsymbol{u}(\boldsymbol{x},t)]\!]) + \eta\,[\![\dot{\boldsymbol{u}}(\boldsymbol{x},t)]\!] && \boldsymbol{x} \in \Gamma_{\mathrm{C}},\ t \in [0,T], && \text{(1d)}\\
\boldsymbol{\sigma}(\boldsymbol{u}(\boldsymbol{x},t))^+ \cdot \boldsymbol{n}(\boldsymbol{x})^+ &= -\boldsymbol{\tau}([\![\boldsymbol{u}(\boldsymbol{x},t)]\!]) - \eta\,[\![\dot{\boldsymbol{u}}(\boldsymbol{x},t)]\!] && \boldsymbol{x} \in \Gamma_{\mathrm{C}},\ t \in [0,T], && \text{(1e)}\\
\boldsymbol{u}(\boldsymbol{x},0) &= \boldsymbol{u}_0(\boldsymbol{x}) && \boldsymbol{x} \in \Omega, && \text{(1f)}
\end{aligned}
$$

where the symbol $[\![\bullet]\!] = (\bullet)^+ - (\bullet)^-$ represents jump in the displacement field across Γ_{C}. A rate-dependent term with viscosity parameter $\eta > 0$ is added to the interfacial traction to render the solution of the above problem unique. Looking at the limit case $\eta \to 0$, we retrieve a standard formulation of the rate-independent cohesive zone model.

The time-dependent problem can be solved using incremental variational approach. To this end, we discretize the time domain $[0,T]$ with N_T time steps with time-step size $\Delta t^k, k = 1,\dots,N_T$. The velocity is approximated using Implicit-Euler scheme as $\dot{\boldsymbol{u}}(\boldsymbol{x},t^k) \approx {}_{\Delta t^k}[\boldsymbol{u}^k(\boldsymbol{x}) - \boldsymbol{u}^{k-1}(\boldsymbol{x})]$.

To have a computationally efficient and robust scheme for solving the structural problem, we use an approximation of the cohesive tractions $\tilde{\boldsymbol{\tau}}$. Here, we approximate the non-linear terms in the exponential cohesive law [4] with the corresponding values resulting from the previous time step. A similar approach is used in phase-field models of fracture [1,3]. The normal and the tangential components of the cohesive traction are given by

$$\tilde{\tau}_{\mathrm{n}}(\delta_{\mathrm{n}}^k, \delta_{\mathrm{s}}^k, \delta_{\mathrm{n}}^{k-1}, \delta_{\mathrm{s}}^{k-1}) := e\,\delta_{\mathrm{n}}^*\,\frac{\delta_{\mathrm{n}}^k}{\delta_{\mathrm{n}}^*}\exp\!\left(-\frac{\delta_{\mathrm{n}}^k}{\delta_{\mathrm{n}}^*}\right)\left\{1 - q\,\frac{\delta_{\mathrm{n}}^{k-1}}{\delta_{\mathrm{n}}^*}\exp\!\left(-\frac{[\delta_{\mathrm{s}}^{k-1}]^2}{\delta_{\mathrm{s}}^{*2}}\right)\right\} + \zeta(\delta_{\mathrm{n}}^k), \tag{2a}$$

$$\tilde{\tau}_{\mathrm{s}}(\delta_{\mathrm{n}}^k, \delta_{\mathrm{s}}^k, \delta_{\mathrm{n}}^{k-1}, \delta_{\mathrm{s}}^{k-1}) := 2e\,\frac{\delta_{\mathrm{s}}^*}{\delta_{\mathrm{s}}^k}\,\delta_{\mathrm{s}}^k\exp\!\left(\frac{[\delta_{\mathrm{s}}^{k-1}]^2}{\delta_{\mathrm{s}}^{*2}}\right)\left[1 + \frac{\delta_{\mathrm{s}}^{k-1}}{\delta_{\mathrm{n}}^*}\right]\exp\!\left(-\frac{\delta_{\mathrm{n}}^{k-1}}{\delta_{\mathrm{n}}^*}\right), \tag{2b}$$

respectively, with a non-interpenetration penalty term $\zeta \in C^1(\mathbb{R};\mathbb{R})$.

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The Capriccio method: a scale bridging approach for polymers extended towards inelasticity

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In this contribution we present an extension of the multiscale Capriccio method towards inelasticity. This enables coupled simulations of a particle domain embedded into a continuum with particular focus on polymer systems. Starting from the method's initial implementation of pure elasticity, we substitute the nonlinear elastic continuum constitutive law by a recently developed viscoelastic-viscoplastic one which is able to capture the mechanical behaviour of the particle system in a much larger strain range. Furthermore, we discuss numerical aspects like the choice of time steps and iteration numbers.

1 Multiscale techniques

Continuum mechanics usually does not take into account the atomistic or molecular structure of matter. This makes it difficult to account for effects that originate from atomistic length and time scales which typically are at the range of nanometers and femtoseconds. Prominent examples for applications where this is of specific interest are interphases in polymer nanocomposites: There, the rather stiff filler particles are embedded into a comparably weak polymer matrix and have significant influence on the mechanical behaviour of the composite, even at low filler contents [1]. This can be traced back, among others, to local changes in the deformability of the polymer chains, which is altered due to the presence of and the interactions with the filler particles. In contrast to continuum mechanics, molecular dynamics (MD) explicitly takes into account the particular structure of matter. It is a well-suited approach to model the material behavior at length and time scales relevant for the description of interphase effects of polymer nanocomposites. A severe drawback of MD is its restriction to very small systems and rather short time intervals: Typical system sizes and time spans, despite of the ongoing increase of computational power, are some nanometers overall length and up to microseconds time intervals. Hence, it is very difficult to incorporate particle-based simulation into problems usually arising in continuum mechanics and thus engineering approaches.

To bring these two strategies together, i.e. the continuum mechanical and the particle-based point of view, multiscale techniques are required. Despite of decades of research in this regard and some well-suited approaches for crystalline materials, a reliable method for polymer systems could not be established so far. An exception is the Capriccio method developed [2] and optimised [3] in recent years: This approach has been designed for the specific needs of polymers and embeds a particle-based region into a much larger continuum domain. The particle region is treated by MD keeping the full complexity of particle-based simulations, i.e. with usual particle numbers, simulation times, parameters, etc. On the other hand, the continuum part employs the Finite Element method to solve the associated differential equations. Both descriptions overlap in a bridging domain which ensures the information exchange between the domains. In addition to an energy blending in the bridging domain governed by a weighting factor α, a kinematic constraint links continuum and particle displacements in a weak form. In the MD domain, anchor points act as auxiliary particles and are the interaction partners for the continuum and the MD domain.

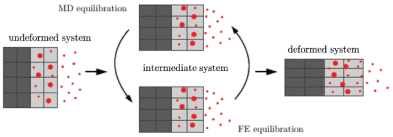

Fig. 1: Spatial set-up and staggered solution scheme of the Capriccio method: the FE domain (grey) overlaps with the MD domain (small red dots) in the bridging domain (light grey) using anchor points (large red circles).

In its first implementation [4], the Capriccio method proved to be stable and reasonable results could be obtained using the staggered scheme depicted in Figure 1: starting from the undeformed configuration, the FE system deforms based on the boundary conditions in the first load step and the anchor points move accordingly. This disturbs the MD part of the system which has to be equilibrated and after a sufficient number of MD-FE steps the system achieves its overall equilibrium. However, deviations with respect to the analytical and a pure FE reference solution could not be sufficiently reduced and thus have been since then subject of further research. One of the significant issues is the profound knowledge of the material

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Submitted / accepted / in press

Journal Articles

[1] **Christof Bauer, Maximilian Ries, Sebastian Pfaller**
Accelerating molecular dynamics simulations by a hybrid molecular dynamics-continuum mechanical approach
Soft Materials, submitted

[2] **Francesc Font-Clos, Marco Zanchi, Stefan Hiemer, Silvia Bonfanti, Roberto Guerra, Michael Zaiser, Stefano Zapperi**
Predicting the failure of two-dimensional silica glasses
Nature Physics, submitted

[3] **Yash Jain, Maximilian Ries, Sebastian Pfaller, Florian Müller-Plathe**
Addressing surface effects at the particle-continuum interface in a molecular dynamics and finite elements coupled multiscale simulation technique
submitted

[4] **Dhananjay Phansalkar, Kerstin Weinberg, Michael Ortiz, Sigrid Leyendecker**
A spatially adaptive phase-field model of fracture
Computer Methods in Applied Mechanics and Engineering, arXiv:2109.10175 [cs, math], submitted

[5] **Maximilian Ries, Christof Bauer, Felix Weber, Paul Steinmann, Sebastian Pfaller**
Characterization of the material behavior and identification of effective elastic moduli based on molecular dynamics simulations of coarse-grained silica
submitted

Conference papers

[1] **S. Elmira Birang O., Ana-Sunčana Smith, Paul Steinmann**
Configurational Forces in Bond Order Potentials
Proceedings in Applied Mathematics and Mechanics, accepted

[2] **Wuyang Zhao, Sebastian Pfaller**
A concurrent MD-FE coupling method towards simulations of fracture of thermoplastic polymers.
In: *16th conference of the Complas (2021), submitted*

In preparation

Journal Articles

[1] **Achraf Atila, Erik Bitzek**
Atomistic origins of deformation-induced structural anisotropy in metaphosphate glasses

[2] **Samaneh Esfandiary, Paolo Moretti, Miguel A. Muñoz**
Spectral signatures of localization in brain networks

[3] **Nosaibeh Esfandiary, Paolo Moretti, Michael Zaiser**
Statistical aspects of interface adhesion and detachment of hierarchically patterned structures

[4] **Nosaibeh Esfandiary, Paolo Moretti, Michael Zaiser**
Spectral analysis of fracture patterns in interface adhesion of hierarchical materials

[5] **Sudheer Ganisetti, Achraf Atila, Julien Guénolé, Aruna Prakash, Jürgen Horbach, Lothar Wondraczek, Erik Bitzek**
The Origin of Deformation Induced Topological Anisotropy in Silica Glass

[6] **Paras Kumar, Maurice Rohracker, Julia Mergheim**
RVEGen: Micro-Structure Configuration to Mesh Generation. A PYTHON Based Open Source Tool to Facilitate the Creation of RVEs with Random Heterogeneous Micro-Structure

[7] **Tarakeshwar Lakshmipathy, Alexander Hartmaier, Erik Bitzek**
Influence of lattice discreteness on fracture mechanics

[8] **Tarakeshwar Lakshmipathy, Alexander Hartmaier, Erik Bitzek**
Influence of crack tip radius on fracture toughness: an atomistic study

[9] **Mattia Livraghi, Sampanna Pahi, David M. Smith, Christian R. Wick, Ana- Sunčana Smith**
Towards a General AMBER Force Field for Amine-Based Epoxy Resins: Liquid and Glassy

[10] **Valentina Marzulli, Ali Mauricio Velasco Sabogal, Thorsten Pöschel**
Local decay of shear strength in granular assemblies

[11] **Valentina Marzulli, Ali Mauricio Velasco Sabogal, Achim Sack, Thorsten Pöschel**
A novel setup to Study the Stress Regime within a layer of Granular Material during a Quasi-Static Penetration Process at Different Gravity Levels

[12] **Sukhminder Singh, Lukas Pflug, Michael Stingl**
Surrogate-based stochastic optimization for enhancing delamination resistance of composites

[13] **Ali Mauricio Velasco Sabogal, Jose Daniel Muñoz, Thorsten Pöschel**
Adaptive method to simulate fractures in solid brittle materials by Multi-sphere DEM and Beam-like bonding forces

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

[15] **Christian R. Wick, Ece Topraksal, Sampanna Pahi, David M. Smith, Ana- Sunčana Smith**
What can we learn from quantum mechano-chemical calculations of small polymer models?

[16] **Michael Zaiser, Seyyed Ahmad Hosseini, Paolo Moretti, Tero Mäkinen, Juha Koivisto, Mahshid Pournajar, Marcus Himmler, Michael Redel, Dirk W. Schubert, Mikko J. Alava**
Hierarchical slice patterns inhibit crack propagation in brittle sheets

2.3 Participation in conferences and workshops

Christof Bauer

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
11.01.2021 / 15.01.2021	14th WCCM-ECCOMAS 2020	virtual	Talk: *Towards adaptive discrete-to-continuum modelling of thermoplastics*
15.03.2021 / 19.03.2021	91st GAMM	virtual	Talk: *Aspects of adaptive discrete-to-continuum modelling of thermoplastics*
22.09.2021 / 24.09.2021	8th ECCOMAS Thematic Conference on the Mechanical Response of Composites - COMPOSITES 2021	virtual	Talk: *Discrete-to-continuum coupling of pre-deformed thermoplastic polymers*

Paras Kumar

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
11.01.2021 / 15.01.2021	14th WCCM-ECCOMAS 2020	virtual	Talk: *Size-Effects in Composite Materials: A Comparison of Interface and Interphase Modelling Approaches*
15.03.2021 / 19.03.2021	91st GAMM	virtual	Talk: *Modeling Size Effect in Polymer Nanocomposites*
07.07.2021 / 09.09. 2021	6th ECCOMAS Young Investigators Conference 2021	virtual	Talk: *RVEGen: A PYTHON Based Tool for Random Particulate Micro-Structure RVE Generation*
23.08.2021 / 27.08.2021	ICTAM 2020+1	virtual	Talk: *Computational Modeling of Size Effects in Polymer Nano-Composites*

Marie Laurien

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
07.09.2021 / 09.09.2021	17th International Symposium on Computer Methods in Biomechanics and Biomedical Engineering	virtual	Talk: *Nonlocal wrinkling instabilities in bilayered systems using peridyanmics*

Dhananjay Phansalkar

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
15.03.2021 / 19.03.2021	91st GAMM	virtual	Talk: *Space-dependent transition zone parameter for a phase-field model of brittle fractures*

Maximilian Ries

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
11.01.2021 / 15.01.2021	14th WCCM-ECCOMAS 2020	virtual	Talk: *Multiscale FE-MD coupling: rethinking the Capriccio method*
22.09.2021 / 24.09.2021	8th ECCOMAS Thematic Conference on the Mechanical Response of Composites - COMPOSITES 2021	virtual	Talk: *Revised boundary conditions for FE-MD multiscale coupling of amorphous polymers (keynote)*

Ina Schmidt

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
15.03.2021 / 19.03.2021	91st GAMM	virtual	Talk: *On the influence of the biological availability on bone remodelling*
07.09.2021 / 09.09.2021	CMBBE 2021	virtual	Poster: *Continuum bone remodelling considering cancellous and cortical bone*
07.10.2021 / 08.10.2021	Understanding and Improving Fracture Healing	virtual	Participation only

Sukhminder Singh

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
15.03.2021 / 19.03.2021	91st GAMM	virtual	Talk: *Computational design of heterogeneous materials to enhance interfacial fracture resistance using gradient-based material optimization*
13.06.2021 / 18.06.2021	WCSMO 14	virtual	Talk: *Material optimization to enhance delamination resistance of composites*

Lucie Spannraft

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
11.01.2021 / 15.01.2021	14th WCCM-ECCOMAS 2020	virtual	Talk: *Grain boundary interaction: Energetic and dissipative microtractions model coupled to a mixed-mode cohesive zone model*
15.03.2021 / 19.03.2021	91st GAMM	virtual	Talk: *Gradient-extended crystal inelasticity with a coupling of a microtractions and decohesion model*

Christian Wick

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
27.01.2021 / 29.01.2021	International Online Workshop on Multi-dimensional Particle Characterization	virtual	Participation only
01.03.2021 / 03.03.2021	Second conference of CRC1114 on "Scaling Cascades in Complex Systems"	virtual	Participation only
04.10.2021 / 06.10.2021	International Online Workshop on Continuous Particle Synthesis and Product Design	virtual	Participation only

Wuyang Zhao

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
11.01.2021 / 15.01.2021	14th WCCM-ECCOMAS 2020	virtual	Talk: *A particle-continuum coupling method for simulations of viscoelastic amorphous polymers and nanocomposites*
07.09.21 / 09.09.21	XVI International Conference on Computational Plasticity, Fundamentals and Applications - COMPLAS 2021	virtual	Talk: *An MD-FE coupling simulation method applied to fracture of viscoelastic-viscoplastic glassy polymers.*
22.09.21 / 24.09.21	8th ECCOMAS Thematic Conference on the Mechanical Response of Composites - COMPOSITES 2021	virtual	Talk: *Partitioned-domain particle-continuum coupling methods for simulations of inelastic amorphous polymer-based nanocomposites.*

2.4 Collaborations with other research institutions

Achraf Atila

Partner institute	Researchers involved	Research topic
Otto Schott Institute of Materials Research, University of Jena, Germany	Lothar Wondraczek	Local elastic moduli of glasses

Christof Bauer

Partner institute	Researchers involved	Research topic
Theoretical Physical Chemistry Group, Technical University of Darmstadt, Germany	Florian Müller-Plathe, Yash Jain, Maximilian Ries, Wuyang Zhao	Collaboration on improving the Capriccio method

Stefan Hiemer

Partner institute	Researchers involved	Research topic
Center for Complexity and Biosystems, University of Milan, Italy	Francesc Font-Klos, Marco Zanchi, Silvia Bonfanti, Roberto Guerra, Stefano Zapperi	Plasticity in atomistic glasses

Tarakeshwar Lakshmipathy

Partner institute	Researchers involved	Research topic
ICAMS, Ruhr-Universität Bochum; Germany	Alexander Hartmaier	Influence of crack tip radius on fracture behaviour
ICAMS, Ruhr-Universität Bochum, Germany	Thomas Hammerschmidt	Benchmarking of interatomic potentials in fracture simulations
Division of Mechanics, Lund University, Sweden	Pär A. T. Olsson	Benchmarking of interatomic potentials in fracture simulations

Maximilian Ries

Partner institute	Researchers involved	Research topic
Theoretical Physical Chemistry Group, Technical University of Darmstadt, Germany	Florian Müller-Plathe, Yash Jain, Christof Bauer, Wuyang Zhao	Collaboration on improving the Capriccio method

Lucie Spannraft

Partner institute	Researchers involved	Research topic
Department of Industrial and Materials Science, Chalmers University of Technology, Gothenburg, Sweden	Fredrik Larsson, Kenneth Runesson	Grain boundary mechanics

Ali Mauricio Velasco Sabogal

Partner institute	Researchers involved	Research topic
Department of Physics, National University of Colombia, Bogotá Colombia	Jose Daniel Muñoz	Adaptative cell refinement for the study of fractures in brittle materials with a multi-sphere DEM approach and beam-like interaction model.

Christian Wick

Partner institute	Researchers involved	Research topic
Institute Ruđer Bošković, Zagreb, Croatia	David M. Smith	Development of Hybrid QM/MM methods for fracture of epoxy resins

Wuyang Zhao

Partner institute	Researchers involved	Research topic
Theoretical Physical Chemistry Group, Technical University of Darmstadt, Germany	Florian Müller-Plathe, Yash Jain,	Coupled MD-FE fracture simulations of coarse-grained polystyrene

3 Qualification Concept

3.1 Qualification programme

The qualification programme includes “qualification days”, “alumni and visitors workshops”, and “RTG retreats” as basic activities. These are accompanied by obligatory participations in 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. Furthermore, all presentations of student theses supervised by FRASCAL doctoral researchers take place within the framework of the so-called student seminar series of FRASCAL (S^3 FRASCAL).

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 used in the doctoral projects and ensures profound interdisciplinary education. It is mandatory for the doctoral researchers / associated doctoral researchers to attend at least ten / five of them within the doctorate.

The mini-lectures are usually given by FRASCAL PAs, sometimes by FRASCAL doctoral researchers or external experts.

Although the guidelines of the GRK 2423 FRASCAL no longer provide for mini lectures for the third year of a cohort, we were able to secure two excellent speakers for a mini lecture each, who perfectly complemented or expanded the previous qualification programme.

Dr.-Ing. Britta Schramm (Applied Mechanics, University of Paderborn, Paderborn, Germany), who is also a sub-project leader in TRR 285, talked in her lecture in January about simulation approaches to crack growth in heterogeneous materials in both basic and application-oriented research. TRR 285 members were also invited to attend this lecture. The digital format of this mini lecture made it easy for a large number of interested people from different locations to attend this joint event of GRK 2423 FRASCAL and TRR 285.

In the second mini lecture, completely different time and length scales for fracture processes were considered than we have known so far in FRASCAL: Prof. Dr. Daniel Koehn (Tectonics Research Group, GeoCentre Northern Bavaria, FAU) spoke in his mini lecture about fracture problems in geology. This exciting topic met with such great interest beyond the GRK that we welcomed participants from all over Germany and even from Switzerland to the digital full-day lecture.

The collaboration with Daniel Koehn has proved so fruitful that we were able to recruit him as project leader for a new sub-project "Modelling of fragmentation and fracturing processes in deformation bands and faults, from single grains to seismic-scale faults" (with Michael Zaiser as co-PA) for FRASCAL from 1 January 2022: FRActure across SCALes: from quantum now up to geological (!) scales.

Table 9: Mini lectures

	Date	Title	Lecturer
01	15 January 2021	Theories, Experimental Investigations and Numerical Modeling regarding Crack Growth	B. Schramm
02	12 March 2021	Fractures, faults and roughening anti-cracks: pattern formation in Geology	D. Koehn

These two lectures, like the previous ones, were also published as a printed script. This serves the doctoral students as a reference work after the lecture.

Figure 54: Impressions of the two mini lectures and photo of the mini lecture notes.

Soft skills trainings

In 2021, two soft skills seminars were held, which were specially designed for FRASCAL doctoral students and tailored to their needs and wishes.

Table 10: Soft skills trainings

	Date	Title	Lecturer
01	08 / 09 February 2021	Attracting successfully research funding! The road from the idea to getting funded!	W. Simoleit
02	16 April 2021	Supervising Thesis Projects	D. Vode

Attracting successfully research funding! The road from the idea to getting funded! (Dr. Wilma Simoleit, Bonn)

To attract funding for the own position or the realization of project ideas is a major basis for success in science and a very topical issue for our FRASCAL doctoral researchers in the last year of their doctorate. Various questions arise, such as: How can I finance my ideas and myself in science by extramural funding? How do I find the right funding program for project support or for a fellowship inland or abroad? How do I write a success promising proposal?

In this online workshop the participants gained insight into the principles of research funding, the structure of proposals and the procedures of proposal submission and evaluation. They received guidelines to find the right funding agency and funding program to finance a scientific project or to attract a fellowship. The participants trained to write a convincing proposal. They could choose a fictional topic, a previous publication, their dissertation or a topic they want to work on in the future. Major focus was on the title of a proposal, a strong summary and the development of an adequate

budget. The participants also learned unwritten rules they should keep in mind, when applying for research funds.

Major subjects of the workshop were:

- Basic principles of the funding system
- Funding institutions and programs
- Writing a promising proposal
- Submission and evaluation procedures

Supervising thesis projects (Dzifa Vode, Nürnberg)

Many doctoral researchers and postdocs supervise, support and coach bachelor and master students during student research projects or theses. In this workshop, FRASCAL doctoral researchers learned how to structure and manage the supervision process a way that is both goal- and process-oriented. They developed their own supervision structure and trained helpful communication techniques. They were given the appropriate tools to tackle typical problems during the supervision process. In addition, various ways of assessing Bachelor's and Master's theses fairly and transparently were discussed. After the workshop, they had acquired skills to approach their next supervision more confidently.

Major subjects of the workshop were:

- Reflecting your own experience with being supervised and supervising
- Characteristics of good supervision
- Roles and tasks of supervisors
- Supervision frequency and rhythm
- Solving difficult supervising situations
- Assessing student theses

S^3 FRASCAL

This student seminar series of FRASCAL (S^3 FRASCAL) is a newly established part of the qualification programme of GRK 2423 FRASCAL.

All bachelor's, project and master's theses supervised by FRASCAL doctoral researchers (incl. associates) and post-docs are from now on part of the FRASCAL qualification programme (for a listing see also chapter 3.3.2). The students' presentations, which must be given as part of their theses, continue to take place at the respective chairs of the supervisors and examiners, but are at the same time part of S^3 FRASCAL and all FRASCAL members are invited to the presentation and subsequent discussion.

Table 11: S^3 FRASCAL

Student	Topic	Supervisor / Date
Vincent Dötschel	Untersuchung des Materialverhaltens von Poly(2-Vinylpyridin) mithilfe molekulardynamischer Simulationen	Maximilian Ries / 12.11.2021
Alexander Müller	Untersuchung des Bruchverhaltens von Polystyrol mit Hilfe molekulardynamischer Simulationen	Maximilian Ries / 19.07.2021
Vinay Nagaraj	A literature review on fracture of graphene	Elmira Birang / 01.02.2021

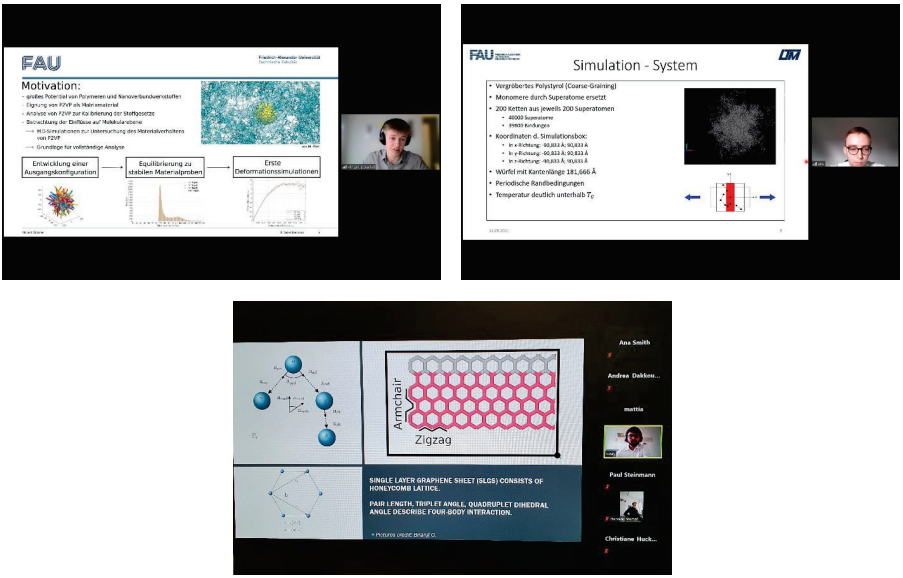


Figure 55: Students during their presentations at S³ FRASCAL: V. Dötschel (top left), A. Müller (top right) and V. Nagaraj (bottom centre).

RTG seminars

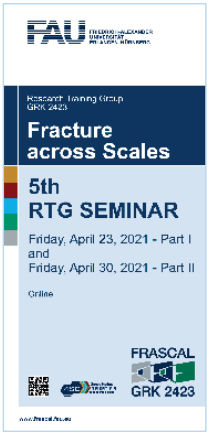
In each lecture period, one qualification day is reserved for an RTG seminar mandatory for the doctoral researchers and associated doctoral researchers. Within the framework of this seminar, the current developments of each doctoral project are presented as talks of 15 min duration with 5 to 10 min subsequent 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 12: RTG seminars

	Date	Subject	Mode
01	23 April 2021 / 30 April 2021	5. RTG Seminar part I / part II	all doctoral researchers and postdoctoral researcher
02	14-15 October 2021	6. RTG Seminar	all doctoral researchers and postdoctoral researcher, four associated doctoral researchers

Programmes see Appendix 1 and Appendix 2

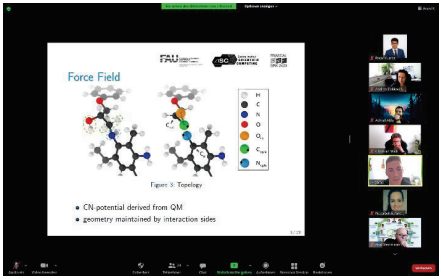
5th RTG Seminar



On April 23 and April 30, 2021, the fifth RTG seminar of the Research Training Group GRK 2423 FRASCAL took place.

This was the first FRASCAL RTG Seminar that had to be held in purely digital form. It was therefore decided to spread the eleven presentations by the doctoral researchers and postdoc over two days.

The associated doctoral researchers took on the role of moderators. At all times, they ensured that each session started on time and that the lecture and discussion time was adhered to in the best possible way.



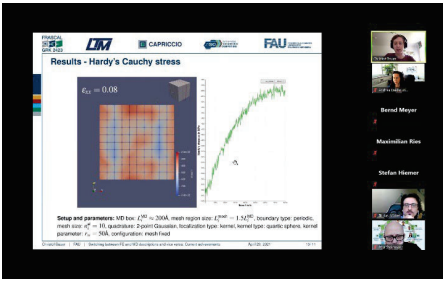


Figure 56: Impressions of the 5th RTG Seminar.

Figure 57: 6th RTG Seminar at the Hotel Riesengebirge in Neuhof an der Zenn. (Image: A. Dakkouri-Baldauf)

As usual at our biannual RTG seminars, all FRASCAL doctoral researchers, the post-doctoral researcher and this time even four of the associated doctoral researchers each gave a talk on their latest research results. The progress of the young researchers compared to the last RTG seminar was very remarkable and clearly visible in all of them! Here you will find the programme.

However, the doctoral researchers not only presented their latest scientific results, but also took turns moderating all the sessions. They all solved this task with excellence and ensured that each of the numerous presentations, including discussion, remained on time during the two days and that the schedule was always kept to in an exemplary manner.

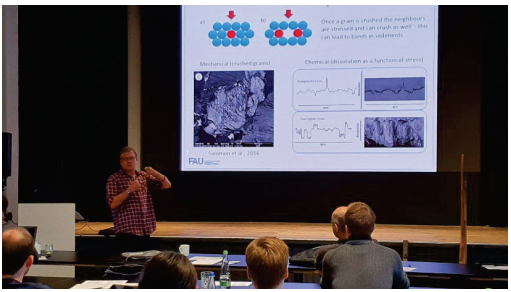


Figure 58: Daniel Koehn is presenting his new project in FRASCAL. (Image: A. Dakkouri-Baldauf)

A very warm welcome was given to Prof. Dr. Daniel Koehn, who will lead a new subproject in the GRK 2423 FRASCAL entitled: “Modelling of fragmentation and fracturing processes in deformation bands and faults, from single grains to seismic-scale faults” from 1 January 2022. He presented this project in a lecture on the second day of the seminar. This project will significantly extend the length scale considered in GRK 2423 FRASCAL, so to speak FRASCAL, Fracture across Scales – from quantum to geological (!) scales. We are very pleased to welcome Daniel Koehn as a new member of FRASCAL!

Since the doctoral researchers of the first cohort of the Research Training Group are almost at the end of their doctoral thesis phase and therefore (have to) think about their professional career after the after the dissertation, another block was reserved at the seminar – divided between the two seminar days – in which the Principal Advisors Julia Mergheim, Paul Steinmann and Ana-Sunčana Smith presented their professional careers in a lively, impressive and entertaining way, using their very different and exciting CVs as examples. In doing so, they wanted to show the doctoral students that there are very different paths to an academic career and that one can take various, sometimes unplanned, forks in the road and still successfully reach one’s destination.

Figure 60: Julia Mergheim (left) and Ana-Sunčana Smith (right) presenting their different and very fascinating CVs. (Images: A. Dakkouri-Baldauf)

Figure 59: Paul Steinmann is presenting a video about fragmentation of candy bars. (Image: A. Dakkouri-Baldauf)

A particular highlight of the RTG seminar was a short workshop by Paul Steinmann entitled „Peer Review – from the perspective of the editor, the reviewer and the author". In it, he very imaginatively and humorously explained the peer review process of a scientific publication using a very illustrative example, the cryo-fracturing and -fragmentation of candy bars (fictional authors: Kurt Kaltbrecher and Vera von der Suess). He explained the entire process from the scientific idea and experiment through the preparation of a manuscript to the accepted publication. From the time of submission, the review process of the manuscript was considered from the perspective of the scientist, the editor, and the reviewer. Among other things, the questions were to which journal the publication should be submitted at all, how this works technically, which reviewers the editor should invite, how the reviewer proceeds professionally and technically, how long such a review process takes, and how the author should deal with criticism or rejection of his or her paper. And finally, it was explained how the confirmation of acceptance of a paper looks like and when and how the author receives the proofs of the article. At the end of the workshop, to the surprise of the participants, everyone received a sample of the chocolate bar that plays a central role in the publication, a so-called FRASCAL chocolate bar.

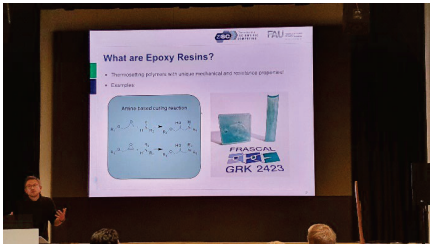
After sitting in the seminar room for a long time and listening attentively to the lectures, it felt good to continue the discussions about science, but also about other important things in life, in small groups quite casually on a hike. We were rewarded with a beautiful view of the autumnal Zenn valley and a small refreshment consisting of drinks and buttered pretzels, with which the hotel staff had surprised us in the middle of the path.

It was highly pleasing that with Marie Laurien, Maurice Rohracker and Felix Weber, three potential doctoral researchers of the 2nd cohort of FRASCAL (start: 1 January 2022) were already present and could thus make first contacts and informally inform themselves about a doctorate in a Research Training Group. At the next, the 7th RTG seminar, the entire second cohort of FRASCAL doctoral researchers will then be present and report on their first results ….









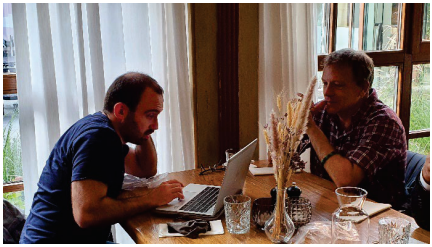



Figure 61: Further impressions of the 6th RTG Seminar. (Images: A. Dakkouri-Baldauf).

Special seminars

For the special seminars, internationally renowned scientists are invited to speak on FRASCAL-relevant research topics in detail and then actively involve FRASCAL researchers in discussions and question-and-answer sessions.

The special seminar with Prof. Adrian Lew was a joint seminar between the Glasgow Computational Engineering Centre (GCEC) and FRASCAL

Table 13: Special seminars

	Date	Title	Lecturer
01	09 February 2021	**High-Fidelity Simulation of Brittle Fracture Problems** Joint GCEC and FRASCAL Special Seminar A number of methods have been presented that have been introduced in 2D and 3D in recent years. Their final results are: (a) stress intensity factors can be computed with arbitrary accuracy (in 2D), (b) the mesh does not need to be refined around the crack tip for accuracy (in 2D), and (c) numerical experiments show convergence of the computed crack paths. These methods were presented with applications to thermally driven cracks in thin glass plates and to the propagation of volcanic dikes from a magma chamber, a hydraulic fracture problem.	Prof. Adrian Lew Stanford University, CA, USA
02	19 March 2021	**Computational analysis of graphene mechanics: deposition, adhesion and fracture** Results of molecular dynamics simulations of the mechanical properties of graphene were presented using three examples with experimental relevance. (a) Deposition of graphene a nanoparticle-decorated substrate, focusing on the formation of wrinkles and their interaction. Consideration of the problem of partial delamination of the sheet due to the presence of regions with high nanoparticle density. (b) Deposition of graphene over a trench and the effects of stresses and thermal fluctuations. (c) Behaviour of defected graphene under tensile loading: discussion of the role of strain rate and temperature on fracture size effects including a proposal of a theory to interpret the results.	Prof. Dr. Stefano Zapperi University of Milan Center for Complexity & Biosystems (CC&B), Department of Physics, Milan, Italy

English language coaching

Publications in international journals, presentations at international conferences and scientific exchange with international researchers require profound knowledge of scientific English.

With Paul Gahman from the "FAU Language Centre", FRASCAL participants have a professional English language coach at their disposal, who trains oral presentations, proofreads English publications and covers many other individually requested topics in his English lessons every lecture period.

Attendance of English classes is optional.

Table 14: English coaching seminars

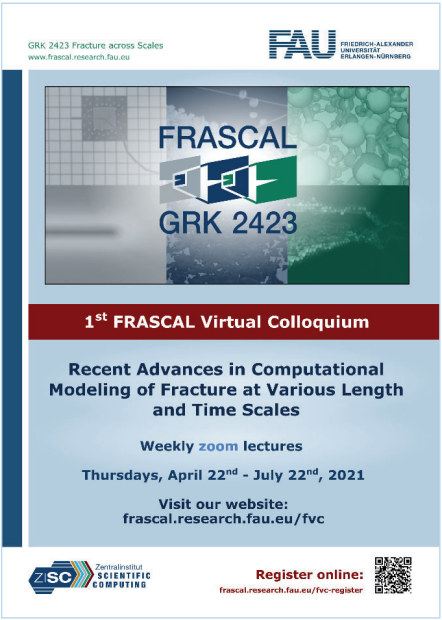
Date	Topic
Winter semester 2020/2021	Individual Language Consultations and Group Classes
	How to Structure a PhD Tesis

Summer semester 2021	Individual Language Consultations and Group Classes
	Online Writing Tools; Recap of Identifying Parts of Speech in Sentences
	Paraphrasing
	Drafting & Revising
	Defending Thesis: Q&A Section
	Describing Data from Various Graph Types, Equations and Related: Bring your questions about equations and such to today's lecture!
	Revisiting Linking, Assimilation and Problematic Consonants
	Establishing and Maintaining Cohesion in Written Work
Winter semester 2021/2022	Preparing for and Practicing a Thesis Defense
	Paraphrasing and Reformulating the Written Word
	Targeting Common Mistakes in Writing
	Intonation and Pausing, Tackling the Q&A Session
	Vocabulary Practice, Identifying Informal Language

Figure 62: English coaching with Paul Gahman. (Images: Jonas Ritter)

3.1.2 1st FRASCAL Virtual Colloquium

In the 1st FRASCAL Virtual Colloquium, recent studies on fracture and the failure of materials were presented by various, international guest speakers, including material instability, crack formation and transition, material adhesion and grain boundary evolution. A wide variety of materials, from brittle to ductile and from crystalline to disordered, were discussed. Along the same vein, different approaches to modelling materials, ranging from molecular dynamics to statistical and continuum mechanics, were addressed. Specifically, the following methods spanning various scales were reviewed in the talks: Atomic-scale and coarse-grained molecular dynamic simulations, line tension models, statistical-mechanics models, fibre bundle models, cohesive zone models, phase-field methods, eigenerosion approaches, smeared methods, continuum disconnections, damage homogenization, and the material point method.



The research training group GRK 2423 FRASCAL brings together researchers from various departments of the Faculty of Sciences and the Faculty of Engineering with the aim to improve the understanding of fracture in heterogeneous materials. This is accomplished by developing simulation methods that are able to capture the multiscale nature of failure.

In keeping with this spirit, our doctoral, associated doctoral and post-doctoral researchers organised this virtual colloquium in 2021 (22 April to 22 July). This event replaced a mini-symposium at CFRAC 2021 that was already in the planning stage at that time, when the conference had been cancelled due to the Corona pandemic. The organisation of a mini-symposium at an international conference is part of the qualification program within FRASCAL. Therefore, the new “FRASCAL Virtual Colloquium” served as a replacement event and provided a platform to discuss recent advances in the computational modelling of fracture at various length and time scales. Ambitious goals were pursued, such as increasing the understanding of fracture behaviour, the optimal design of structures, failure time prediction and the design of smart materials.

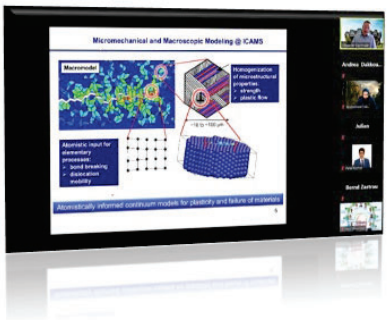
The programme of events was comprised of a weekly series of 12 guest talks in total by experts tackling the aforementioned problems from different viewpoints, such as mechanics, materials science, mathematics, physics and chemistry. Each 45-minute talk was followed by a public discussion with a multinational audience spanning from FAU members to members from other national and international research institutions. Afterwards, an in-depth exchange between the doctoral students from FRASCAL and the invited experts took place.

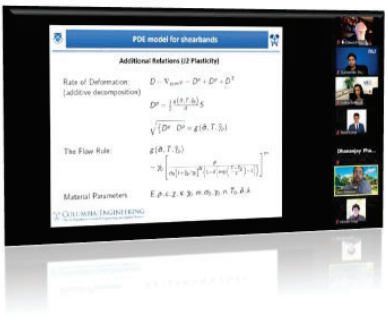
The format of this colloquium was an absolute success. A large number of international participants, mostly well over 100, attended the engrossing talks by well-known experts and joined the lively discussions. To that end, we would like to take this opportunity to thank all our speakers and attendees who contributed to our 1st Virtual Colloquium and made it a great success. Thanks to this highly stimulating and positive experience, we plan to hold a similar FRASCAL colloquium series on a yearly basis.

As for the organisation of the event, each of the 12 FRASCAL projects invited a speaker. The respective doctoral student chaired the session, while an anchor team of FRASCAL students provided technical support. Flyers and posters for advertisement were designed and printed by our students. In addition, a book of abstracts was provided as an overview of the entire event.

Table 15: Programme of the 1st FRASCAL Virtual Colloquium

Date	Title	Lecturer
22 April 2021	Bridging the scales in fracture and damage mechanics	**Alexander Hartmaier** Ruhr-Universität Bochum, Germany
29 April 2021	Computational modeling and design optimization of structures using the phase field fracture method	**Haim Waisman** Columbia University, USA
06 May 2021	Predictability of failure in disordered solids using fiber bundle models	**Soumyajyoti Biswas** SRM University, India
20 May 2021	How disorder affects the failure: Fractures on models inspired by Bamboo Guadua angustifolia	**Jose Daniel Muñoz** National University of Colombia, Colombia
27 May 2021	From sub-Rayleigh anticrack to supershear crack propagation in snow slab avalanche release	**Johan Gaume** EPFL, Switzerland
10 June 2021	Modelling fracture with eigenerosion versus phase-field	**Anna Pandolfi** Politecnico di Milano, Italy
17 June 2021	Fracture of random media from atoms to the continuum	**Lars Pastewka** Albert-Ludwigs-Universität Freiburg, Germany
24 June 2021	Discrete and smeared approaches in computational fracture mechanics	**René de Borst** University of Sheffield, United Kingdom
01 July 2021	Phase-field fracture models for linearized and finite elasticity	**Kerstin Weinberg** Universität Siegen, Germany
08 July 2021	Continuum modeling of grain boundary plasticity using dislocations and disconnections	**Nikhil Admal** University of Illinois Urbana-Champaign, USA
15 July 2021	Ionic polymer nanocomposites under deformation	**Ahmad Moghimikheirabadi** ETH Zürich, Switzerland
22 July 2021	A molecular simulation approach of epoxy resins: From curing to deformation and fracture	**Robert Meißner** Technische Universität Hamburg and Helmholtz-Zentrum Geesthacht, Germany





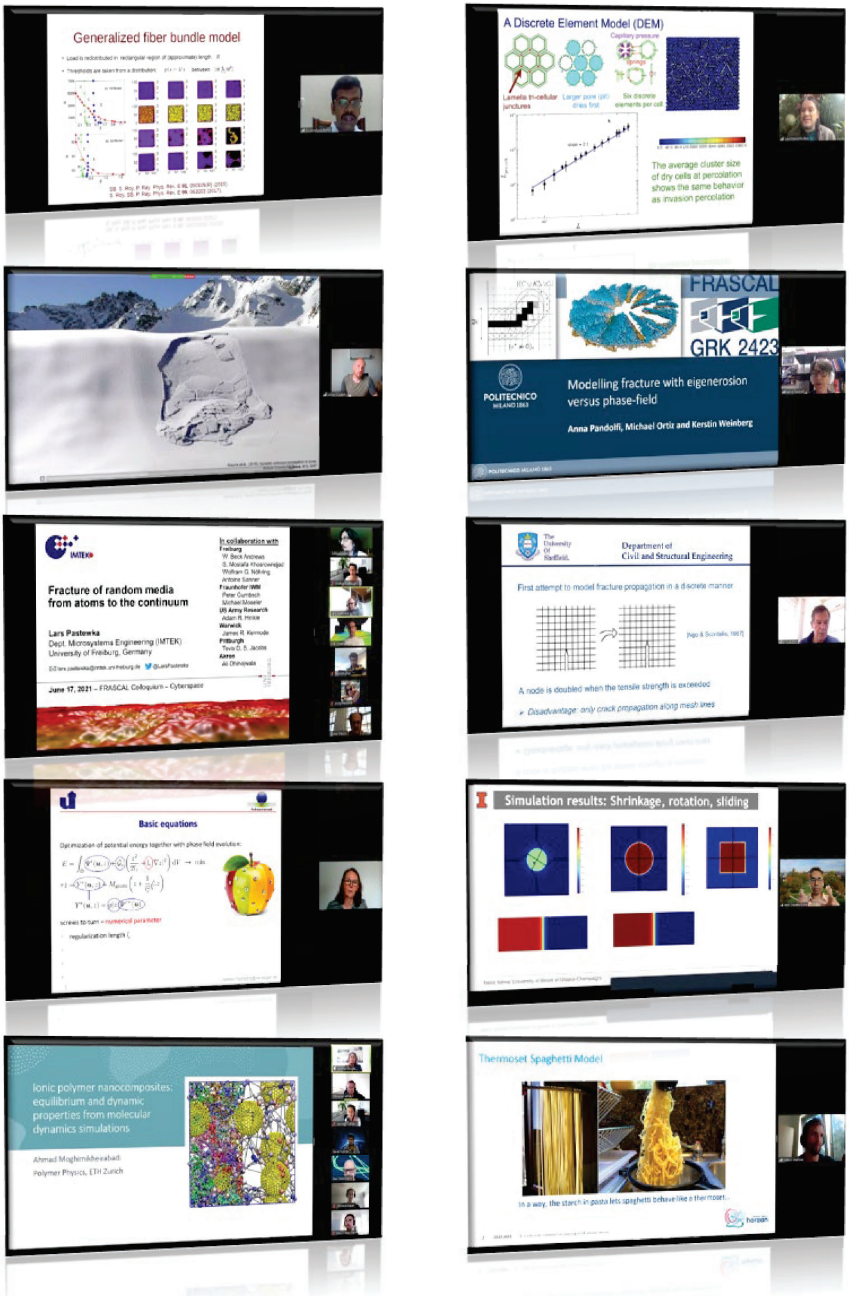


Figure 63: Speakers of the 1st FRASCAL Virtual Colloquium in chronological order.

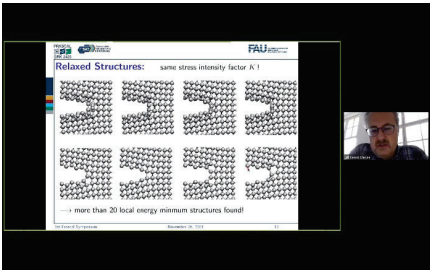
3.1.3 1st (virtual) FRASCAL Symposium

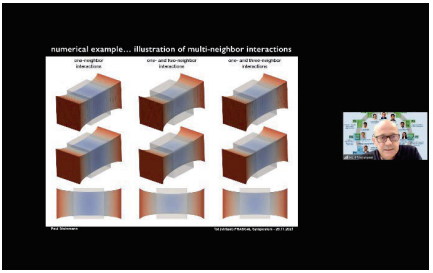
In addition to the 1st FRASCAL Virtual Colloquium (FVC), a new, (digital) lecture format was established in GRK 2423 FRASCAL this year:

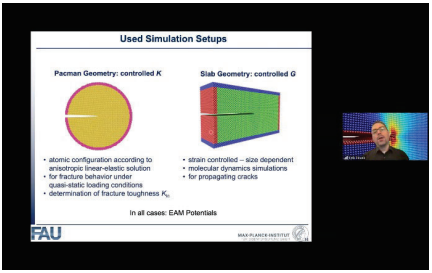
On 26 November 2021 the so-called "1st (virtual) FRASCAL Symposium" took place.

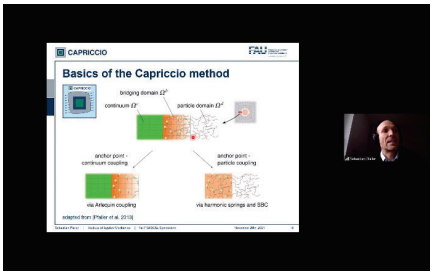
While the 1st FVC provided a platform for international researchers to present their recent studies and results on fracture and material failure, the 1st (virtual) FRASCAL Symposium, on the other hand, served to present the research priorities and latest results of GRK 2423 FRASCAL to the fracture community: Within the framework of this symposium, the principal advisors of the GRK 2423 FRASCAL projects contributed their own insights into the fracture problem from a higher-level perspective in six presentations and provided a basis for stimulating discussions and interaction with colleagues from around the world.

In a sense, the 1st (virtual) FRASCAL Symposium of Research Training Group 2423 was born out of necessity, as the annual FRASCAL Visitors Workshop – usually held as two-day events at secluded venues outside the FAU campus accompanied by social activities – could not take place due to Covid-9-related travel restrictions for international guests.









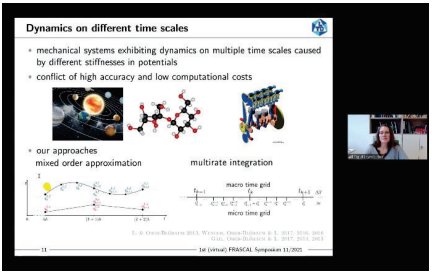


Figure 64: Speakers of the 1st (virtual) FRASCAL Symposium: Bernd Meyer, Paul Steinmann, Stefano Zapperi, Erik Bitzek, Sebastian Pfaller, Sigrid Leyendecker (from left to right and from top to bottom).

3.2 Visiting researcher programme

Table 16: Visiting researchers

From / to	Guest	Research Subject
15.01.2021	**Dr.-Ing. Britta Schramm** University of Paderborn Angewandte Mechanik, Paderborn, Germany	Joint Mini Lecture of GRK 2423 FRASCAL and TRR 285 *via Zoom*: *"Fracture Mechanics - Theories, Experimental Investigations and Numerical Modeling Regarding Crack Growth"* **Host:** Prof. Paul Steinmann (LTM)
09.02.2021	**Prof. Adrian Lew** Stanford University Mechanical Engineering Stanford, CA, USA	Invited Lecture at the Joint GCEC and FRASCAL Special Seminar *via Zoom:* *"High-Fidelity Simulation of Brittle Fracture Problems"* **Host:** Prof. Paul Steinmann (LTM)
12.03.2021	**Prof. Dr. Daniel Koehn** Friedrich-Alexander University of Erlangen-Nuremberg GeoZentrum Nordbayern Erlangen, Germany	Mini Lecture *via Zoom*: *"Fractures, faults and roughening anti-cracks: pattern formation in Geology"* Introduction to geological "fracture" problems: pattern formation and scaling from atoms to tectonic plates **Host:** Prof. Paul Steinmann (LTM)
19.03.2021	**Prof. Dr. Stefano Zapperi** University of Milan Center for Complexity & Biosystems (CC&B), Department of Physics Milan, Italy	Invited Lecture *via Zoom:* *"Computational analysis of graphene mechanics: deposition, adhesion and fracture"* **Host:** Prof. Michael Zaiser (WW8)
22.04.2021	**Prof. Dr. Alexander Hartmaier** Ruhr-Universität Bochum Department of Micromechanical and Macroscopic Modelling Bochum, Germany	Invited Lecture *via Zoom* at the 1st FRASCAL Virtual Colloquium: *"Bridging The scales in fracture and damage mechanics"* **Host:** Tarakeshwar Lakshmipathy / Prof. Erik Bitzek (WW1)
29.04.2021	**Prof. Haim Waisman** Columbia University Civil Engineering & Engineering Mechanics New York, NY, USA	Invited Lecture *via Zoom* at the 1st FRASCAL Virtual Colloquium: *"Computational modeling and design optimization of structures using the phase field fracture method"* **Host:** Sukhminder Singh / Prof. Michael Stingl (Applied Mathematics, (Continuous Optimization)
06.05.2021	**Dr. Soumyajyoti Biswas** SRM University-AP Department of Physics Andhra Pradesh, India	Invited Lecture *via Zoom* at the 1st FRASCAL Virtual Colloquium: *"Predictability of failure in disordered solids using fiber bundle models"* **Host:** Nosaibeh Esfandiary / Dr. Paolo Moretti (WW8)
20.05.2021	**Prof. Jose Daniel Muñoz Castaño** National University of Colombia Department of Physics Bogotá, Colombia, South America	Invited Lecture *via Zoom* at the 1st FRASCAL Virtual Colloquium: *"How disorder affects the failure: Fractures on models inspired by Bamboo Guadua angustifolia"*

		Host: Ali Mauricio Velasco Sabogal / Prof. Thorsten Pöschel (CBI)
27.05.2021	**Prof. Johan Gaume** SLAB - Snow and Avalanche Simulation Laboratory EPFL, ENAC School Lausanne, Switzerland	Invited Lecture *via Zoom* at the 1st FRASCAL Virtual Colloquium: *"From sub-Rayleigh anticrack to supershear crack propagation in snow slab avalanche release"* **Host:** Jonas Ritter / Prof. Michael Zaiser (WW8)
10.06.2021	**Prof. Anna Pandolfi** Polytechnic University of Milan Department of Civil and Environmental Engineering Milano, Italy	Invited Lecture *via Zoom* at the 1st FRASCAL Virtual Colloquium: *"Modelling fracture with eigenerosion versus phase-field"* **Host:** Paras Kumar / Prof. Julia Mergheim (LTM)
17.06.2021	**Prof. Dr. Lars Pastewka** Albert-Ludwigs-Universität IMTEK - Institut für Mikrosystemtechnik Freiburg, Germany	Invited Lecture *via Zoom* at the 1st FRASCAL Virtual Colloquium: *"Fracture of random media from atoms to the continuum"* **Host:** Tobias Müller / Prof. Bernd Meyer (CCC)
24.06.2021	**Prof. René de Borst** University of Sheffield Department of Civil and Structural Engineering Sheffield, United Kingdom	Invited Lecture *via Zoom* at the 1st FRASCAL Virtual Colloquium: *"Discrete and smeared approaches in computational fracture mechanics"* **Host:** Paras Kumar / Prof. Julia Mergheim (LTM)
01.07.2021	**Prof. Dr.-Ing. PD Kerstin Weinberg** Universität Siegen Lehrstuhl für Festkörpermechanik Siegen, Germany	Invited Lecture *via Zoom* at the 1st FRASCAL Virtual Colloquium: *"Phase-field fracture models for linearized and finite elasticity"* **Host:** Dhananjay Phansalkar / Prof. Sigrid Leyendecker (LTD)
08.07.2021	**Prof. Nikhil Chandra Admal** University of Illinois Mechanical Science & Engineering Urbana, IL, USA	Invited Lecture *via Zoom* at the 1st FRASCAL Virtual Colloquium: *"Continuum modeling of grain boundary plasticity using dislocations and disconnections"* **Host:** Christof Bauer / PD Dr. Sebastian Pfaller (LTM)
15.07.2021	**Dr. Ahmad Moghimikheirabadi** ETH Zurich Department of Materials, Polymer Physics Zurich, Switzerland	Invited Lecture *via Zoom* at the 1st FRASCAL Virtual Colloquium: *"Ionic polymer nanocomposites under deformation"* **Host:** Dr. Christian Wick / Prof. Ana-S. Smith (PULS Group)
22.07.2021	**Prof. Dr.-Ing. Robert Meißner** Technische Universität Hamburg Molekulardynamische Simulation weicher Materie Hamburg, Germany	Invited Lecture *via Zoom* at the 1st FRASCAL Virtual Colloquium: *"A molecular simulation approach of epoxy resins: from curing to deformation and fracture"* **Host:** Julian Konrad / Prof. Dirk Zahn (CCC)
09.11.2021 / 13.11.2021	**Prof. Michael Ortiz** California Institute of Technology, Pasadena, CA, USA	Collaboration with S. Leyendecker, D. Phansalkar (P9) and K. Weinberg (University of Siegen): the content and structure of a joint paper was determined and the following points discussed:

		1. Energy splits in quasi-static phase field formulations 2. Small deformation versus finite kinematics in fracture models 3. Dynamic phase field simulations, theory and numerics 4. Convergence study of adaptive dynamic phase field simulation **Host:** Prof. Sigrid Leyendecker (LTD)

3.3 Additional qualification measures

3.3.1 Summer schools / Winter schools

Paras Kumar

From / to	Name of school	Location
06.09.2021 / 10.09.2021	Advanced Course on Modeling of Localized Inelastic Deformation	Czech Technical University, Prague, Czech Republic

Sukhminder Singh

From / to	Name of school	Location
12.04.2021 / 16.04.2021	Optimization of Shape and Material Properties: Advanced Mathematical Methods and 3D Printing	virtual
06.09.2021 / 10.09.2021	Advanced Course on Modeling of Localized Inelastic Deformation	Czech Technical University, Prague, Czech Republic

Lucie Spannraft

From / to	Name of school	Location
06.09.2021 / 10.09.2021	Advanced Course on Modeling of Localized Inelastic Deformation	Czech Technical University, Prague, Czech Republic

3.3.2 Student projects and theses

Student work completed in 2021 that were supervised by FRASCAL doctoral researchers.

Bachelor theses

Student	Topic	Supervisor / Date
Omar Aldowajy	Multiscale simulations of inelastic polymers under shear deformation using the Capriccio method	Wuyang Zhao / 11.10.2021
Maximilian Dejori	Simulation of fracture in collagen-based materials	Nosaibeh Esfandiary / 15.07.2021
Vincent Dötschel	Untersuchung des Materialverhaltens von Poly(2-Vinylpyridin) mithilfe molekulardynamischer Simulationen	Maximilian Ries / 12.11.2021
Alexander Müller	Untersuchung des Bruchverhaltens von Polystyrol mit Hilfe molekulardynamischer Simulationen	Maximilian Ries / 19.07.2021

Project theses

Student	Topic	Supervisor / Date
Jacqueline Albertsen	Untersuchung des Deformationsverhaltens eines amorphen Thermoplasten unter Scherdeformation mittels molekulardynamischer und kontinuumsmechanischer Betrachtung	Christof Bauer / 21.06.2021
Maurice Rohracker	Determining Macroscopic Behavior of Hyperelastic Heterogeneous Materials	Paras Kumar / 10.09.2021
Zheng Wang	Characterization of amorphous polystyrene under isotropic volumetric deformation using molecular dynamics simulations	Wuyang Zhao / 31.07.2021

Master theses

Student	Topic	Supervisor / Date
Christian Greff	Machine Learning of the Solubility of Liquids	Stefan Hiemer / 19.05.2021
Swetha Ramesh	Convolutional Long Short-Term Memory: Views and Perspectives in Atomistic Fracture Mechanics	Dr. Paolo Moretti, S. Elmira Birang O., Nosaibeh Esfandiary / 15.09.2021
Yujie Zhang	Investigation of deformation-induced anisotropy of polystyrene using molecular dynamics simulations	Wuyang Zhao / 30.08.2021

4 Equal Opportunity Measures

Equal opportunities for women and men as well as career promotion and development of doctoral and postdoctoral researchers is a central concern of the Research Training Group. To this end, the Research Training Group GRK 2423 FRASCAL offers comprehensive measures for equal opportunities, career promotion and development of young scientists, as well as for the compatibility of a scientific career and professional life.

4.1 Workshops, seminars

The F^{3}G network (Research Associations of Friedrich-Alexander-Universität Erlangen-Nürnberg for the promotion of equality) offers lectures and seminars on the topics of women's advancement, gender sensitization, etc., in addition to a variety of other gender equality measures, in which members of the affiliated research associations can participate. Thus, some FRASCAL members have also taken advantage of these training measures and participated in the following workshops:

Table 17: Workshops organized by F^{3}G with participation of GRK 2423 FRASCAL members

	Date	Title	Lecturer
01	26 - 29 January 2021	PhD, and next? Career options, skills and orientation for scientists (workshop and individual coaching)	Dr. Karin Bodewits & Dr. Philipp Gramlich (München)
02	10 March 2021	Small Talk? It's nice to be connected!	Deborah Ruggieri (Berlin)

4.2 Virtual film screening and discussion

On 14 June 2021, GRK 2423 FRASCAL, in collaboration with IGK 2495, screened the documentary film „PICTURE A SCIENTIST" followed by a (digital) panel discussion.

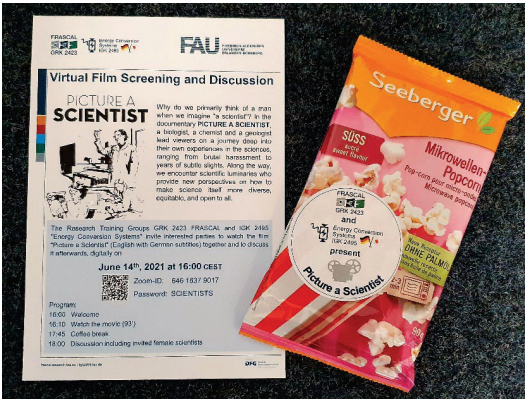


Figure 65: Invitation to the film event incl. snack given to each participant beforehand. (Image: A. Dakkouri-Baldauf)

The film tells of the spirit of optimism among women researchers who are writing a new chapter for women scientists. A biologist, a chemist, and a geologist take the audience on a journey through the experiences of their academic careers – as women in science. In their careers, they have faced discrimination from the beginning. From cramped labs to spectacular field stations, however, they also encounter scientific luminaries who reveal new perspectives on how science itself can become more diverse, equitable, and open to all.

After watching the film together in virtual screening, there was a discussion led by Dr. Julia Will, Women's Representative at FAU's Department of Materials Science and Engineering. For this purpose, we invited three outstanding female scientists associated with GRK 2423 FRASCAL and asked them about their experiences with the problems addressed in the film:

Prof. Dr. Julia Mergheim is a Professor at the Institute of Applied Mechanics at FAU and head of the research group „Numerical Mechanics“. Prof. Mergheim is a member of IGK 2495 „Energy Conversion Systems“ and GRK 2423 FRASCAL.

Prof. Dr. Areti Papastavrou is a Professor of Mathematics and Technical Mathematics at the Nuremberg University of Technology, where she is also the current Vice Dean and Women's Representative. One of Prof. Papastavrou's doctoral students, Ina Schmidt, is an associated doctoral researcher in GRK 2423 FRASCAL.

Prof. Dr. Ana-Sunčana Smith is a Professor of Theoretical Physics at FAU and works part-time as a Senior Researcher at the Ruđer Bošković Institute in Zagreb, Croatia. Prof. Smith is principal advisor of project P12 in GRK 2423 FRASCAL.

In addition, participants could anonymously leave their thoughts and comments on the film on a digital bulletin board, which was also very actively used. Even before the film, the audience had the opportunity to answer the question, „How do you picture a typical scientist?“. The same question was asked after the film to see if the image had changed. Examples of comments before the movie: *„Kind of a nerdy person who is curious and analytical.“* or *„Hair full of smoke from an explosion in the lab, wears either a lab coat or the same old-fashioned sweater every day.“* … The same question was answered after the movie with, for example, *„You may very well be a flawed and prejudiced person. You can be the oppressor or one who is silent about it. Not very ‚rational' or ‚logical' as they may see themselves“* or with *„Problem solvers in science and society.“* …

In response to the question or request for comments „Something I saw in the film that I was totally surprised about:“ there was an extremely large number of responses, such as *„that women were silent about what happened to them“* or *„that I couldn't pass the implicit bias test and my reaction time was longer than I would have thought“* or *„Nowadays, women are more visible in science, but there is still a lot to do to reach the same state as men in science. There are many aspects that still need to change“* and many more.

This very lively and emotional participation shows how stirring and important this topic is for all scientists, how much need for action and discussion there still is, and how important it is therefore to offer such events. Hopefully, there will be many more such activities and the path will continue in a positive direction.

4.3 Project: Female STEM scientists at FAU as role models

In a joint project of the *GRK 2423 FRASCAL* and the *Office for Gender and Diversity*, female STEM scientists at FAU and their success stories are presented as part of the "Innovationsbündnis Hochschule 4.0". The aim is to show not only unattainable role models, but a panorama of female scientists of different qualification levels and academic positions. This is to be realised in the form of a printed brochure.

The aim of the publication project is to interest schoolgirls and (potential) young female scientists in an academic career and to motivate them through concrete role models and examples. Women achieve outstanding results in studies and science. Nevertheless, women are still underrepresented in technical and scientific fields at the higher career levels. By concretely showing individual career paths, a long career path appears less abstract and more feasible.

By the end of 2021, all of the interviews with the selected female FAU scientists had already been conducted and the majority of the photos taken. The result is extremely diverse, exciting and entertaining CVs. The printed brochure will appear in spring 2022.

4.4 Further measures

- Financial support for vacation care for the children of our FRASCAL members.
- Financial support of specific F^3G projects in FAU holiday childcare programmes.
- Pedagogic improvement of the infrastructure at FAU day care facilities for children.
- Participation in F^3G coordination costs.
- Purchase of two toy boxes for temporary children's employment for FRASCAL members.
- Contingent option of one occupancy place in the day care centre “Pfauennest II”.

5 Selected Highlights

5.1 Awards

Sebastian Pfaller

2nd place at the Science Slam TF 2021

Figure 66: Sebastian Pfaller during his science slam talk at the "Tag der Technischen Fakultät" 2021. (Image: Erich Malter)

FAU's "Tag der Technischen Fakultät" took place on 19 November 2021 in a hybrid format and was broadcast via livestream.

A science slam competition was also held as part of this event. A total of twelve slammers gave their best and presented their research topics within three minutes in an extremely creative and entertaining way. At the end, the winner was determined by a digital vote of the audience.

Our PA Sebastian Pfaller also took part in the competition and performed “Die Ballade von den multiplen Skalen" (“The Ballad of Multiple Scales") in rhyme. In doing so, he highlighted the scientific challenge of the multi-scale nature of failure and the important role of GRK 2423 FRASCAL in researching this problem.

From the beginning, Sebastian Pfaller led the vote - at times with a large lead. Only at literally the last second was he overtaken and slipped to a still excellent second place by a narrow margin.

As a prize, Sebastian Pfaller received the coveted FAU owl and a voucher for a balloon ride!

Congratulations, Sebastian!

Ina Schmidt

BayWISS prize for “Herausragende oder zukunftsweisende Forschungsleistung im jeweiligen Wissenschaftsbereich“.

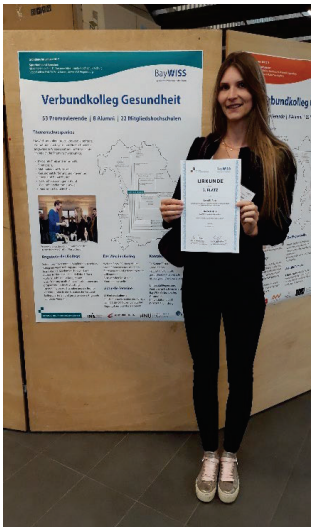


Figure 67: Ina Schmidt with her certificate on the occasion of the BayWISS Award for "Outstanding or forward-looking research achievement in the respective field of science" on 07 October 2021. (Image: Sabine Fütterer-Akili)

Ina Schmidt was awarded for her doctorate on the topic of "Biomechanics of the Bone". As part of the BayWISS annual colloquium, the BayWISS prizes were awarded for "Outstanding or forward-looking research achievement in the respective scientific field", in which she took third place.

In her doctorate, she is working on the modelling and simulation of bone remodelling processes that take place due to external stress and under different conditions. The aim is to predict the development of bone density on a patient-specific basis and thus predict the risk of fracture or prevent possible fractures. This is of particular interest in degenerative diseases such as osteoporosis or in high-performance sports.

Congratulations, Ina!

5.2 BayIND online seminar for young researchers with FRASCAL doctoral researcher

On 5 May 2021, the Bavarian-Indian Centre for Business and University Cooperation (BayIND) organised an online seminar for PhD aspirants from India.

The aim was to encourage young Indian researchers to choose Bavaria as a location for their research careers. To effectively address their questions and concerns, BayIND organised an online seminar on “PhD in Bavaria”. In this seminar, participants had the opportunity to interact with two current Indian doctoral researchers from Bavaria:

One doctoral researcher from TUM (Munich) and one doctoral researcher from FAU (Erlangen-Nuremberg) were invited. It was a great honour that one of our FRASCAL doctoral researchers, **Paras Kumar**, was invited to explain the advantages of doing a doctoral thesis in Bavaria to potentially interested Indian students. The main focus was on the following aspects:

1. Why did I choose Bavaria to do my research?
2. My research and life at my university
3. Why would I recommend to do research in Bavaria?

Figure 68: Paras Kumar during his presentation at the online seminar "PhD in Bavaria".

Due to this good contact to BayIND and through it also to the Bavarian state initiative "Research in Bavaria", we were also able to use the latter's platform in the summer to recruit doctoral researchers for the new FRASCAL cohort (start 1 January 2022), e.g. via their social media channels such as Twitter.

5.3 Mini-retreat of FRASCAL project P6 (Capriccio group)

In July 2021 - as in the summer of 2020 - the P6 project members (Christof Bauer, Sebastian Pfaller, Maximilian Ries and Wuyang Zhao), the so-called Capriccio group, met for a mini-retreat to discuss various scientific, organisational and strategic issues. Due to the ongoing Covid-19 restrictions, the meeting did not take place in a secluded location outside the university campus like last time, but in a sufficiently large seminar room on FAU's South Campus to ensure enough distance.

Each of the three P6 doctoral researchers gave a presentation on a topic they were currently working on in order to initiate discussions on these subjects.

The scientific part was complemented by another FRASCAL member, Dhananjay Phansalkar, who is doctoral researcher under the P9 project. He was invited to give a talk on his ongoing work on phase field modelling.

In between, the participants of the mini-retreat fortified themselves with a homemade snack outside and also continued their discussions during a hike between Erlangen and Nuremberg.

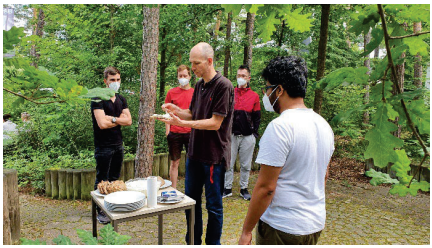


Figure 69: Members of the P6 project during a break in their mini retreat. (Images: A. Dakkouri-Baldauf)

5.4 1st virtual Peridynamic Mini-Symposium

(Text: Marie Laurien) On 21 December 2021, the 1st virtual Peridynamic Mini-Symposium took place, organized by members of GRK 2423 FRASCAL.

Research in the field of peridynamics has experienced tremendous growth in recent years. However, in one's close surrounding, fellow peridynamic researchers are still not that easy to find. Since two doctoral researchers of GRK 2423 FRASCAL, Jonas Ritter and Marie Laurien, employ the theory in their projects, the idea emerged to arrange an event where peridynamic researchers can exchange views and insights. The aim was to build a network of PhD students and bring together different peridynamic approaches and applications.

Thus, on a December afternoon, doctoral researchers and students from FAU Erlangen-Nürnberg, Bilkent University in Ankara and University of Strathclyde in Glasgow as well as Professor Paul Steinmann (spokesperson of the GRK 2423 FRASCAL) and Professor Ali Javili (Bilkent University) came together via Zoom. In six interesting talks, the participants reported on different aspects of continuum-kinematics-inspired peridynamics and various applications of PD, e.g. homogenization and nonlocal bone remodeling. Jonas Ritter, doctoral researcher of project P5 of GRK 2423 FRASCAL, presented his work on "Simulating fracture of resolved microstructures in porous brittle solids by means of peridynamics" Marie Laurien, doctoral researcher of project P10 of GRK 2423 FRASCAL gave a talk entitled "Peridynamic analysis of nonlocal wrinkling instabilities in bilayered systems". Each talk was followed by a lively discussion about the specific work of the researcher as well as challenges using peridynamics in general.

It was a great pleasure to meet the researchers and an active exchange about peridynamic topics will hopefully be continued in the future.

Figure 70: Researchers in the field of peridynamics coming together at the 1st Peridynamic Mini-Symposium via Zoom.

5.5 FRASCAL goes ART

Inspired by the images of the doctoral researchers' simulations, which are not only scientifically impressive but also extremely valuable from an artistic point of view, we have launched the project "FRASCAL goes ART".

The initial plan is for the (associated) doctoral researchers and postdocs (or together as a project) to illustrate their simulation motifs on a poster template, which will then be exhibited in the CSC building at FAU - the first exhibits are even already hanging there (see Figure 72) - and will soon also be available in a gallery on our website. We will see what further develops from this ...

Our gallery is still under construction, but you can already admire the first artworks.

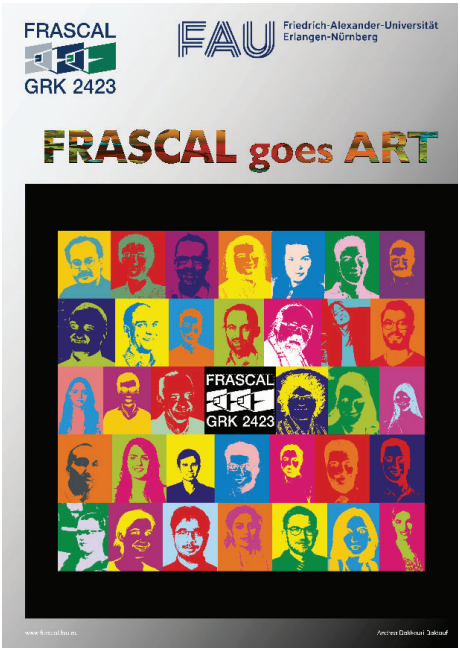


Figure 71: All FRASCAL members of the first cohort, depicted in pop art. (Image: A. Dakkouri-Baldauf)

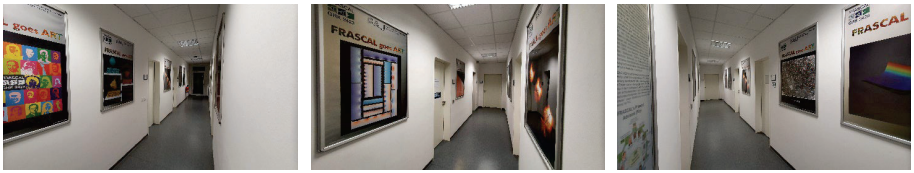


Figure 72: "FRASCAL goes ART" gallery in the CSC building. (Images: A. Dakkouri-Baldauf)

Figure 73: Atomistic simulation of sound waves emitted from a propagating crack in a harmonic crystal. The colours of the atoms represent their velocity magnitudes. (Tarakeshwar Lakshmipathy).

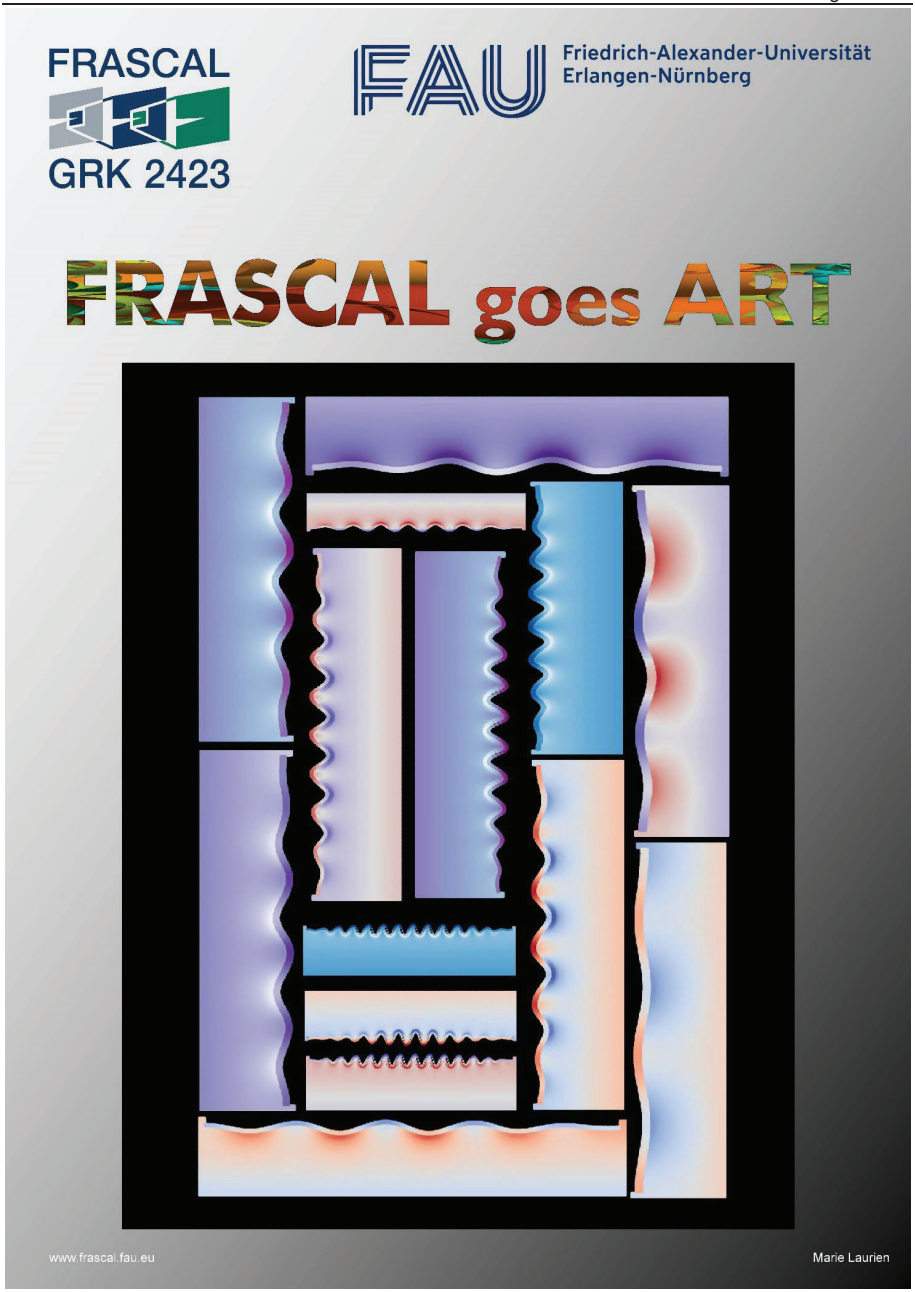


Figure 74: Nonlocal wrinkling instabilities. (Marie Laurien).

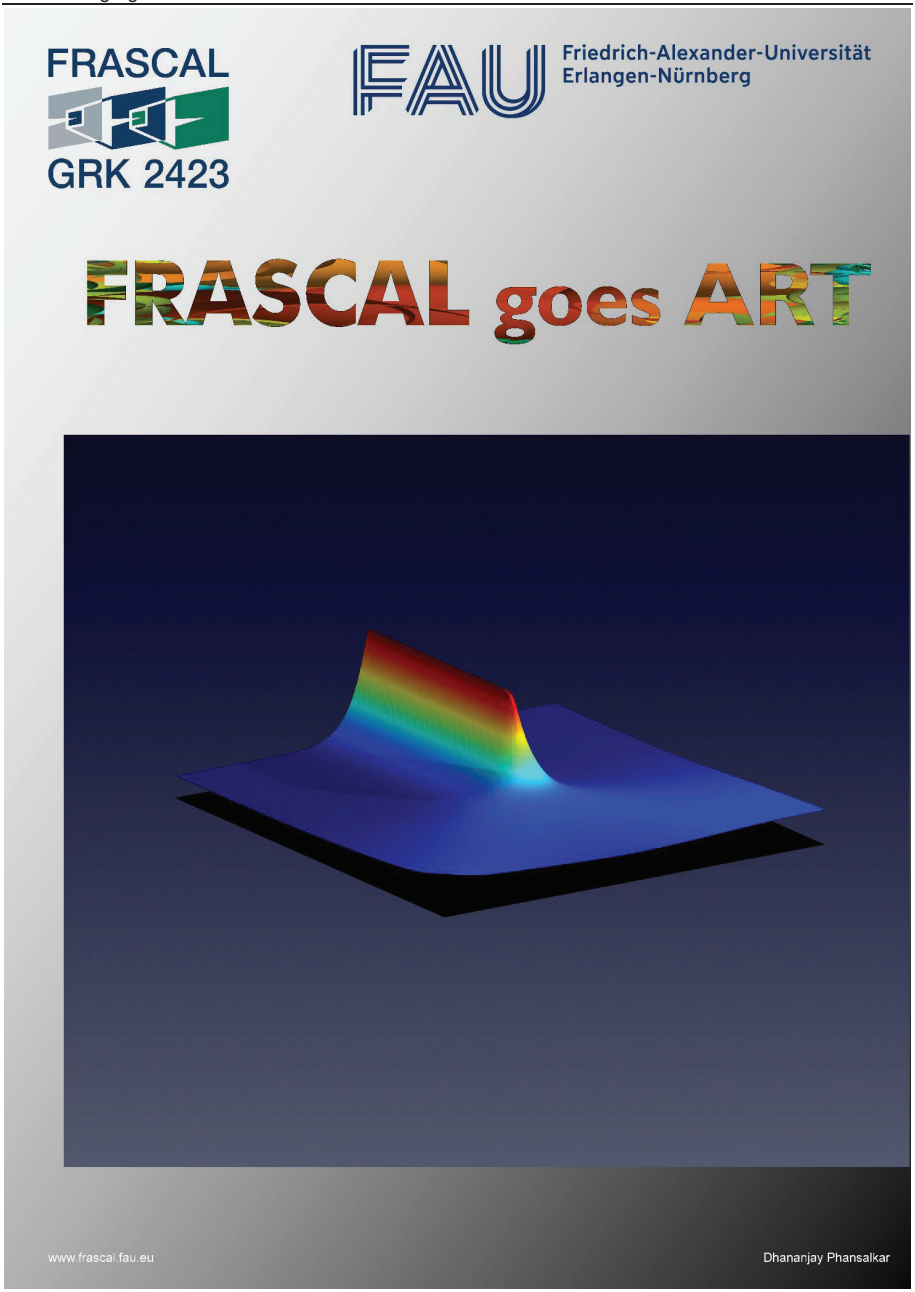


Figure 75: Phase-field model simulating the evolution of smeared crack in the 2D edge-crack panel. The red colour stands for the crack, the blue for the undamaged region with a transition zone in between. (Dhananjay Phansalkar).

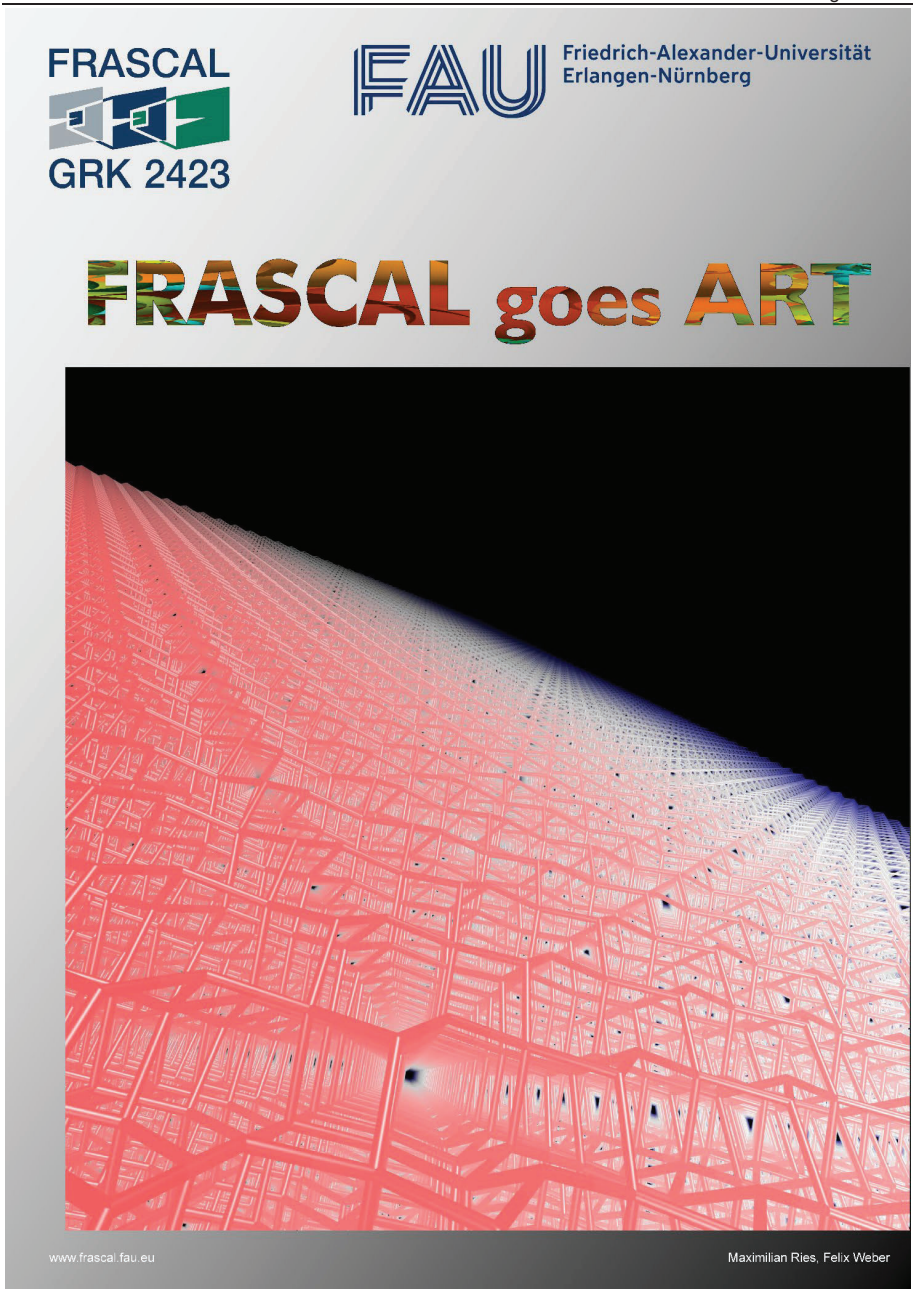


Figure 76: Silica nanofiller in coarse-grained resolution (Maximilian Ries, Felix Weber).

Figure 77: Direct shear tests on granular materials with different grain shapes. Simulated with the Multisphere Discrete Element Method. (Ali Mauricio Velasco Sabogal).

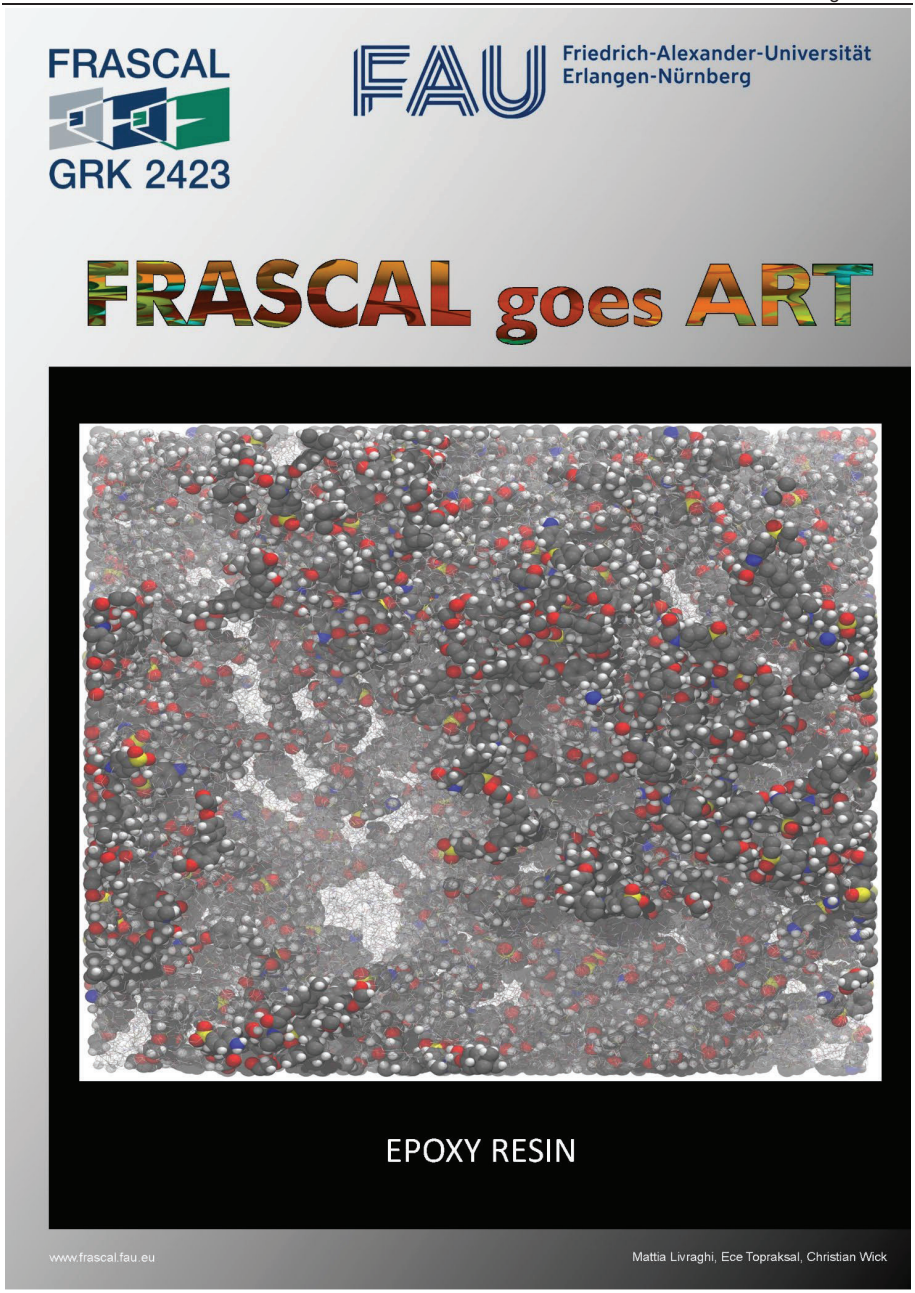


Figure 78: Curing epoxies in molecular dynamics. Only the largest, reacted molecular group is portrayed as balls and sticks, while every-thing else is shown as transparent wireframes. (Mattia Livraghi, Ece Topraksal, Christian Wick).

5.6 Weekly FRASCAL meetings

Usually, people met in person at the full-day events of the qualification programme and thus had the opportunity to exchange views on scientific, but also organisational, administrative and personal topics in a relaxed atmosphere before and after the events as well as during the breaks. Due to the pandemic-related changeover of the qualification programme from face-to-face to digital, these personal meetings suddenly fell away. Therefore, we initiated a weekly digital "FRASCAL "coffee break". There, FRASCAL-internal social contacts were cultivated, but also professional topics were discussed.

TOPZ

At the end of July 2020, the "FRASCAL coffee break" was transformed into a so-called TOPZ. In this "**T**opical **O**verview **P**resentation **Z**oomposium", every week a FRASCAL doctoral researcher presents her/his own latest research or current problems in a five- to ten-minute talk and discusses them with the interested audience. After these usually very helpful and fruitful discussions, organisational or personal matters are further discussed informally. In 2021, a total of 21 TOPZ took place, so that each doctoral researcher had her/his turn about twice.

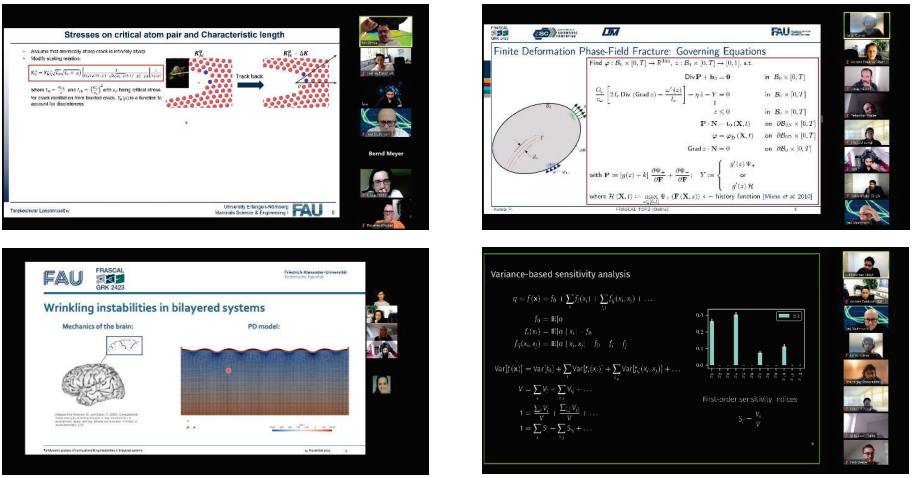


Figure 79: Topical Overview Presentation Zoomposium (TOPZ): Tarakeshwar Lakshmipathy (top left), Paras Kumar (top right), Marie Laurien (bottom left) and Sukhminder Singh (bottom right).

5.7 FRASCAL library

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.

82 new books have already been acquired in the first three years of FRASCAL.

For a complete list, see Appendix 3.

The library is very well received by FRASCAL members and usually at least a quarter to a third of the books are on loan.

Figure 80: FRASCAL library. (Image: A. Dakkouri-Baldauf)

6 Appendices

6.1 Appendix 1: Programme of the 5th RTG Seminar

Programme of the 5th RTG Seminar			
Date	23 April and 30 April 2021	Time	14:10 – 17:00
Venue	Zoom		

Lectures: 15 min + 5 min discussion

Time	Name	Title of Presentation
23 April 2021 – Part I		
14:10 – 14:20	WELCOME and INTRODUCTION	
Chairperson: **Achraf Atila**		
14:20 – 14:40	Julian Konrad (P3)	*Reorganization Processes in Epoxy Resins along Tensile Deformation*
14:40 – 15:00	Tarakeshwar Lakshmipathy (P2)	*On the Influence of Lattice Discreteness on Fracture Mechanics*
15:00 – 15:20	BREAK	
Chairperson: **Florian Wullschläger**		
15:20 – 15:40	Tobias Müller (P1)	*The Ongoing Quest for the Correct Boundary Conditions*
15:40 – 16:00	Sukhminder Singh (P11)	*Material Optimization to Enhance Delamination Resistance of Heterogeneous Structures*
16:00 – 16:20	BREAK	
Chairperson: **Maximilian Ries**		
16:20 – 16:40	Christian Wick (P12)	*Towards Understanding Mechanochemistry in Epoxy Resins*
16:40 – 17:00	Christof Bauer (P6)	*Switching Between FE and MD Descriptions and Vice Versa: Current Achievements*

Programme of the 5th RTG Seminar			
Date	23 April and 30 April 2021	Time	14:15 – 16:40
Venue	Zoom		

Lectures: 15 min + 5 min discussion

Time	Name	Title of Presentation
30 April 2021 – Part II		
14:15 – 14:20	WELCOME and INTRODUCTION	
Chairperson: **Samaneh Esfandiary**		
14:20 – 14:40	Jonas Ritter (P5)	*The Anisotropic Elastic Behaviour of Porous Snow under Compression*
14:40 – 15:00	Ali Mauricio Velasco Sabogal (P4)	*Modelling Grain Fracture within DEM Simulations*
15:00 – 15:20	BREAK	
Chairperson: **Wuyang Zhao**		
15:20 – 15:40	Paras Kumar (P8)	*Phase-Field Fracture Models in Finite Deformation Setting*
15:40 – 16:00	Nosaibeh Esfandiary (P7)	*Adhesion and Detachment of Hierarchical Structures: Critical and Subcritical Failure*
16:00 – 16:20	BREAK	
Chairperson: **Stefan Hiemer**		
16:20 – 16:40	Dhananjay Phansalkar (P9)	*Uniform and Adaptive ϵ in Phase-Field Models for Brittle Fractures*

6.2 Appendix 2: Programme of the 6th RTG Seminar

Programme of the 6th RTG Seminar			
Date	14 – 15 October 2021	Time	9:00 – 16:40
Venue	Hotel Riesengebirge, Neuhof a. d. Zenn		

Lectures: 20 min + 10 min discussion, associates: 15 min + 5 min discussion

Time	Name	Title of Presentation
14 October 2021		
9:00 – 9:30	CHECK IN & COFFEE	
9:30 – 9:40	WELCOME & INTRODUCTION	
Chairperson: **Christof Bauer**		
9:40 – 10:10	Nosaibeh Esfandiary (P7)	*Crack morphology and adhesion properties of hierarchical structures*
10:10 – 10:40	Paras Kumar (P8)	*Computational modeling of fracture in finite deformation setting via variational approaches*
10:40 – 11:00	COFFEE	
Chairperson: **Tarakeshwar Lakshmipathy**		
11:00 – 11:30	Jonas Ritter (P5)	*High strain rate compression of porous brittle snow structures*
11:30 – 12:30	*CVs and experiences of FRASCAL PAs: Julia Mergheim and Paul Steinmann*	
12:30 – 14:00	LUNCH BREAK	
Chairperson: **Ina Schmidt**		
14:00 – 14:30	Dhananjay Phansalkar (P9)	*Dynamic simulation of a phase-field fracture with the Newmark method*
14:30 – 15:00	Paul Steinmann	*Peer Review - from the Perspective of the Editor, the Reviewer and the Author*
15:15 – 18:30	HIKING	
18:30	DINNER	

Programme of the 6th RTG Seminar			
Date	14 – 15 October 2021	Time	9:00 – 16:40
	Hotel Riesengebirge, Neuhof a. d. Zenn		

Lectures: 20 min + 10 min discussion, associates: 15 min + 5 min discussion

Time	Name	Title of Presentation
15 October 2021		
8:00 – 9:00	BREAKFAST	
Chairperson: **Ahmad Hosseini**		
9:10 – 9:40	Julian Konrad (P3)	*Interfaces & nano-particles in epoxy resins*
9:40 – 10:10	Tarakeshwar Lakshmipathy (P2)	*Influence of crack tip radius on fracture behavior*
10:10 – 10:40	Christof Bauer (P6)	*Adaptive switching between FE and MD according to the current load level*
10:40 – 11:00	COFFEE BREAK	
Chairperson: **Nosaibeh Esfandiary**		
11:00 – 11:20	Wuyang Zhao (P6)	*A concurrent MD-FE coupling method towards fracture simulations of amorphous glassy polymers*
11:20 – 11:40	Prof. Dr. Daniel Koehn	*Deformation bands and fragmentation processes in faults across scales in Earth Sciences*
11:40 – 12:10	*CVs and experiences of FRASCAL PAs: Ana-Sunčana Smith*	
12:10 – 13:40	LUNCH BREAK	
Chairperson: **Lucie Spannraft**		
13:40 – 14:10	Sukhminder Singh (P11)	*Stochastic material optimization for enhancing delamination resistance of composites*
14:10 – 14:40	Tobias Müller (P1)	*How to determine the minimum energy pathway for crack propagation with correct boundary conditions*
14:40 – 15:10	Christian Wick (P12)	*Towards understanding mechanochemistry in epoxy resins - Part II*
15:10 – 15:30	COFFEE BREAK	
Chairperson: **Dhananjay Phansalkar**		
15:30 – 15:50	Ina Schmidt (P10)	*Bone fracture healing within continuum bone remodeling*
15:50 – 16:10	Samaneh Esfandiary (P7)	*Spectral signatures of fault tolerant neural architectures*
16:10 – 16:30	Stefan Hiemer (P5)	*Exploiting machine learning for the prediction of failure in microstructurally disordered materials*
16:30 – 16:40	OUTLOOK & CLOSING	

6.3 Appendix 3: List of book inventory

	Author	Title	Publishing Year
1	Anandarajah, Annalingam	Computational Methods in Elasticity and Plasticity: Solids and Porous Media	2010
2	Antman, Stuart S.	Nonlinear Problems of Elasticity	2005
3	Başar, Yavuz; Weichert, Dieter	Nonlinear Continuum Mechanics of Solids: Fundamental Mathematical and Physical Concepts	2010
4	Bažant, Zdeněk P.; Le, Jia-Liang; Salviato, Marco	Quasibrittle Fracture Mechanics and Size Effect	2021
5	Bergström, Jörgen	Mechanics of Solid Polymers: Theory and Computational Modeling	2015
6	Bertram, Albrecht	Elasticity and Plasticity of Large Deformations	2012
7	Bertram, Albrecht; Glüge, Rainer	Solid Mechanics: Theory, Modeling, and Problems	2015
8	Bland, David Russell	The Theory of Linear Viscoelasticity	2016
9	Bobaru, Florin; Foster, John T.; Geubelle, Philippe H.; Silling, Stewart A. (eds.)	Handbook of Peridynamic Modeling	2017
10	Bonet, Javier; Wood, Richard D.	Nonlinear Continuum Mechanics for Finite Element Analysis	2008
11	Borja, Ronaldo I.	Plasticity: Modeling & Computation	2013
12	Braides, Andrea	Γ-Convergence for Beginners	2002
13	Brázdová, Veronika; Bowler, David R.	Atomistic Computer Simulations; A Practical Guide	2013
14	Broberg, K. Bertram	Cracks and Fracture	1999
15	Bui, Huy Duong	Fracture Mechanics: Inverse Problems and Solutions	2006
16	Chadwick, Peter	Continuum Mechanics: Concise Theory and Problems	1999
17	Chakrabarty, Jagabanduhu	Theory of Plasticity	2006
18	Chatzigeorgiou, George; Charalambakis, Nicholas; Chemisky, Yves; Meraghni, Fodil	Thermomechanical Behavior of Dissipative Composite Materials	2018
19	Chen, Wai-Fah; Han, Da-Jian	Plasticity for Structural Engineers	2007

	Author	Title	Publishing Year
20	Chipot, Michel; Quittner, Pavol (eds.)	Handbook of Differential Equations – Stationary Partial Differential Equations Vol. 3	2006
21	Cho, Kwang Soo	Viscoelasticity of Polymers: Theory and Numerical Algorithms	2016
22	Christensen, Richard M.	Theory of Viscoelasticity	2003
23	Coussy, Olivier	Mechanics and Physics of Porous Solids	2010
24	Drozdov, Aleksey D.	Finite Elasticity and Viscoelasticity: A Course in the Nonlinear Mechanics of Solids	1996
25	Epstein, Marcelo	The Elements of Continuum Biomechanics	2012
26	Eringen, A. Cemal; Maugin, Gerard A.	Electrodynamics of Continua I: Foundations and Solid Media	1990
27	Eringen, A. Cemal; Maugin, Gerard A.	Electrodynamics of Continua II: Fluids and Complex Media	1990
28	Freeman, Eric; Robson, Elisabeth; Sierra, Kathy; Bates, Bert	Head First Design Patterns: Building Extensi-ble and Maintainable Object-Oriented Software	2020
29	Freund, Lambert B.	Dynamic Fracture Mechanics	1990
30	Goedecker, Stefan; Hoisie, Adolfy	Performance Optimization of Numerically Intensive Codes	2001
31	Goriely, Alain	The Mathematics and Mechanics of Biological Growth	2017
32	Green, Albert E.; Zerna, Wolfgang	Theoretical Elasticity	2012
33	Gross, Dietmar; Seelig, Thomas	Fracture Mechanics	2018
34	Gross, Dietmar; Seelig, Thomas	Fracture Mechanics	2018
35	Gurtin, Morton E.	Configurational Forces as Basic Concepts of Continuum Physics	2000
36	Han, Weimin; Reddy, B. Daya	Plasticity: Mathematical Theory and Numerical Analysis	2013
37	Hashiguchi, Koichi	Elastoplasticity Theory	2014
38	Haupt, Peter	Continuum Mechanics and Theory of Materials	2002
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