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Friedrich-Alexander-Universität
Erlangen-Nürnberg

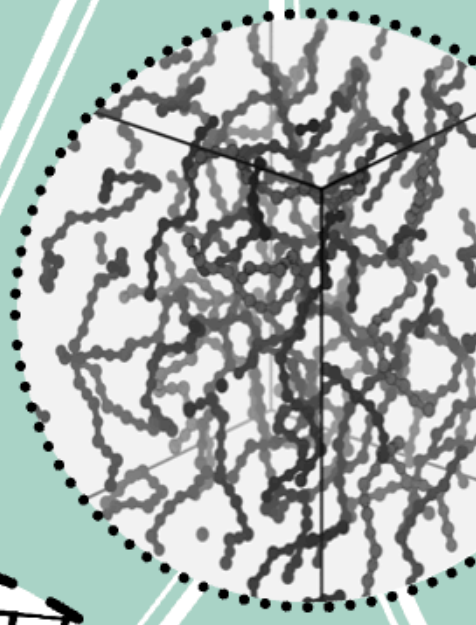
FRACTURE ACROSS SCALES

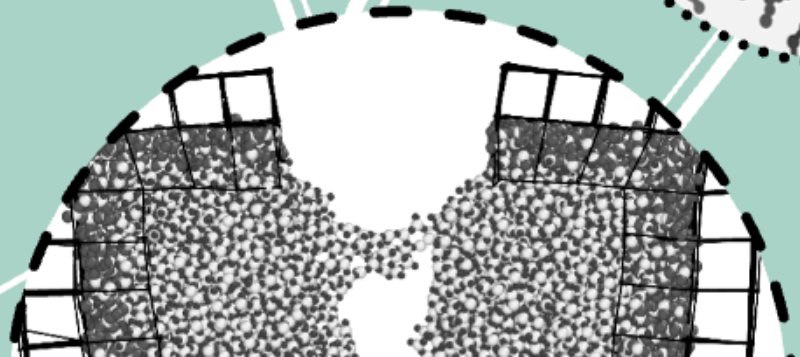
Integrating Mechanics, Materials Science, Mathematics, Chemistry and Physics

ANNUAL REPORT 2024

FRASCAL

GRK 2423





Annual Report
of the Research Training Group GRK 2423

FRASCAL

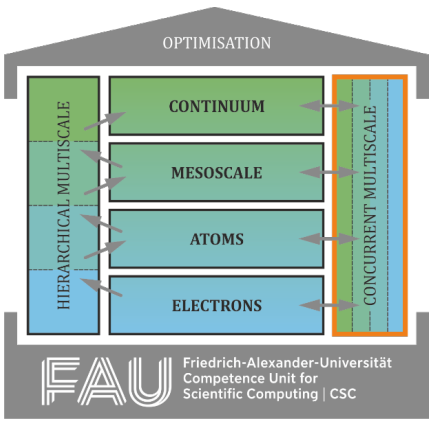
Fracture across Scales

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

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

Prof. Dr.-Ing. Paul Steinmann (spokesperson)
Prof. Dr. rer. nat. Michael Stingl (co-spokesperson)

2024



www.frascal.fau.de

IMPRESSUM

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Preface

The year 2024 marked a significant transition for FRASCAL as we experience the handover from one cohort of doctoral researchers to the next. This course but defining moment in our program was shaped by both the achievements of our outgoing researchers and the promising aspirations of those joining us. A key highlight of the year was our Recruitment Symposium, which played a crucial role in selecting the next generation of talented scientists. This event provided a vibrant platform for intellectual exchange, fostering discussions between prospective candidates, PAs, and current doctoral researchers. It was inspiring to see how new ideas and research ambitions took shape during this process, setting the foundation for the future of our graduate program.

As we look back on 2024, we also celebrate the achievements of our outgoing cohort. Their dedication, perseverance and contributions to their respective fields have enriched our academic community, and we are proud that they are on their finishing line and will move on to their next professional and personal goals.

We extend our gratitude to all doctoral researchers, PAs, coordinating and administrative staff who have supported this transition, ensuring a seamless handover and continued excellence in research and academic training. With renewed energy and enthusiasm, we look forward to the journey ahead, welcoming new perspectives and fostering a dynamic research environment in the years to come.

We hope this annual report provides valuable insights into the milestones, events, and achievements of FRASCAL throughout the past year.

Erlangen, January 2025

Paul Steinmann & Michael Stingl

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. rer. nat. Michael Stingl

Doctoral researchers' spokesperson:

Deepak Balasaheb Jadhav

Doctoral researchers' gender representative:

Shucheta Shegufta

Participating supervisors

Principal Advisors (PAs)	Chair, Department, Work Address	Contact Data	Research Area
Friedrich, Manuel, Prof. Dr. rer. nat.	Modeling and Numerics, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen	+49 9131 85-67 214 / - 67 225, manuel.friedrich@fau.de, www.mso.math.fau.de	**Applied Analysis, Calculus of Variations**
Koehn, Daniel, Prof. Dr. rer. nat.	Tectonics, Dep. of Geography and Geosciences, Schlossgarten 5, 91054 Erlangen	+49 9131 85-22626 daniel.koehn@fau.de, www.gzn.nat.fau.eu	**Structural Geology and Tectonics**
Leyendecker Sigrid, Prof. Dr.-Ing.	Applied Dynamics, Dep. of Mechanical Engineering, Immerwahrstraße 1, 91058 Erlangen	+49 9131 85-61 001, sigrid.leyendecker@fau.de, www.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, www.chemistry.nat.fau.eu/ccc/groups	**Surface Science**
Moretti, Paolo, PD 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, www.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**
Pflug, Lukas Dr. rer. nat.	FAU Competence Center Scientific Computing, Cauerstr. 11, 91058 Erlangen	+49 9131 85-67139 lukas.pflug@fau.de www.zisc.fau.de/zisc/staff	**Optimisation**
Pöschel, Thorsten, Prof. Dr. rer. nat.	Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraβe 3, 91058 Erlangen	+49 9131 85-70 501, thorsten.poeschel@fau.de, www.mss.cbi.fau.de	**Granular Media**
Smith, Ana-Sunčana, Prof. Dr. rer. nat.	Theoretical Physics, Dep. of Physics, Cauerstraβe 3, 91058 Erlangen	+49 9131 85 70 565 / -518, smith@physik.uni-erlangen.de, www.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, Cauerstraβe 11, 91058 Erlangen	+49 9131 85-67 141 / -20785, michael.stingl@fau.de, www.mso.math.fau.de	**Optimisation**
Wick, Christian R. Dr.	IZNF, Cauerstr. 3, 91058 Erlangen	+49 09131 85-70567, christian.wick@fau.de, www.puls.physik.fau.de	**Quantum-to-continuum model of thermoset**
Zahn, Dirk, Prof. Dr. rer. nat.	Theoretical Chemistry, ComputerChemistryCenter, Nägelsbachstr. 25, 91052 Erlangen	+49 9131 85-20 205 / 404, dirk.zahn@fau.de, www.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, www.matsim.techfak.uni-erlangen.de	**Statistical Mechanics of Materials**

Doctoral & postdoctoral researchers

Post Doc	Chair, Department, Work Address	Contact Data	Research Area
Hantal, György, Dr. rer. nat.	Theoretische Physik I, Dep. of Physics, Cauerstr. 3., 91058 Erlangen	+49 9131 85-70563 György.hantal@fau.de	**Quantum-to-Continuum Model of Thermoset**
Kumar, Paras, Dr. rer. nat.	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**
Ries, Maximilian Dr. rer. nat.	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**

Doctoral Researchers	Chair, Department, Work Address	Contact Data	Research Area
Canbolat, Utku	Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraße 3, 91058 Erlangen	+49 9131 85-70 490 / -518, utku.canbolat@fau.de, www.mss.cbi.fau.de	**Large Scale Simulations for Fragmentation of Granular Materials**
Greff, Christian	Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65 063 / -066, christian.greff@fau.de, www.matsim.techfak.uni-erlangen.de	**Tuning Adhesion Properties of Hierarchical Materials**
Igel, Lennart	Mathematical Optimisation, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen	+49 9131 85-67 083 / -20785, lennart.g.igel@fau.de, www.mso.math.fau.de	**Fracture Control by Material Optimisation**
Jadhav, Deepak Balasaheb	Applied Dynamics, Dep. of Mechanical Engineering, Immerwahrstraße 1, 91058 Erlangen	+49 9131 85-61 002 / -011, deepak.jadhav@fau.de, www.ltd.tf.uni-erlangen.de	**Adaptive Dynamic Fracture Simulation**
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**
Mathur, Bakul	Tectonics, Dep. of Geography and Geosciences, Schlossgarten 5, 91054 Erlangen	+49 1765 78 24271 bakul.mathur@fau.de, www.gzn.nat.fau.eu	**Fragmentation and Fracture in Geological Rocks**
Puhlmann, Pascal	Theoretical Chemistry, Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen	+49 9131 85-20422 pascal.puhlmann@fau.de www.chemistry.nat.fau.eu/ccc/groups/zahn-group/	**Fracture in Polymer Composites: Nano to Meso**
Ritterhoff, Christian	Computational Chemistry, Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen	+49 9131 85-20 421 / -404, christian.ritterhoff@fau.de, www.chemistry.nat.fau.eu/ccc/groups	**Chemistry at the Crack Tip**
Rohracker, Maurice	Applied Mechanics, Dep. of Mechanical Engineering, Paul-Gordan-Str. 3, 91052 Erlangen	+49 9131 85-64 410 / -413, mau.rohracker@fau.de, www.ltm.tf.fau.eu	**Fracture in Polymer Composites: Meso to Macro**
Seutter, Joscha	Modeling and Numerics, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen	+49 9131 85-67 215 / - 67 225, joscha.seutter@fau.de, www.mso.math.fau.de	**Discrete-to-Continuum Passage for Variational Fracture Models**
Shegufta, Shucheta	Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65 065 / -066, shucheta.shegufta@fau.de, www.matsim.techfak.uni-erlangen.de	**Failure in Porous Materials**
Weber, Felix	Applied Mechanics, Dep. of Mechanical Engineering, Paul-Gordan-Str. 3, 91052 Erlangen	+49 9131 85-64 410 / -413, felix.w.weber@fau.de, www.ltm.tf.fau.eu	**Multiscale Fracture of Thermoplastic Polymers**

Associated doctoral researchers

Associated Doctoral Researchers	Chair, Department, Work Address	Contact Data	Research Area
Laubert, Lukas	Applied Mechanics, Dep. of Mechanical Engineering, Paul-Gordan-Str. 3, 91052 Erlangen	+49 9131 85-644/ -10, lukas.laubert@fau.de, www.ltm.tf.fau.eu	**Multiscale Fracture of Thermoplastic Polymers**
Santarossa, Angel	Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraβe 3, 91058 Erlangen	+49 9131 85-70 482, angel.santarossa@fau.de, www.mss.cbi.fau.de	**Crack Front Segmentation in I+III Mixed Mode Loading**
Smith, Ruaridh	Tectonics, Dep. of Geography and Geosciences, Schlossgarten 5 91054 Erlangen	+49 9131 85 25915 ruaridh.smith@fau.de, www.gzn.nat.fau.eu	**Modelling Geothermal Systems through Fractured Media**
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	**Mechanics of Generalised Interfaces and Grain Boundaries**
Titlbach, Anna	Faculty of Mechanical Engineering Kesslerplatz 12, 90489 Nürnberg	+49 157 59611854 anna.titlbach@th-nuernberg.de	**Computational Bone Remodelling**

Mercator Fellows

Mercator Fellows	Affiliation	Expertise
Bitzek, Erik Prof. Dr.-Ing.	Max-Planck-Institut für Eisenforschung, Germany	Atomistic simulations of fracture processes with particular emphasis on 3D crack modelling and crack-microstructure interactions
De Lorenzis, Laura, Prof.	Eidgenössische Technische Hochschule Zürich, Switzerland	Computational fracture mechanics, variational phase-field modelling of brittle and ductile fracture, fracture in shells, multifield fracture problems, and fatigue
Pandolfi, Anna, Dr.	Politecnico di Milano, Italy	Computational mechanics, development of advanced fracture techniques (cohesive elements, eigenerosion), particle methods for the discretization of failure of solids and diffusion of fluids, and multiscale material models for porous brittle materials (brittle damage) to simulate fracking

External Advisory Board

External Advisory Board	Affiliation	Expertise
Bangerth, Wolfgang, Prof.	Colorado State Universtiy, CO, US	**Open source software development**
Kouznetsova, Varvara, Prof.	Eindhoven University of Technology, NL	**Optimization**
Ortiz, Michael, Prof.	California Institute of Technology, CA, US	**Data-driven mechanics**
Walther, Andrea, Prof.	Humboldt University Berlin, DE	**Industrial and applied mathematics**

1.3 Coordination and administration

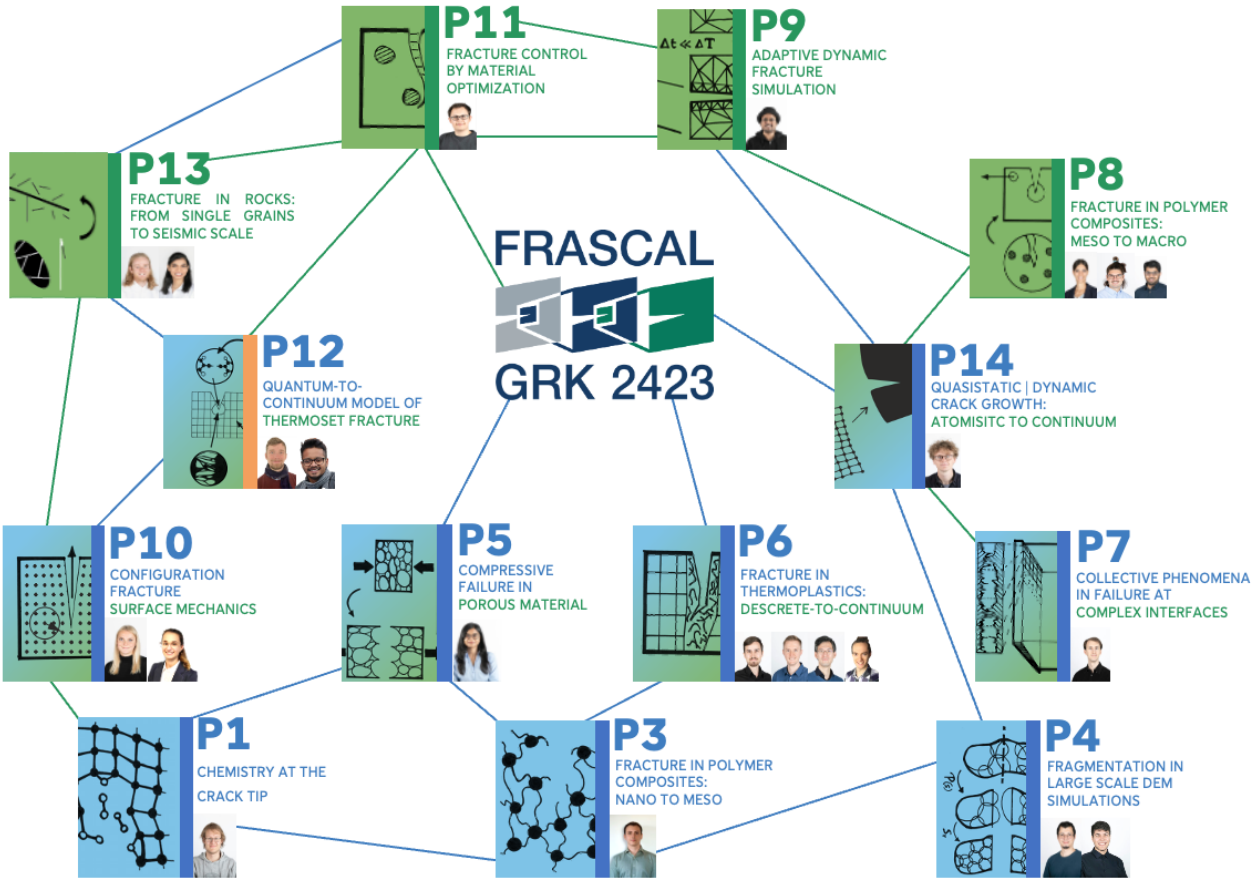
Coordination and administration of GRK 2423 FRASCAL

	Work Address	Contact Data	Work Area
Donhauser, Anna, Dr. rer. nat.	Competence Center Scientific Computing, CSC, Martensstraße 5a, 91058 Erlangen	+49 9131 85-20782 / -20785, www.frascal.fau.eu	**FRASCAL Coordination**
Güthlein, Nicole	Competence Center Scientific Computing, CSC, Martensstraße 5a, 91058 Erlangen	+49 9131 85 20780 / -20785, guethlein@math.fau.de, www.csc.fau.eu	**CSC-Administration**
Herzner, Ann-Sophie	Competence Center Scientific Computing, CSC, Martensstraße 5a, 91058 Erlangen	ann-sophie.herzner@fau.de, www.csc.fau.eu	**CSC Administration student assistant**

1.4 Reporting period

01 January 2024 to 31 December 2024

2 Research Programme



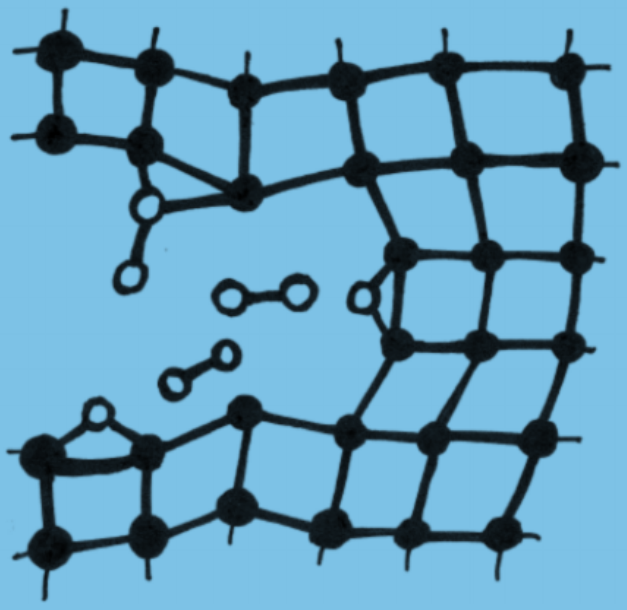
2.1 Research projects

Since the second cohort, FRASCAL comprises 12 doctoral projects (P1, P3-P11, P13 and P14), and one overarching postdoctoral project (P12). These range from quantum mechanics (P1) to atomistic and particle-based methods (P1-P4) and continuum mechanics (P8-P11, P13). Several projects (P5-P7, P12, P14) are dedicated to bridging atomistic and particle-based approaches to continuum-based techniques. The postdoctoral project P12 integrates the results and expertise developed in the doctoral projects to realise a concurrent multiscale modelling approach for fracture, ranging from quantum to continuum treatment. The effect of heterogeneities on fracture behavior is a common scientific question underlying all projects. Heterogeneities can exist on an atomic scale in the form of locally changed bonding or density (P1, P12, P14), or on larger scales, where heterogeneities include second phases as in composites (P3, P6, P8, P11), porous and geological structures (P5, P13), as well as interfaces, surfaces and/or (micro) cracks (P4, P7, P9, P10).

FRASCAL's projects:

	Projects – Short Title
P1	Chemistry at the Crack Tip
P2	Atomistics of Crack-Heterogeneity Interactions
P3	Fracture in Polymer Composites: Nano to Meso
P4	Fragmentation in Large Scale DEM Simulations
P5	Compressive Failure in Porous Materials
P6	Fracture in Thermoplastics: Discrete-to-Continuum
P7	Collective Phenomena in Failure at Complex Interfaces
P8	Fracture in Polymer Composites: Meso to Macro
P9	Adaptive Dynamic Fracture Simulation
P10	Configurational Fracture of Discrete Systems
P11	Fracture Control by Material Optimisation
P12	Quantum-to-Continuum Model of Thermoset Fracture
P13	Fracture in Rocks: From Single Grains to Seismic Scale
P14	Quasistatic/Dynamic Crack Growth: Atomistic to Continuum

	Associated Projects – Short Title
aPA	Mechanical and chemical properties of 2D materials
aPB	Deformation Behaviour and Fracture of Oxide Glasses
aPC	Hydraulic Fracturing in Hydrogels
aPD	Multiscale Mechanics of Granular Materials
aPE	Fracture and Failure Properties of Hierarchical Materials
aPF	AI for Predicting Subcritical Failure of Disordered Materials
aPG	Polymer Nanocomposites across the Scales
aPH	Fracture of Amorphous Polymers across the Scales
aPI	Spectral Signatures of Fault Tolerant Neural Architectures
aPJ	Mechanics of Generalised Interfaces and Grain Boundaries
aPK	Modelling and Simulation of Bone Adaption Processes
aPL	Modelling and Simulation of Flexoelectricity in Bone Fracture
aPM	Modelling Geothermal Systems in Faulted & Fractured Media



P 1

CHEMISTRY AT THE CRACK TIP

Christian Ritterhoff

Prof. Dr. Bernd Meyer
Computational Chemistry
Department of Chemistry and Pharmacy

P1: Chemistry at the Crack Tip

Christian L. Ritterhoff and Bernd Meyer

In my PhD project I extend the work of Tobias Müller to more complex materials, in particular, oxides, perovskites, and minerals relevant in geological processes (see project P13). The aim is to calculate fracture toughness of real materials from first-principles without using input data from experiment. The crucial requirement is the ability to perform atomistic simulations for large "pacman" cutouts around the crack tip using a flexible boundary scheme.

To achieve this on a feasible timescale for the more complex oxide perovskite SrTiO3, I decided last year to switch from a pure quantum mechanical approach to machine-learned interatomic potentials. Using the newly developed atomic cluster expansion (ACE),[1] the plan is to train the potential on DFT data, capturing the effects needed to describe the crack propagation and then use this to calculate larger cutouts to circumvent finite size effects. Experimental data gathered from the cleavage of SrTiO3 in ultra-high-vacuum indicated, however, a strain-induced ferroelectric effect during cleavage. The resulting polarization needs to be quenched on the emerging surfaces and thus has an effect on any finite cutout around the crack tip. Studying this with the previously mentioned "pacman" approach (the embedding of a finite cutout into the far-field solution from anisotropic linear elasticity continuum theory) is difficult, since the polarization leads to long-range electrostatic interactions, which have to be included in the boundary conditions as well as the machine-learned atomic potential.

In light of this, I decided to determine first an upper limit of the induced polarization during cleavage by going back to DFT calculations and studying the deformation of the ideal crystal during fracture using just a few bulk unit cells. Mode 1 fracture can be simply modelled by extending the [001]-direction of a cubic perovskite unit cell. By gradually increasing the [001] basis vector I can increase the strain until the material breaks and thus determine the polarization at the point of fracture. Using this polarization, I can estimate the charge which would build up at the fracture surface and thus suggest a surface reconstruction to quench this charge which can be compared to the experimental findings mentioned above.

First one has to determine the critical strain when fracture occurs. Utilizing my previous experience with the "pacman" approach I can get an estimation of the elongation of the last bond at the crack tip, which yields a value of roughly 10.3% of the cubic lattice constant. I can compare this value with the one from a traction–separation curve which is calculated by stacking multiple unit cells on-top of each other to simulate a bulk structure. By subsequently increasing the distance between two neighbouring (001) lattice planes,

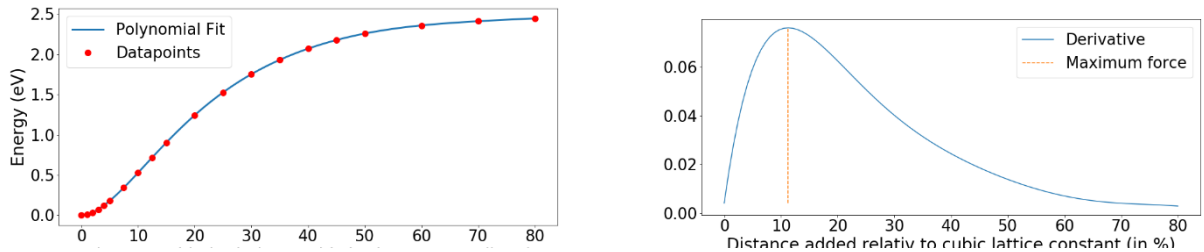


Figure 1 Left: Energy change from static DFT calculations for increasing separation of two neighbouring (001) lattice planes. Right: The derivative of the energy gives the corresponding stress. The maximum stress is reached at a strain of 11.3% of the cubic lattice constant.

the energy profile shown in Figure 1 is obtained. By taking the derivative of this separation curve, I can estimate the elongation at which the maximum stress
is required to further pull the material apart. This critical stress is reached at 11.3% of the cubic lattice constant and represents the strain at which the material would fracture. This is very close to my previous estimate taken from the “pacman” approach.
With this in hand I can calculate the optimized geometry of the strained structure. However, due to the increase of the lattice constant in the [001]-direction, the lattice constant in the other two directions can also change and therefore need to be optimized. The left graph in Figure 2 shows an example for the procedure used for this: Multiple different lateral lattice constants are probed, and the optimum is determined through a polynomial fit. Furthermore, the symmetry of the unit cell needs to be accounted for. The geometry optimizer will keep whichever symmetry was present at the start of the calculation and thus offers us the chance to selectively turn on and off different structural effects. The two most prominent are the ferroelectric (FE) effect and the antiferrodistortive (AFD) effect. The former is the source of the emerging polarization and is simply a relative displacement of the sublattices of the anions and cations in direction of the strain. A sketch of the AFD effect is included on the right side of Figure 2. The octahedrons of oxygen atoms around each Ti ion are rotated against each other with the layer below mirroring this rotation in the opposite direction.

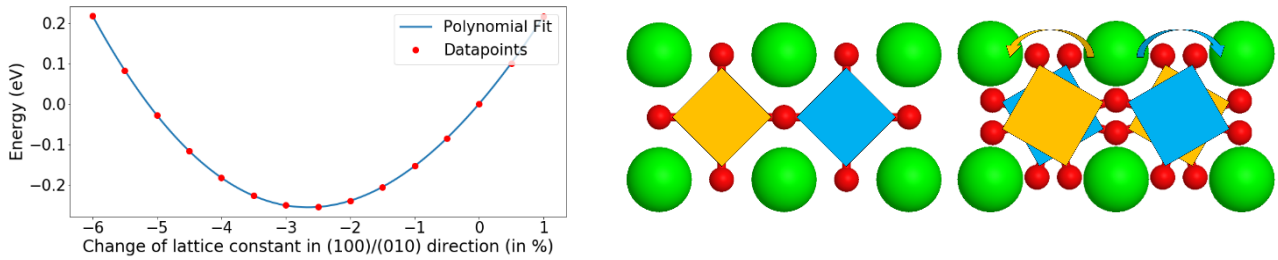


Figure 2 Left: Energy of a tetragonal centrosymmetric SrTiO3 crystal at 20% strain in [001]-direction with different in-plane lattice constant. Right: Sketch of the antiferrodistortive effect.

Selectively turning on or off the antiferrodistortive and ferroelectric effect by means of the initial configuration in the geometry optimization, I can gradually strain the material, optimize the lateral lattice constant as described above, and receive the four different energy profiles shown in Figure 3. The graphs show that while the AFD effect substantially changes the geometry of the purely tetragonal structure, the ferroelectric distortions are barely influenced by it.

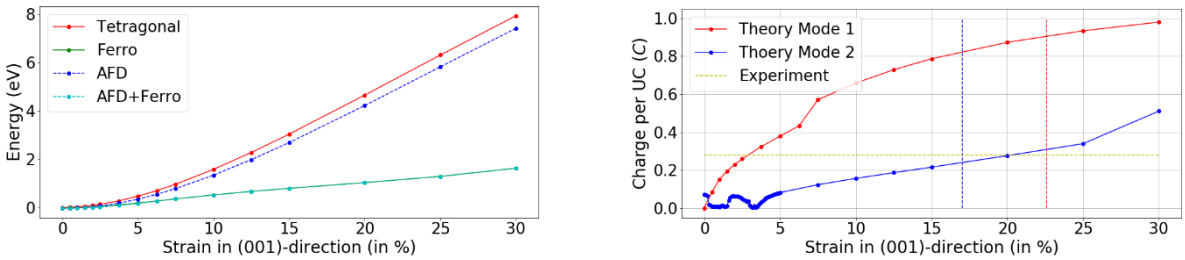
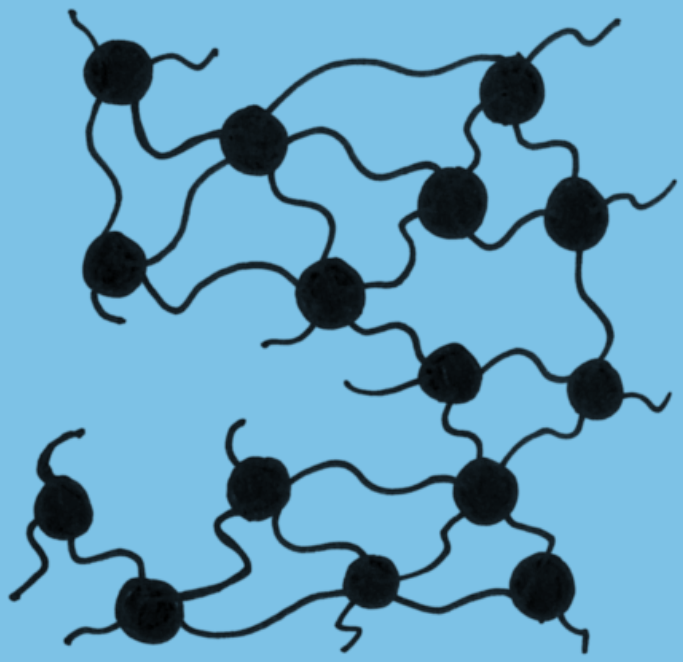


Figure 3 Left: Energy change of a SrTiO3 crystal experiencing increasing tensile strain. The different coloured curves differ by the allowed symmetry. Right: Charge per surface unit cell calculated for SrTiO3 at increasing strain for Mode 1 and Mode 2 fracture. The vertical lines indicate the critical strain during fracture for both fracture modes.

In the next step, the polarization of the structures with the lowest energy for each strain is calculated. Using this polarization, I can calculate the surface charge that will built up due to the strain-induced polarization during fracture. The right graph in Figure 3 shows the resulting curve for Mode 1 as well as Mode 2 fracture. This can be compared now to the surface charge found in experiment (see yellow horizontal line).[2] The cleavage setup in the experiments results dominantly in Mode 2 fracture. And indeed, for this fracture mode, our predicted surface charge agrees very well with the experimental observation. Even though SrTiO3 is centrosymmetric and not ferroelectric in the unstrained state, this result strongly suggests that the high strain at a crack tip induces locally a transition to a ferroelectric state, which leads to residual charges at the crack surfaces.

References

[1] Y. Lysogorskiy, et al. "Performant implementation of the atomic cluster expansion (PACE) and application to copper and silicon", npj Computational Materials 7, 97 (2021).
[2] I. Sokolović, et al. "Incipient ferroelectricity: A route towards bulk-terminated SrTiO3", Physical Review Materials 3, 034407 (2019).



P3

FRACTURE IN POLYMER COMPOSITES: NANO TO MESO

Pascal Puhlmann

Prof. Dr. Dirk Zahn
Theoretical Chemistry
Department of Chemistry and Pharmacy

P3: MD Simulation of Polymer Fracture: Polysiloxanes, Epoxy-Silica Composites

Pascal Puhlmann, Sviataslau Bakhmetau, Patrick Duchstein and Dirk Zahn

Polysiloxanes are mainly known as silicones and are polymers whose molecules have a backbone chain of alternating silicon and oxygen atoms instead of pure carbon atoms as in conventional organic polymers. This composition of an inorganic main chain with additional organic functional groups (e.g. methyl, -CH3) gives silicones a wide range of outstanding properties such as chemical inertness, elasticity and water resistance, as well as exceptional stability at high and low temperatures. These and other material-specific properties have given silicones a wide range of applications, from lubricating greases and electrical cable insulation to biomedical applications.

In the case of an elastomer, for example, it is of course also interesting to investigate the fracture behaviour in more detail. To this end, we have developed an MD force field based on quantum mechanics that allows bond breakage. To make this possible, the silicon-oxygen bond described usually by a harmonic potential was replaced by a Buckingham potential [1]. This theoretically results in the possibility of simple decay at a sufficiently large distance and tensile force. Once the new force field had been successfully set up and tested. The next step was to work on the polymerisation. In the polymerisation of siloxanes, simply spoken two silanols react to form a siloxane by splitting off water.

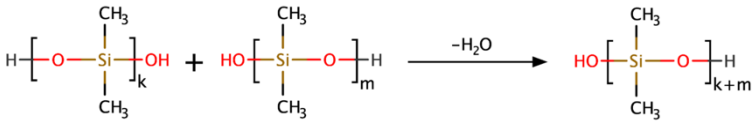


Fig 1: Polymerisation of PDMS by condensation reactions. In our simulation protocol, the gas phase reaction for k = m = 1 (and imposing vaporization of the formed water molecule) is used as the QM subsystem, whereas all other degrees of freedom are treated from MM calculations.

For the MD simulation of the polymerisation, a distance-angle criterion was implemented to find potential reaction partners to identify hydrogen bonds that enable a theoretical proton transfer. The water produced during the reaction is neglected in the MD simulation and removed from the reaction box. The reactions are additionally checked using a correction term based on quantum mechanics, so that only quantum mechanically allowed reactions are accepted. After successful identification and completion of the reactions in the MD simulation, the polymerisation of exclusively linear crosslinking monomers (Dimethylsilandiole; Si(OH)2(CH3)2), the simplest case of polymerisation, resulted in the following picture of polymer chains [2].

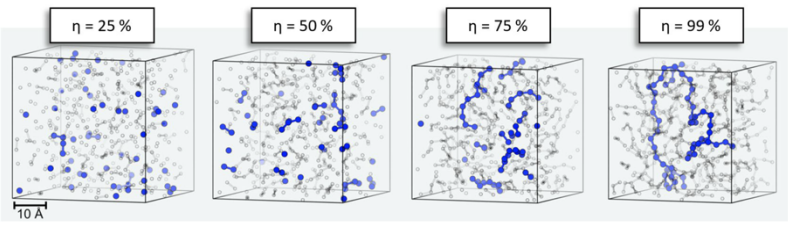


Fig 2: Curing of PDMS at 300 K and 1 atm using 3D periodic simulation cells. Starting from 500 DMSD precursor species, curing up to η = 99% is achieved, leading to a density increase from 0.91 g/cm3 to 1.04 g/cm3, respectively. Only Si atoms are shown. In the final system, a siloxane chain of 54 DMSD building blocks is highlighted in blue. To illustrate the formation process via reactions of monomers and oligomers, the same coloring is applied to earlier stages of polymerisation.

Parallel, we simulated setups of different weigh-ins of DMSD and TMS (Trimethylsilanol, monofunctional, chain terminator). We found strong dependencies of molecular mobility as function of the ratio DMSD/TMS and the cured polymers show the behaviour of silicone

oils. Indeed, for 0/10/20% TMS, we find ν = 65/15/9 and diffusion constants of 0.3/0.6/2.3 · 10−7 cm2s−1, respectively [2]. Next, we focus on mainly two projects. Firstly, the condensation process with higher functional silicone monomers like monomethylsilanetriol to produce three-dimensional networks followed by tensile testing and fracturing of the formed elastomers. Second, the mechanical aging process of the above-described silicone oils.

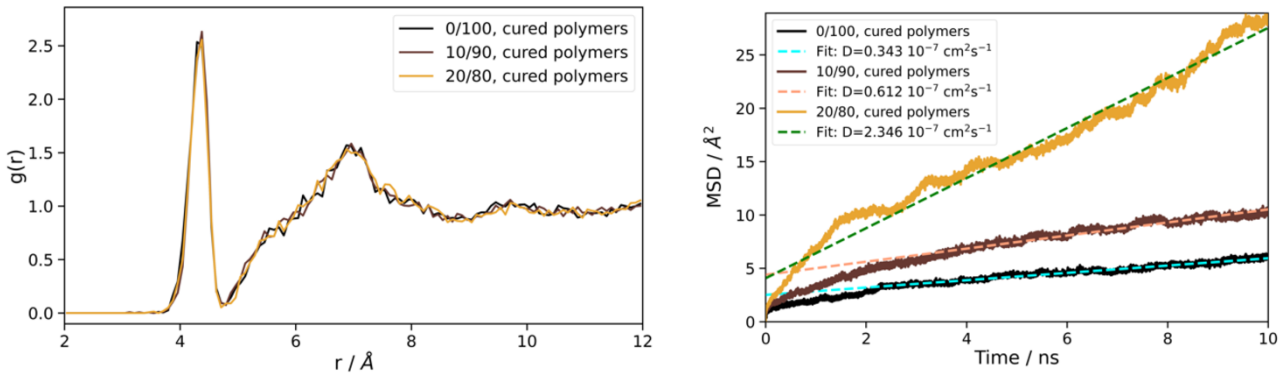


Fig 3: Characterization of the finally obtained silicone oil models from curing the precursor systems of 0/10/20% TMS content at 300 K and 1 atm. Left: radial distribution functions of the Si-O distances. Right: mean-squared-deviation profiles as function of time as used for assessing the diffusion constants. For the latter, linear fits are applied to the last 7 ns, as indicated by the dashed lines.

Epoxy-Silica composites are widely used construction materials as they offer appealing combination of light-weight materials with tailor-made stiffness, resilience and fracture characteristics. Based on the atomic scale modelling from Julian Konrad (doctoral researcher in the 1st round of the RTG) we collected in-depth understanding of the binding (epoxy curing) and unbinding (bond rupture) of epoxy resins and epoxy-silica interfaces [3-7]. This lead to the formulation of a coarse-grained (CG) model that effectively describes 10 nm scale building blocks by means of a single CG particle [8,9]. Therein, the interaction profiles (force-field) of the CG particles are derived for the quantum chemical and molecular

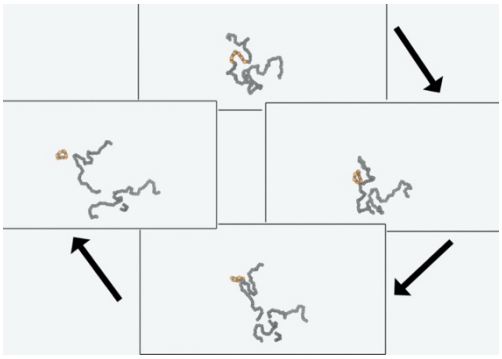


Fig 4: Preview for cyclic deformation as a simulation for mechanical ageing with two edges kept constant. Over a total of 100 cycles (large forces needed, thus only 10 ps per cycle), it was shown that molecules can react with each other through purely mechanical stress to form smaller (possibly also larger) new molecules. The figure also shows the possibility of rings (orange) splitting off from the strands (black) over time. For simplification, only the backbone is highlighted.

mechanics calculations reported in – and thus do not reflect empirical inputs but ab-initio-derived forces. On this basis, stress-strain diagrams of epoxy deformation and fracture were obtained in excellent agreement with tensile testing experiments available from the literature. The underlying µm scale models thus provide a realistic account of visco-elastic and plastic modes of deformation, crack nucleation and propagation of bulk epoxy [9]. Current efforts are directed in transferring the CG model of bulk epoxy for modelling composites with silica particles. While already offering nice insights into the role of local epoxy-silica interfaces as preferred regions of plastic deformations and crack nucleation, the full account of the tensile testing profiles still lacks from finite size effects. Using

massively parallel high-performance computing, we therefore explore the extension of the yet preliminary composite models shown below.

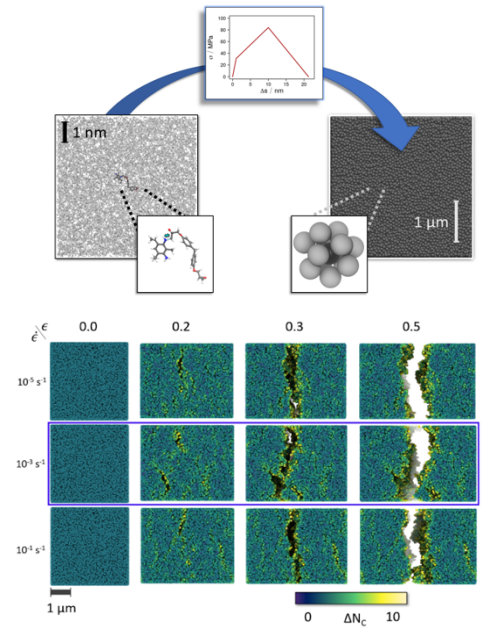


Fig 5: Transferring molecular simulation systems of a 98% cross-linked bisphenol-F-diglycidy-ether / 3,5-diethyltoluene-2,4-diamine epoxy resin model to a CG model of a single type of beads (right), thus reaching from nm to µm scales, respectively. The effective interactions of the beads are derived from the elastic properties and stress profiles as obtained from tensile testing of the MM models.

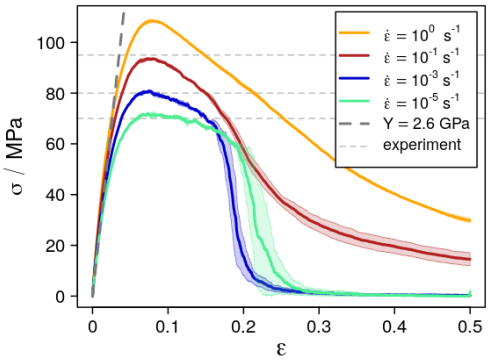


Fig 6: *Left*: snapshots of the tensile testing MD runs mimicking strain rates of 10^{-5} s^{-1} (upper panel), 10^{-3} s^{-1} (blue box) and 10^{-1} s^{-1} (lower panel), respectively. All runs were stared from the same initial configuration (ε = 0, left). While yielding starts ε = 0.1, the underlying damage pattern is best seen at ε = 0.2, respectively. To highlight the differences in damage and crack patterns, the particles are colored according to their net loss of nearest neighbor contacts as compared to the starting point (ε = 0). At the slowest strain rate (10^{-5} s^{-1}), the material has more time for relaxation processes, resulting in the formation of a comparably smooth crack surface. In turn, significantly rougher cracks and coexisting micro-crack formation is observed for tensile testing at 10^{-3} s^{-1} and 10^{-1} s^{-1}, respectively. *Right:* Stress-strain diagrams of the CG simulation model as compared to experimental benchmarks. Apart from the Youngs modulus, we also find the yielding characteristics in excellent agreement.

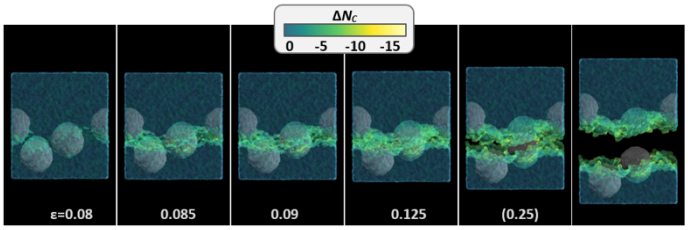


Fig 7: Tensile testing of the epoxy model featuring three randomly placed silica particles of 775 nm diameter. The epoxy resin is described by 10^5 beads of 105 nm diameter using a transparent representation for the individual spheres. The color scheme indicates the loss in nearest neighbor coordination upon tensile testing. Left-to-right: deformed system at ε=0.08, yielding and crack nucleation at the epoxy-silica interfaces (near ε=0.1), followed by fracture (ε>0.1). The crack pathway is determined by the merging of microcracks. Note that the current simulation model is too small to show crack bifurcation, blunting or coexisting microcracks as observed for the pure epoxy model.

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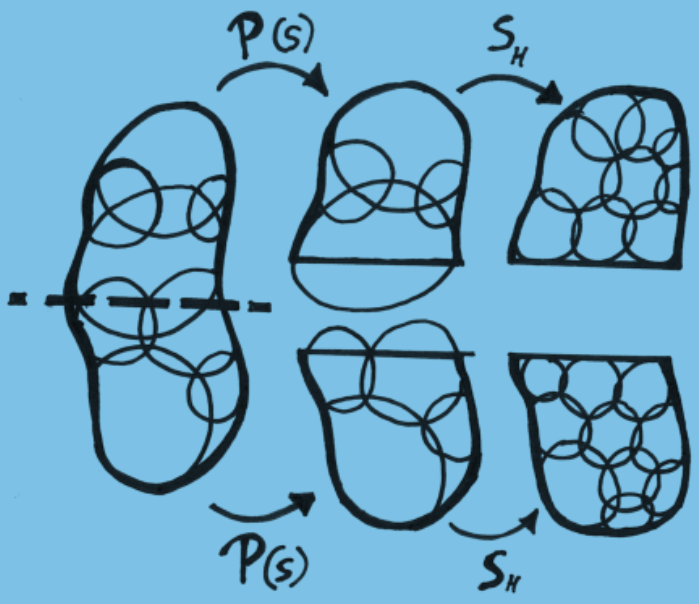

P4

FRAGMENTATION IN LARGE SCALE DEM SIMULATIONS

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P4: Modelling Fragmentation in Large Scale DEM Simulations

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The Python package for clump generation mentioned in the previous annual report is now available online. It includes a surface extraction method for clumps and three multispheres generation models: Favier, Ferellec-McDowell, and Euclidean Distance Transform (EDT). Being open-source aligns with FRASCAL's vision, and the package can easily be downloaded using pip install clump-python. It addresses the need for a clump generation package in the DEM community. The corresponding paper, which describes the models in detail, has been published in the February 2025 issue of SoftwareX. Additionally, we have improved the EDT model by adding two new functionalities. First, we introduced an option to set the maximum radius for spheres, which is particularly advantageous for bonded particle methods. Second, we added a postprocessing layer for multisphere creation to eliminate discretization errors at the particle boundaries. To create multispheres using surface meshes (e.g., STLs), we first discretize the geometry using voxelization. The precision of this process depends on the voxel size: smaller voxels yield higher precision. However, the speed of the method scales with the cube of the voxel size. The modification we introduced rescales the spheres in the multisphere representation so that their boundaries touch the surface mesh without exceeding it. This eliminates discretization errors at the boundaries and ensures that the spheres remain inside the surface mesh, which is especially critical for simulations involving stiff materials. The rescaling algorithm utilizes a spatial partitioning algorithm called k-Trees to find the closest surface mesh vertex, so it has minimal impact on the speed of multisphere creation. Additionally, this approach allows for the use of larger voxel sizes, which significantly improves the speed of multisphere creation without compromising accuracy. This is particularly

Figure 1: Multisphere representations of different geometries created by three clump generation method. From left to right, Favier, Ferellec-McDowell and Euclidean Distance Transform

important because our model requires multisphere creation to occur in real-time during every fracture event, making speed a critical factor.

The previous annual report mentioned that the model has a discrepancy in the particle size distribution (PSD). This issue arises from how the particles are split. In DEM, it is a common challenge to determine fracture planes for models using breakage criteria such as Mohr-Coulomb, Von Mises, or Tresca. These criteria only calculate whether a particle should fracture but do not describe how the particle should be split. Initially, we employed a commonly used model in the literature where the shear within a particle is calculated to determine the orientation of the fracture plane. The particle is then split such that the fracture plane passes through its centroid. However, this model fails to capture the chipping mechanism during fracture, as it always divides the particle into two halves. Chipping refers to the small loss of material from a particle (approximately 10% or less of the total particle volume). This splitting model not only provides an incorrect PSD but also affects the mechanical behavior of the system, as particle shape plays a crucial role. To address this issue, we implemented a new splitting model that identifies the three largest forces acting on a particle. These three points define a plane, and the particle is split along this plane. The motivation for this model comes from experimental studies, which show that fractures in granular materials

often initiate at contact points. This new method enables us to capture the chipping effect, resulting in more realistic outcomes.

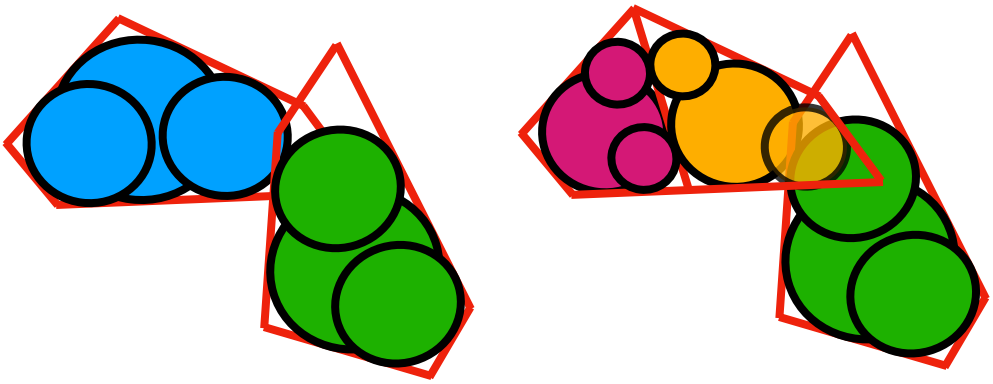

Figure 2: Two-dimensional illustration of the overlapping sphere problem. The outer red lines represent the surface mesh, while the interior circles depict multisphere approximations. The right image highlights the issue of large overlaps between spheres

Splitting the meshes in this way yields sharp edges, which are inherently problematic to approximate using the multisphere approach. This issue becomes more pronounced in our model. Figure 2 illustrates a two-dimensional sketch of the problem. The outer red lines indicate the surface mesh, while the interior circles correspond to their multisphere representations. Since contact detection is performed over the spheres, surface meshes may overlap independently of the spheres. If the number of spheres is insufficient, this overlap becomes more significant. For sharp-edged particles, this effect becomes even more evident, as such shapes require more spheres to accurately represent their geometry. When a fracture occurs, a sphere may be created with a large overlap with a neighbouring particle, as shown on the right-hand side of Figure 2. This introduces a significant amount of artificial energy into the system because the force is proportional to the overlap between the spheres. During bulk numerical simulations, we observed that this effect causes unrealistic behavior, such as particles escaping the system and destabilizing the simulation. To address this issue, we modified the contact model by introducing a cutoff mechanism. If the overlap between spheres exceeds a certain threshold, we replace the force between the particles with a constant value. This modification prevents the introduction of artificial energy into the system and ensures the simulation runs stably.

Another challenge when splitting geometries is the mesh on the surface of the fracture plane. Python modules typically close open surfaces by connecting the vertices along the edges. However, these modules use only a limited number of vertices, resulting in low surface resolution. This, in turn, impacts the multisphere creation after breakage. To address this issue, we developed a code that isolates the edge vertices, adds new vertices to the surface, and performs Delaunay triangulation. Additionally, this approach allows us to manipulate the surface geometry, enabling the creation of not only flat surfaces but also arbitrary ones to better mimic complex fracture planes.

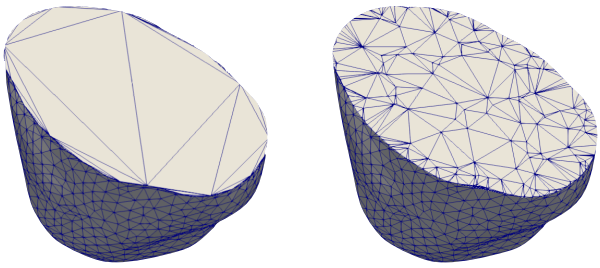

Figure 3: Remeshing STLs

P4C: Crack front segmentation in mixed-mode I+III fluid-induced fractures

Angel Santarossa, Leopoldo R. Gómez, Laureano Ortellado, Anabella Abate and Thorsten Pöschel

When a brittle material is subjected to tensile stress, cracks propagate perpendicular to the maximum direction of the principal stress [1]. However, when out-of-plane shear stress is applied (mixed-mode I+III), the crack front becomes unstable and segments in an array of facets inclined respectively to the mother planar crack [2]. The underlying physical mechanisms responsible for this phenomenon remain, however, unclear due to the lack of a complete 3D theory of crack propagation [3-4].
The main objective of this project is to study the leading mechanism controlling the fracture's geometry for systems under mixed loading. In particular, we aim to study mix-mode I+III fractures in hydro-gels in 3D.
Initially, we designed and developed a novel experimental setup to produce such mix-mode I+III fractures in soft materials (as illustrated in Fig.1). The apparatus is specially designed to be used in X-ray scanners, allowing the non-invasive reconstruction of complex fracture morphologies in 3D. Examples of different crack geometries obtained for different combinations of tension and shear stress are shown in Fig. 2. Furthermore, the apparatus is made of 3D-printed components, making it affordable and adaptable. A detailed

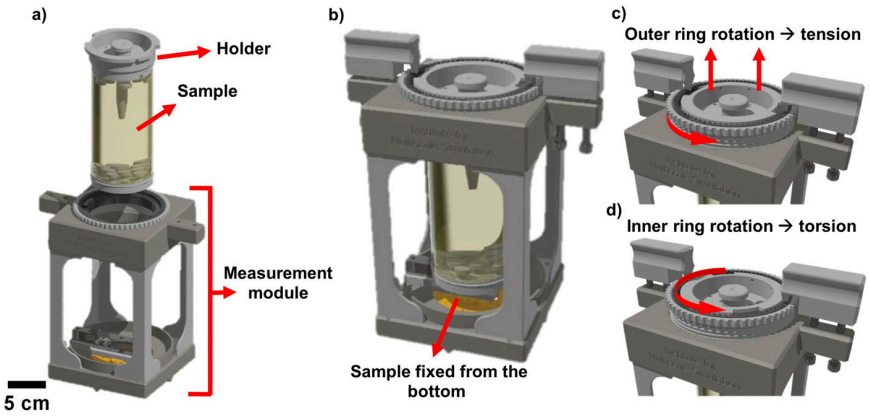

Fig 1: Experimental setup. The sample is mounted to the measurement module (a) and is fixed at the base (b). Two modes of loading can be applied: tension (c), by elongating the sample through the rotation of an outer ring, and shear stress (d), by rotating an inner ring that induces torsion. From: Rev. Sci. Instrum.. 2023;94(7). doi:10.1063/5.0145709.

description of its parts, functioning, and examples demonstrating its capabilities are published in an open-access research article [5].

The device can also be utilized for in situ measurements, i.e., the sample is scanned sequentially after deforming the sample in steps, enabling the examination of fracture growth at consecutive stages. Examples of 3D reconstructions of a mixed-mode I+III fracture in different steps of the fracture evolution are shown in Fig.3.

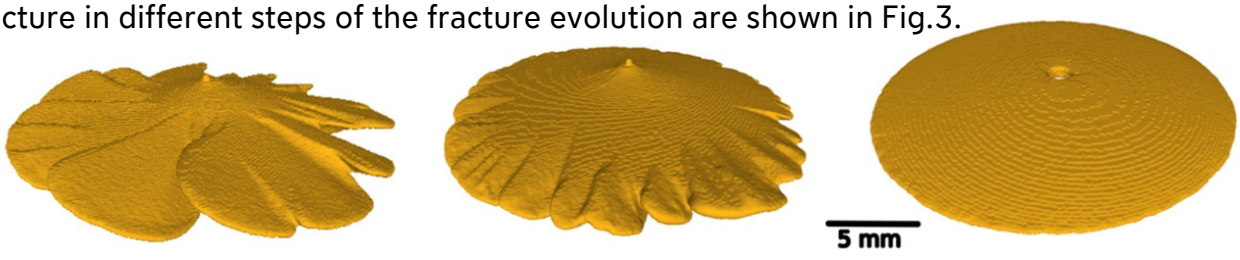

Fig. 2. Visualization of crack geometries in mixed modes I+III fractures using air and an 8 mm elongation of the gel. Cracks were obtained for different values of the torsion angle: 50°(left), 30° (middle), a zero torsion (a mode I driven fracture) (right). From: Rev. Sci. Instrum.. 2023;94(7). doi:10.1063/5.0145709.

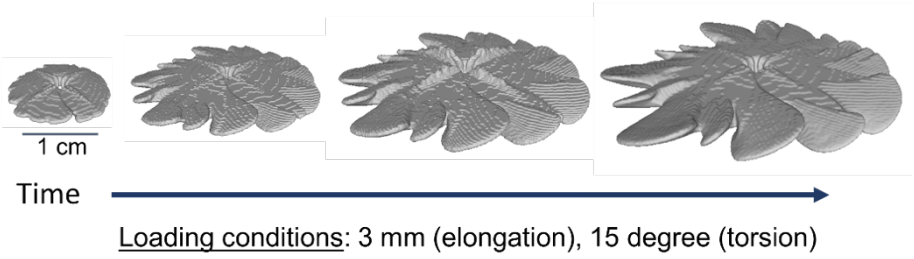

Fig 3: Reconstructions of a crack geometries under mixed mode I+III loading in different steps of the crack propagation. Initial loading conditions are described in the image. To propagate the fracture, the elongation of the sample was increased sequentially

The obtained reconstructed geometry of the cracks in combination with the experimental conditions (angle of torsion, gel's elongation) are used in FEM simulations to determine the stress intensity factors at the crack tip, as shown in Fig. 4. We observed that, locally, the opening mode KI remains dominant along the fracture tips, while the shear modes KII and KIII are significantly smaller. Our experimental and numerical results provide clear evidence that the Principle of Local Symmetry (PLS), which states that fractures propagate in directions that locally cancel shear stresses, governs the fragmentation of brittle

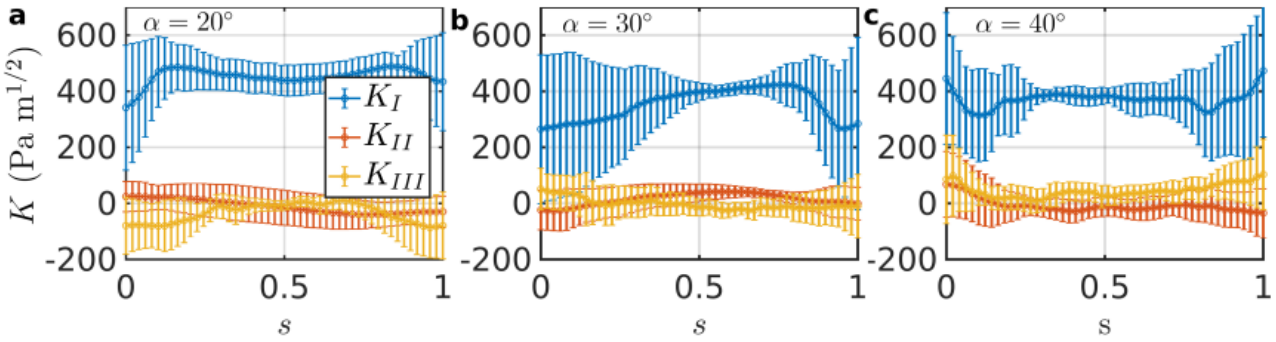

Fig. 4. Stress intensity factors of facets for fractures under different torsion angles. Modes of K over the normalized length, s, of the fracture tip, where $s \in [0, 1]$ covers one of the crack's facets. The solid lines show the mean over the crack's facets; the error bars represent one standard deviation. For all tests shown in this figure the samples were elongated by 4 mm and twisted by α = 20°, α = 30°, and α = 40°. The distributions of stresses were obtained by finite element analysis and the stress intensity factors through stress matching.

hydrogels under mixed-mode I+III loading.

Deviations from the PLS were observed near the edges of the facets, where fluctuations in the stress intensity factors became more pronounced. Large fluctuations near the edges of the facets, $s \gtrsim 0$ and $s \lesssim 1$, suggest that the systematic deviations from the PLS are due to elastic interactions between the facets. To test such a hypothesis, the stress intensity factors for early and well-evolved segmented fractures were compared. To that aim the detailed geometry of evolving cracks was obtained through X-ray tomography and used to compute the local stress intensity factors using finite element simulations. Figure 5 shows a crack at two successive stages of a mixed-mode I+III fracture test, with a sample rotation of α = 30°. In the early stages of its evolution, after an initial stretch of the sample by 3 mm, the fracture reveals numerous small facets resulting from the segmentation of the initially coin-shaped fracture with a circular tip. As the crack progresses, after further stretching to a total of 4 mm, the facets grow and thicken. Furthermore, the coarsening of the facets leads to a reduction in their number. The corresponding stress intensity factors

along the crack tip are shown in the lower part of Fig. 5. The fluctuations in the stress intensity factors near the edges are much greater for developed cracks than for cracks in an early stage of development. Growing facets can be seen as cracks that interact with the initial disc-shaped parent crack and with neighboring facets. Small facets whose tips are distant from one another grow independently. At a later stage, the tips of adjacent facets are less distant. Thus, their mechanical interaction results in a stress amplification (left panel of Fig. 6).

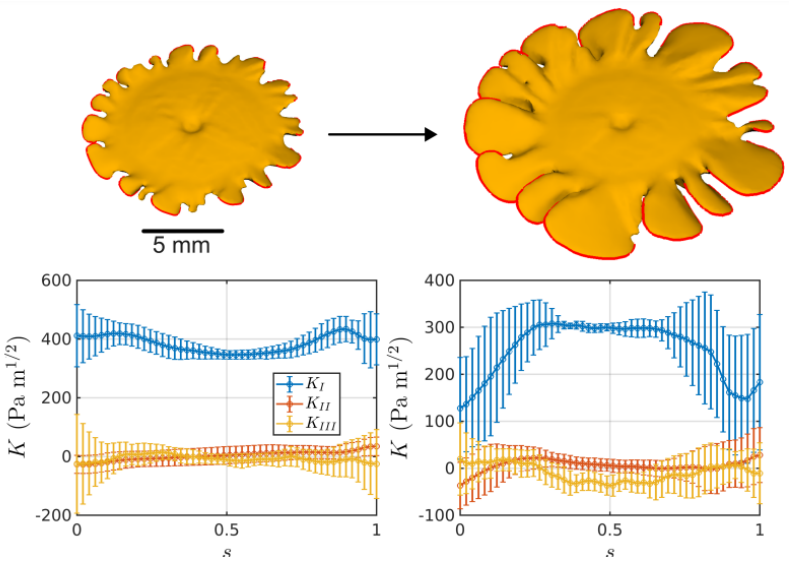

Fig. 5. Stress intensity factors of early and developed facets. Left and right panels show the same fracture at different stages of its evolution. The rotation of the sample is α = 30°, left: elongation is 3 mm; right: 4 mm. The top panels display the fracture as obtained from x-ray tomography, with the red curves indicating the fracture tip. The bottom panels show the averaged stress intensity factors K as a function of the normalized length of the fracture tip, s.

Further growth can lead facets to structure in echelon configurations, as schematically shown in the right panel of Fig. 6, leading to a stress shielding configuration. Overall, facet-facet interactions can either amplify or shield the stress intensity factors near the crack tips, depending on the geometric configuration and the proximity of the facets.

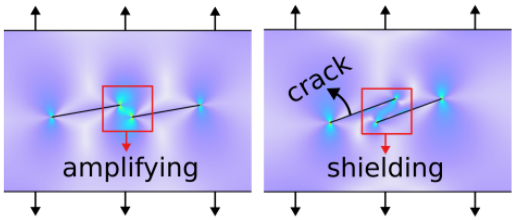

Fig. 6: Facet Interaction. Illustration of the facet interactions for a growing crack. Small facets formed at an early stage grow independently. At later stages, large facets can align, causing amplification of the stress (left panel). Further facet growth can lead to overlapping configurations, which reduces the stress at the tips due to shielding (right panel).

The obtained results suggest that while the PLS provides a robust framework for understanding crack propagation in brittle materials under mixed-mode loading, considerations of facet size and elastic interactions are essential for accurately predicting fracture behavior.

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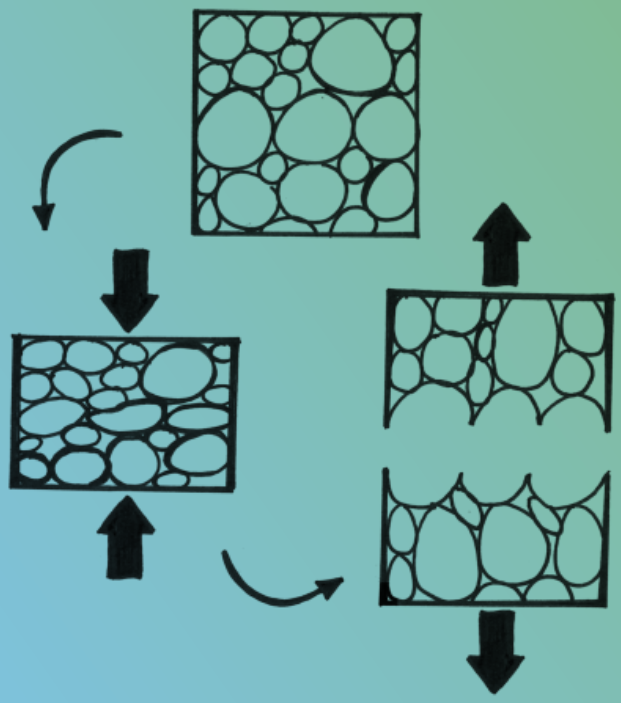

P5

COMPRESSIVE FAILURE IN POROUS MATERIAL

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P5: Modeling failure of disordered porous material with homogenized microstructure using Peridynamics

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While porosity and pore distribution play a crucial role in the mechanical behaviour of porous materials, modeling porous microstructure comes with very high computational costs, making computation at larger scales almost impossible. To address this challenges, we investigate the suitability of the Intermediate Homogenization method proposed by Chen et al [1]. In this technique, a certain percentage of peridynamic bonds of a material point, corresponding the the porosity ϕ, is deleted randomly, as shown in Figure 1a. For each bond, a random number is generated from an uniform distribution in (0,1). If the random number is smaller than $\phi/\phi c$, where ϕc is the critical porosity, the bond is deleted. Bond deletion reduces the elastic modulus of the material, corresponding to porosity, and the stochastic nature of bond deletion introduces disorder into the model.

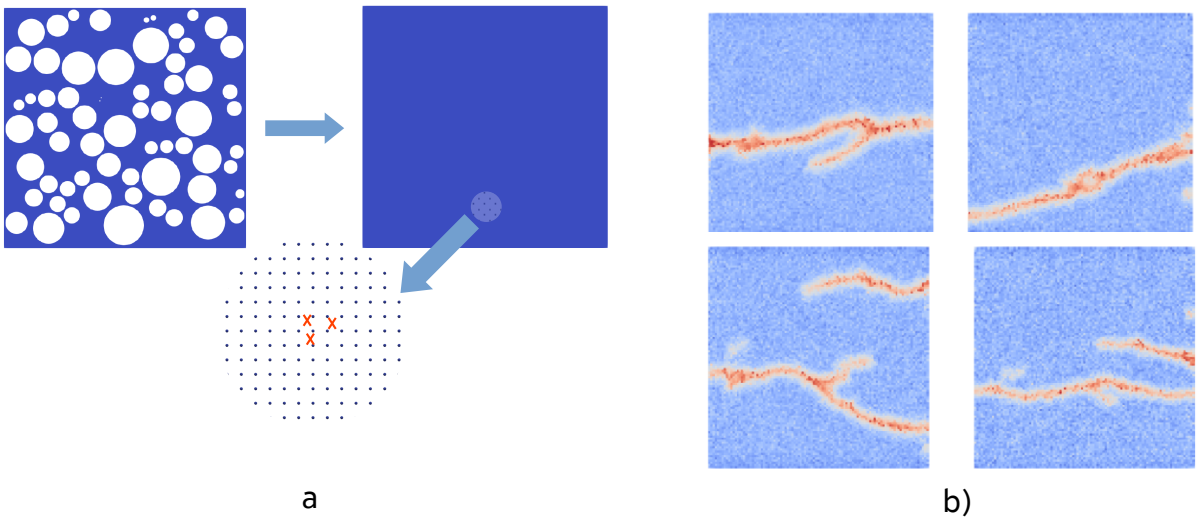

Fig 1: Intermediate Homogenization. a) Instead of resolving the porous microstructure, bonds are deleted randomly from a solid specimen; b) Damage patterns for homogenized specimen with 15% porosity for quasi-static tention tests. Each specimen shows significant variation in damage pattern, highlighting the fluctuation introduced by the intermediate homogenization method

We apply this method for different porosities and compare the results to materials with artificially generated porous microstructure [2]. Bond-based peridynamics is used to model elastic behaviour and damage is introduced by a critical stretch that is calibrated from fracture energy release rate and horizon [3]. The elastic modulus and fracture energy of the homogenized material without bond deletion is the same as that of the matrix of the resolved microstructure. Results show good agreement for both elastic modulus and peak stress, corresponding to a relatively high disordered porous microstructure, as shown in Figure 2. However, it is also observed that these results are sensitive to the value of m, which is the ratio of horizon and discretization size, indicating that the intermediate homogenization method is influenced by discretization. A closer inspection of the bond deletion process reveals that this dependence is inherent to the model. Since each bond is deleted based on independent probability, for an increasing number of bonds per material point, the variance of the ratio of deleted bonds is decreased. The coefficient of

variance of bond retention in a material point can be expressed as,

$$C_v = \frac{1}{m\left(1-\frac{\varphi}{\varphi_c}\right)^2}\sqrt{\frac{1-\left(1-\frac{\varphi}{\varphi_c}\right)^2}{\pi}}, \quad (1)$$

which may be used as a measure of disorder in the system. Therefore for this particular method of bond deletion, disorder the structure gets more homogenized as m increases, as shown in figure 3.

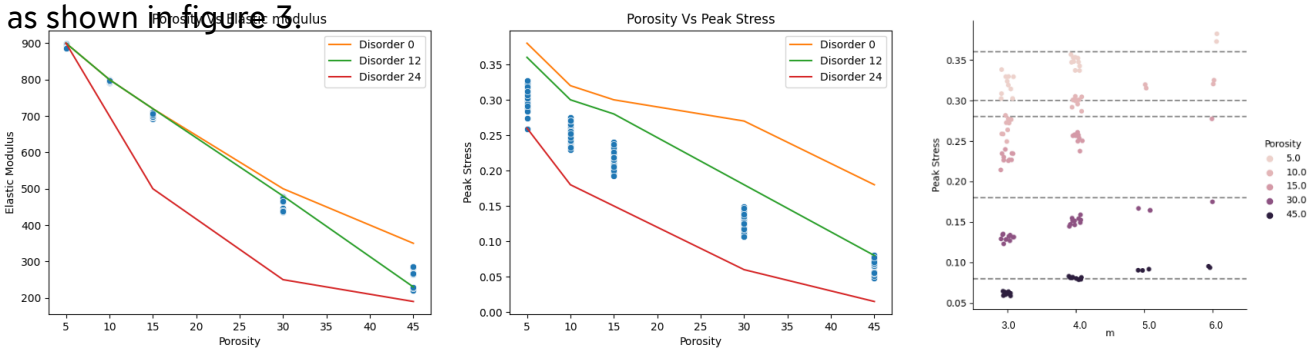

Fig 2: Results of quasi-static tension tests. a) Comparison with results from resolved microstructure; b) Peak stress vs m, where results show an increase of these values with increasing m. The dashed lines indicate the reference values for corresponding porosity for disorder 12 for resolved microstructure (see [2] for definition of disorder).

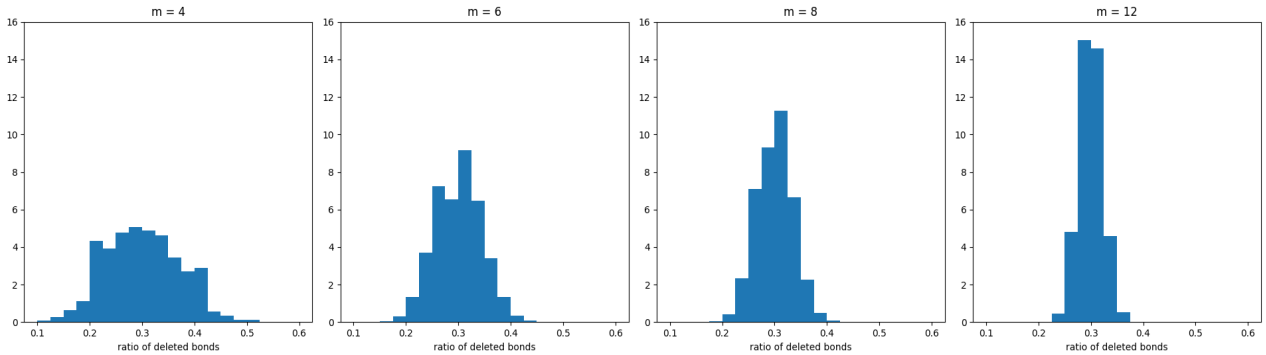

Fig 3: Probability distribution of the ratio of the deleted bonds per node for structures with 30% porosity, highlighting homogenization with m.

make disorder independent of number of bonds and m, we modify the IH model by rescaling the elastic modulus by a factor ηϕ,Cv, where ηϕ,Cv is a function of porosity, m and coefficient of variance, and at the same time delete a fraction 1-p of bonds. The factor ηϕ,Cv is given by

$$\eta_{\varphi,C_v} = (1-\varphi)^2\left(1+\pi m^2 {C_v}^2\right). \quad (2)$$

We apply this to model anticrack type failure of foam glass [4], which has a porosity of 95%. In our model, for m value of 4.0 and a coeffiecient of variance 0.2, this corresponds to 66.78% of the bonds being deleted and a 99.25% reduction of the elastic modulus, damage pattern shown in figure 4.

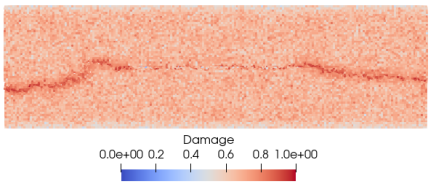

Fig 4: Anticrack type fracture in foam glass specimen with a central notch.

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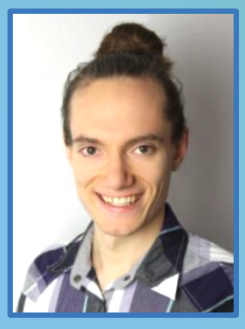
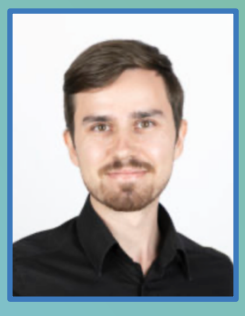
P6

FRACTURE IN THERMOPLASTICS: DISCRETE-TO-CONTINUUM

Felix Weber



Lukas Laubert



Maximilian Ries

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P6.2: Multiscale Fracture Simulations of Glassy Materials

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In P6, we develop and perform multiscale simulations of glassy materials using the Capriccio method [1], which couples molecular dynamics (MD) and the finite element method (FE) concurrently. One of our long-term goals is to use the Capriccio method to study the fracture of polymers and polymer nanocomposites. However, for generic studies of feasibility of multiscale fracture simulations, inorganic glasses are particularly suitable as sample materials because they have a much smaller fracture process zone compared to polymers. In [2], we perform three-dimensional plane strain mode I and mode III fracture simulations of silicon dioxide glass (silica) by applying surface tractions to an FE domain to propagate a crack through a pre-notched MD region.
Figure 1 shows the general setup of the simulations, where the inner silicon and oxygen atoms are described by classical Newtonian particle dynamics (ND), while the outermost particles are equipped with additional dissipative particle dynamics (DPD) terms to subject the atomic domain to a heat bath that controls the temperature. In this study, we use the MD model of Sundararaman et al. [3], the so-called SHIK potential, in which the short-range interactions are modeled by a Buckingham term and the long-range interactions are calculated using the Wolf truncation method. We attach the anchor points to some of the DPD atoms using harmonic springs, which act as auxiliary particles between the FE and MD domains to transfer forces and displacements. The stiffness of the anchor point springs and the load step size applied to the FE domain are determined in quasi-1D simulations, which are a simple means of examining the coupling method from a fundamental point of view. Since the material properties of the FE and MD domains must match to achieve physically meaningful results, we derive the Young's modulus and Poisson's ratio a priori

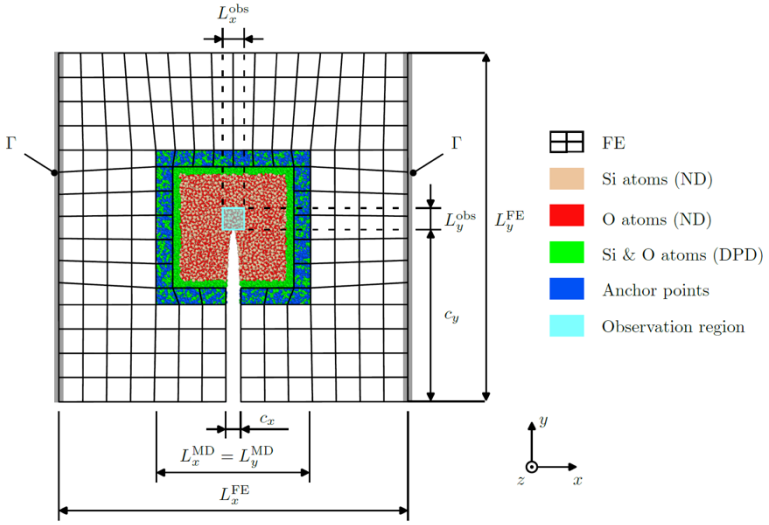

Fig 1: Setup of the particle-to-continuum fracture simulations using the Capriccio method [2].

for specimens prepared at different cooling rates from uniaxial tensile tests using pure MD under periodic boundary conditions (PBC).
The FE-MD specimens contain a notch of width cx and length cy, where we test different configurations: i) a single edge crack in a rectangular panel, ii) three- and four-point bending, and iii) mode III (applying longitudinal shear to the rectangular panels). In the mode III simulations, we fix the distance of the two loaded surfaces of the FE region to

prevent the system from rotating about the y-axis. However, the reaction stress resulting from this constraint is small compared to the applied load on the samples.
The quantities of interest are evaluated in an observation region in front of the crack tip. An external tensile load is applied by imposing a surface traction, which is defined in the material configuration Ti at different load rates and for samples synthesized at different cooling rates. Using linear elastic fracture mechanics (LEFM), we derive fracture toughness and crack opening displacement (COD) values that are in the range of the experimental data. In this context, we use the formulas for the stress intensity factors under the conditions of modes I and III given in [4], which depend on the external mechanical loading of the samples and the geometry of the test setups. Figure 2 shows a) the virial stress and b) the number of pairwise interactions, i.e. the number of bonds, evaluated in observation regions in front of the crack tip of different sizes. Since fracture toughness corresponds to the first bond breakages [5], the size of the observation region should be chosen as small as possible. At a size of 5.0 Å, the virial stress drops to a value of KI equal to approximately $0.8\ MPa\sqrt{m}$, which roughly corresponds to the value at which the number of bonds also begins to decrease rapidly. Therefore, we consider this value to be our prediction for the fracture toughness KIc. Since the temperature is only controlled in the outer part of the particle domain in the Capriccio method, an increase in temperature during fracture can

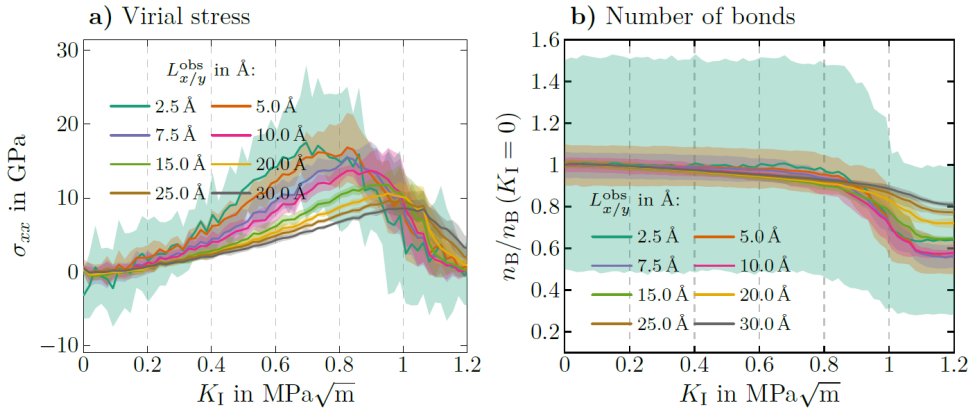

Fig 2: a) Virial stress σ_{xx} and b) number of bonds n_B over stress intensity factor K_I for different sizes of the observation region at the crack tip. The standard deviation over five replicas is given by the shaded areas [2].

be observed. However, this only occurs when a significant number of bonds have been broken, and is therefore not considered as suitable for determining the fracture toughness. For the simulations of mode III, we obtain values of approximately $0.4\ MPa\sqrt{m}$ for KIIIc.
In future studies, we will compare structural properties such as radial/angular distribution functions and ring sizes and relate them to the different fracture modes. The insights gained in this study, both in terms of fracture properties and the Capriccio method, will also help to advance our fracture simulations of polymers.

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Assessment of the Capriccio method via coupled continuum-particle simulations for conducting fracture simulations of amorphous materials

Lukas Laubert, Felix Weber and Sebastian Pfaller

To counter recurring inconsistencies observed in various loading scenarios and material models when applying the Capriccio method, a highly simplified one-dimensional (1D) representation is employed. The Capriccio method is a concurrent continuum-particle coupling technique that relies on force-transmitting anchor points (APs) to couple a finite element (FE) with a molecular dynamics (MD) material description. The 1D replica comprises the essential features, as, e.g., the staggered solution scheme, but solves all its coupled domains with the direct stiffness method to achieve maximum efficiency. Its coupling mechanism also relies on APs, which are massless particles that follow the motion of a continuum and transmit forces via harmonic potentials to particles from the particle-based domain.
In parallel, analogous coupled systems in a three-dimensional space using the original Capriccio method are mapped to a one-dimensional representation. Using a developed comparison framework, we visualize the strain states of the system domains along the loading direction as shown in Figures 1 and 2 (left) for direct comparison with the 1D systems. For more detailed investigation of the system at specific strain states, the weighted mean displacement of particle subdivisions along the direction of loading are

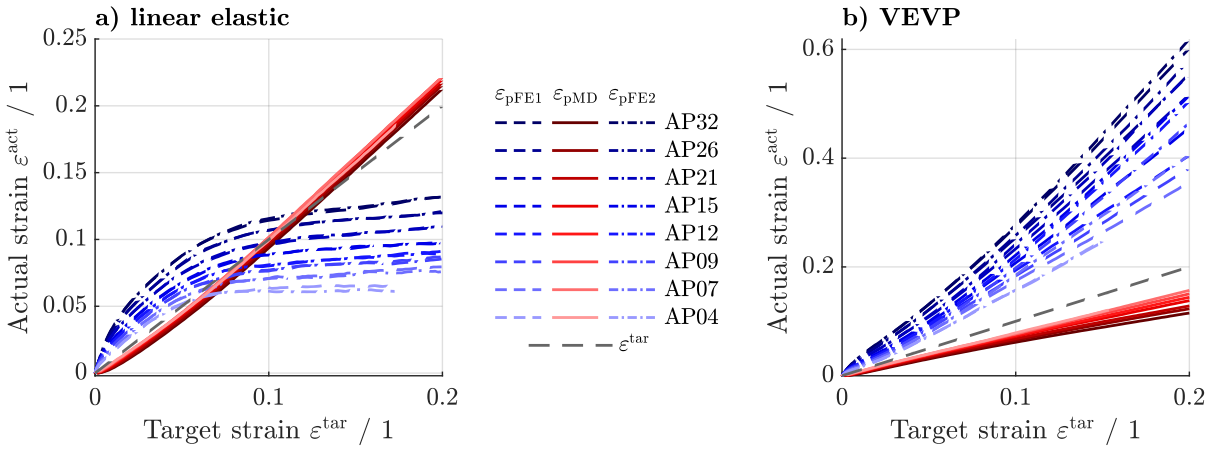

Fig 1: Actual strain over target strain from tensile tests in a variation study on the number of APs using a polystyrene MD model, coupled to a) a linear elastic and b) a viscoelastic-viscoplastic (VEVP) FE domain.

visualized over the initial box center positions of these subdivisions as displayed in Figure 2 (right).

Investigation of various load types using the staggered solution scheme in 1D systems reveals the motion resistance of the coupling region (CR) as the fundamental cause of the strain inconsistencies. This motion resistance especially leads to adverse relaxation effects when using viscous material models in any domain, which further increase the deviating strains between the domains as displayed in Figure 1: We here employ a polystyrene MD model and vary the number of APs in order to adapt the cumulative AP stiffness within the

CR. The CR extends the setup to two enveloping FE regions. When using a linear elastic material description for only the FE part as shown in Figure 2 a), the responding MD domain exhibits a smaller deviation from the black-dashed target reference strain. When employing a viscoelastic-viscoplastic (VEVP) material model in the FE domains, which is accurately calibrated based on pure MD simulations under periodic boundary conditions, the influence of the number of APs, becomes more obvious: A lower number of APs, resulting in a lower cumulative AP stiffness, significantly reduces the strain deviations, however, does not lead to a satisfactory alignment with the target strain. Furthermore, this

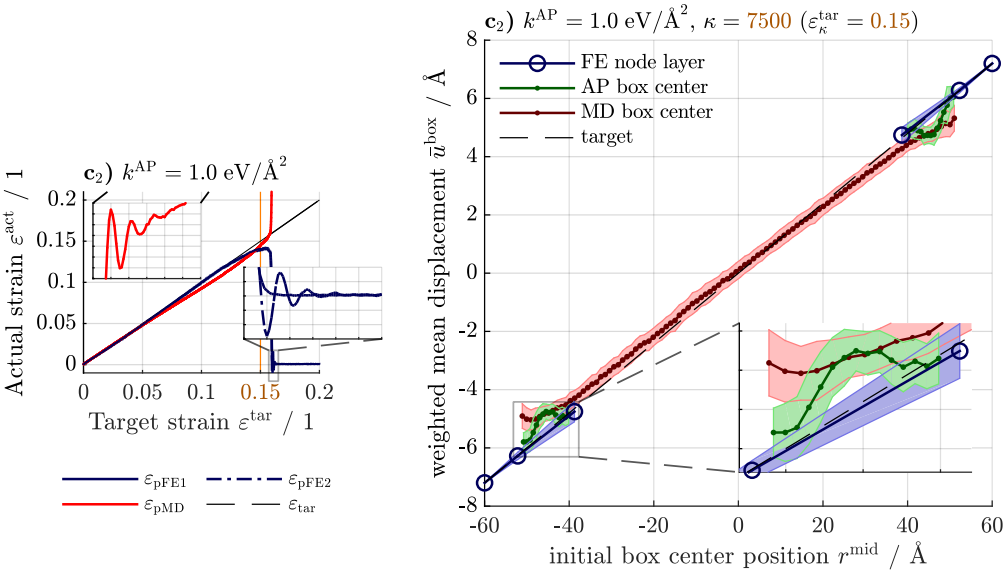

Fig 2*: Right:* furthermore shows the system state shortly before the occurrence of breakage: The CR (see inlet) still exhibits some shortcomings, but overall allows for a sound domain adherence and thus enables a proper coupled tensile test of the silica model.

approach is strongly limited, as a sufficient number of APs as well as cumulative AP stiffness is necessary to remain a sound coupling of the domains, particularly for the investigation of thermoplastics. Further sensitivity analyses using the 1D systems identified the most significant influencing parameters and system settings on the identified motion resistance: A higher number of load steps (leading to smaller strain increments per load step), a reduced AP stiffness, a lower total number of anchor points (see Figure 1) or using stiffer material models, respectively, have the biggest impact on reducing the motion resistance. Furthermore, reducing the length of the coupling region and concentrating the APs (or their stiffnesses) on the side closer to the reacting (usually MD) domain inside the coupling region also have a mentionable impact on the reduction of the motion resistance. To explore the limits of using the Capriccio methodology and testing its suitability for conducting advanced fracture simulations, we furthermore employ a silica model, using an equivalent setup to the polystyrene and 1D investigations. This silica model mostly behaves linearly elastic. Using the 1D mapping approach mentioned, we locate an optimal cumulative AP stiffness, enabling consistent strains in both the FE and MD domains during load application as shown in Figure 2 (left): Until rupture closely after 15% strain, the domains are almost identically elongated, following the target strain reliably. After rupture, the FE domain to which the larger MD part is attached undergoes oscillatory deformation, caused by the energy release during rupture, which is transmitted from the MD region through the CR, as highlighted in the inlets of Figure 2 (left).

Overall, however, all the measures mentioned of enhancing the performance of the classic Capriccio method are subject to limitations or associated drawbacks. Still, the discoveries

contribute significantly to the understanding of the Capriccio method and its application in multiscale modeling, especially for the investigation of the fracture mechanics of organic and inorganic amorphous materials. In a next step, the findings will, in particular, be used to investigate the fracture behavior of bio-sourced epoxies in depth.

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P6: Revealing the percolationagglomeration transition in polymer nanocomposites

Eva Maria Richter, Gunnar Possart, Paul Steinmann, Sebastian Pfaller and Maximilian Ries

This contribution [1] builds the concluding step of a multiscale approach to effectively capture the mechanical behavior of polymer nanocomposites (PNCs), in this case, silica-modified polystyrene, cf. Fig. 1. By introducing continuum-based representative volume elements (RVEs) that employ previously identified elastoplastic property gradients for the interphases surrounding the fillers [2,3], the effects of particle size, particle volume fraction, and agglomeration on the mechanical performance are investigated. Uniaxial tension tests are simulated with the respective finite-element RVEs, and stress-strain curves are derived. The elastic and plastic material properties of the RVE can then be

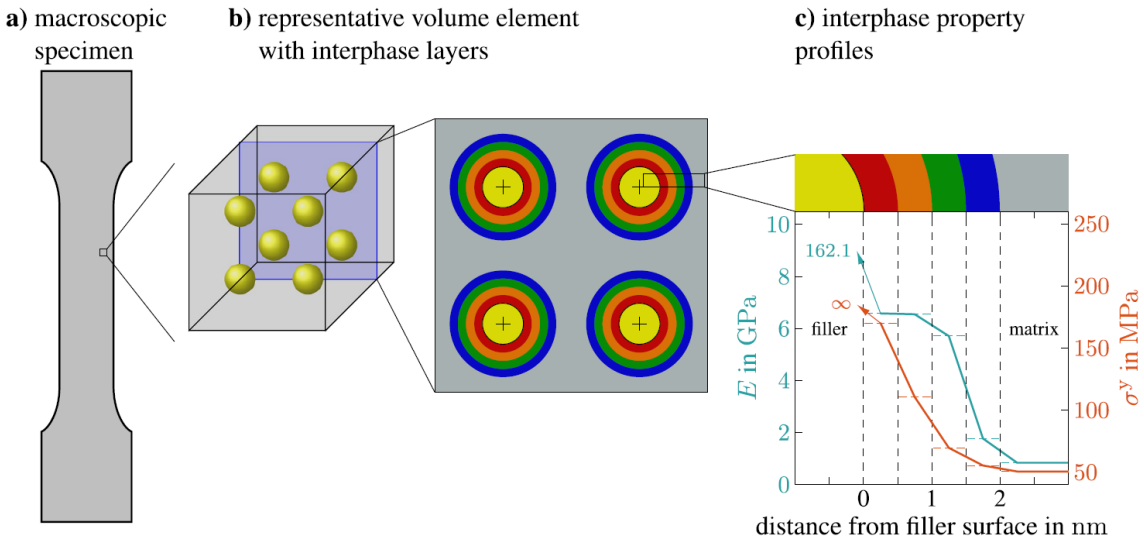

Fig 1: Multiscale nature of polymer nanocomposites: (a) the macroscopic material behavior is governed by the microstructure (b) that comprises matrix polymer (grey), filler particles (yellow), and surrounding interphase layers IP1 (blue, at the matrix) to IP4 (red, at the particle surface); (c) the interphase features elastoplastic property profiles, exemplarily shown for Young's modulus E and yield stress σ^y in silica-enforced polystyrene [2]; reprinted from [1].

extracted and analyzed quantitatively by fitting the stress-strain curves with a Voce-type elastoplasticity formulation.

At small degrees of agglomeration, i.e., good particle dispersion, in combination with a sufficiently large particle volume fraction, percolation bands form, leading to improved elastic and plastic properties (cf. Figs. 2 and 3, respectively). Higher degrees of agglomeration or particle clusters behave like large single particles, which has an adverse effect, i.e., the nanoscale size effect is thereby neutralized. Therefore, the precise MD-informed elastoplastic interphase representation of our RVEs enables the investigation of the transition from beneficial percolation to unfavorable agglomeration. Ultimately, this contribution establishes a link between the effects of particle size, particle volume fraction, agglomeration, and percolation, which have so far only been discussed separately in the literature.

Our methodology offers new insights into the structure-property relations of PNCs and their resulting mechanical behavior. The underlying multiscale approach with a systematic transition from molecular to microscopic scales is required to complement experimental observations and exploit the full potential of PNCs.

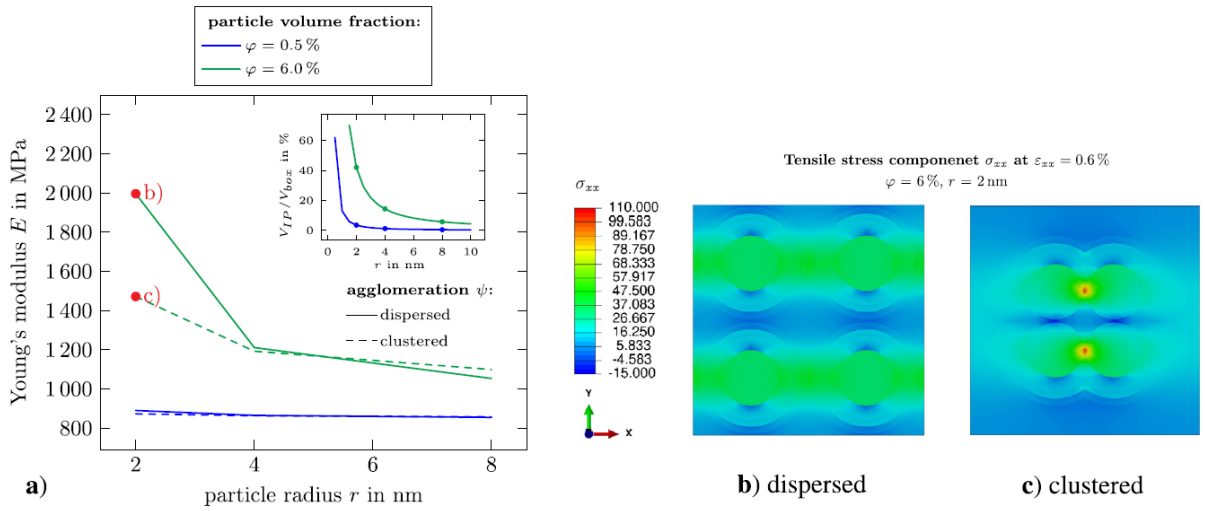

Fig 2: (a) Influence of particle radius r on Young's modulus E for particle volume fractions φ = 0.5 and 6% at extreme degrees of agglomeration ψ, showing the adverse size effect; inset: interface volume fraction with respect to total RVE volume $VIP/Vbox$. (b) and (c) Contour plots of Cauchy stress σ_{xx} at ε_{xx} = 0.6% for φ = 6%, r = 2 nm, dispersed and clustered, xy-plane through particle centers, showing the transition from beneficial percolation to disadvantageous agglomeration; reprinted from [1].

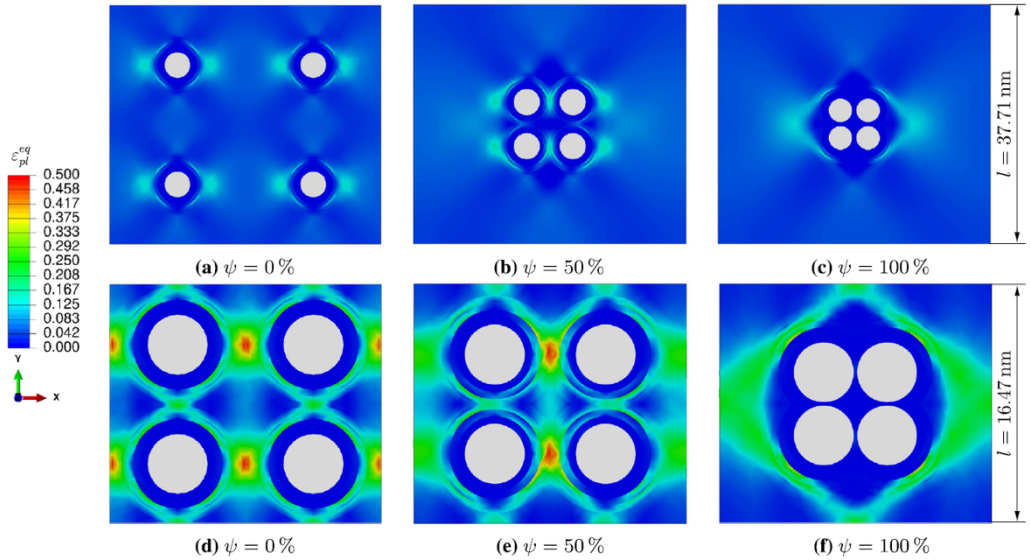

Fig 3: *Contour plots of equivalent plastic strain ε^{eq}_{pl} in xy-planes through the particle centers, evaluated at maximum strain ε_{xx} = 10% and for different degrees of agglomeration. The particles are greyed out and all have r = 2 nm. Top row: minimum particle volume fraction φ = 0.5%. Bottom row: maximum particle volume fraction φ = 6%; reprinted from [1]*

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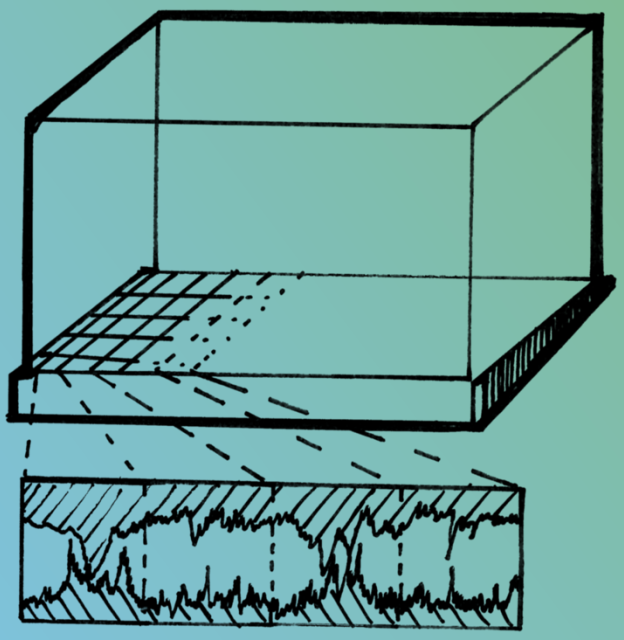

P7

COLLECTIVE PHENOMENA IN FAILURE AT COMPLEX INTERFACES

Christian Greff

PD Dr. Paolo Moretti
Materials Simulations
Department Material Science and Engineering

P7: Tuning load redistribution near heterogeneous

Christian Greff and Paolo Moretti

The research subject of this project is the connection between material structure and material behaviour in hierarchically structured thin films under tension. Simulations are performed with a network model based on a regular cubic grid of nodes. Each edge connects two of these nodes and is assigned a randomly distributed failure threshold to model the local strength in a brittle material. The systems are structured by removing chosen edges from the network such that cut-like 'gaps' create a hierarchical structure.
Earlier research in this project showed that a hierarchical structuring of the thin film could enable a localization of damage without reduction in work of fracture in nearly all cases of disorder of local strength [1]. This might be of interest for introducing a predetermined location of failure without creating a weakness. In the case of a weak layer being already present, it could be shown that hierarchical structuring would outperform work of fracture in reference systems without hierarchical structuring for all cases. This could be traced back to different primary mechanisms determining the necessary work of failure, crack roughening in non hierarchical systems compared to crack arrest and coalescing individual cracks in hierarchically structured systems. These different mechanisms lead to different fracture profiles, as shown by scaling analysis of the fracture interfaces and now added to with investigation of the correlation of crack heights. The correlation C of the crack interface height was calculated according to the equation C(r)=⟨hh'⟩_r-⟨h⟩⟨h'⟩, Here, r is the

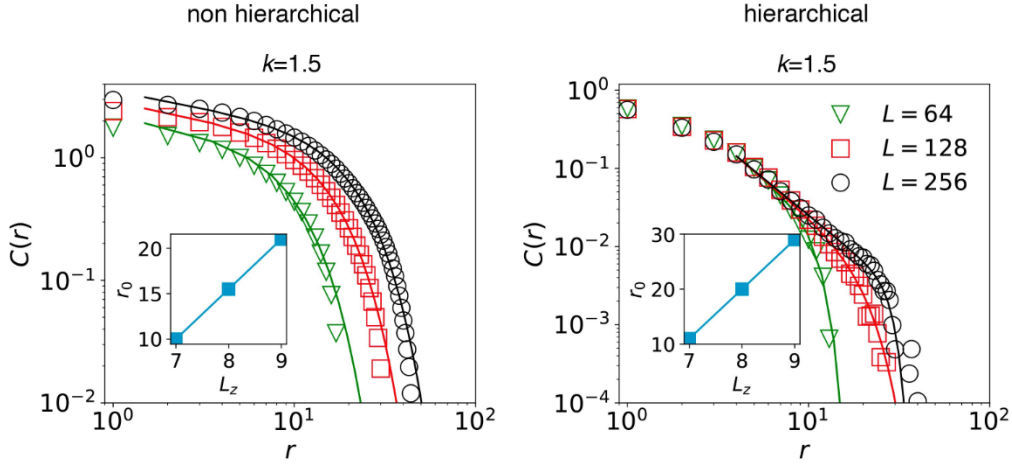

Fig. 1: Correlation analysis of crack surfaces in network systems

distance between the points with h and h'. The results of this are shown in figure 1 for systems with high disorder of local strength (k=1.5).
The correlations follow a truncated power law:

$$C(r) = r^{-\eta} exp\left[-\left(\frac{r}{r_0}\right)^{\zeta}\right]$$

with dependence on distance r and a short distance cut-off r0, which in turn depends on the thickness of the system Lz. This shows that the thin film nature of the systems influences their failure behaviour. The actual correlation values show that further mechanisms must be in effect, since for equal Lz, the values in the hierarchical system are approximately two orders of magnitude smaller than those in the non hierarchical system. It is of note that the analysis of fracture profiles represents a look into the interplay between both the elastic behaviour and the failure behaviour of the system. While the former is influenced by the structure, the latter is based on failure criteria like the threshold

assigned to each edge. A clearer understanding of the role of structure on the active mechanisms can therefore be achieved by instead focusing on the correlations of displacements in the system which are based purely on elastic behaviour. To this end, we formulated the Green's function of the network, its elastic kernel, which describes the elastic response of the system in point x, y, z to a force applied in a point x′, y′, z′:

$$u_i = \sum G_{ij} f_j; G_{ij} = G(x, y, z, x', y', z')$$

Here, u_i is the displacement in node i as caused by a force f in node j. We then investigated the behaviour of the system when a point force is applied in the centre of the system, as visualized in figure 2.

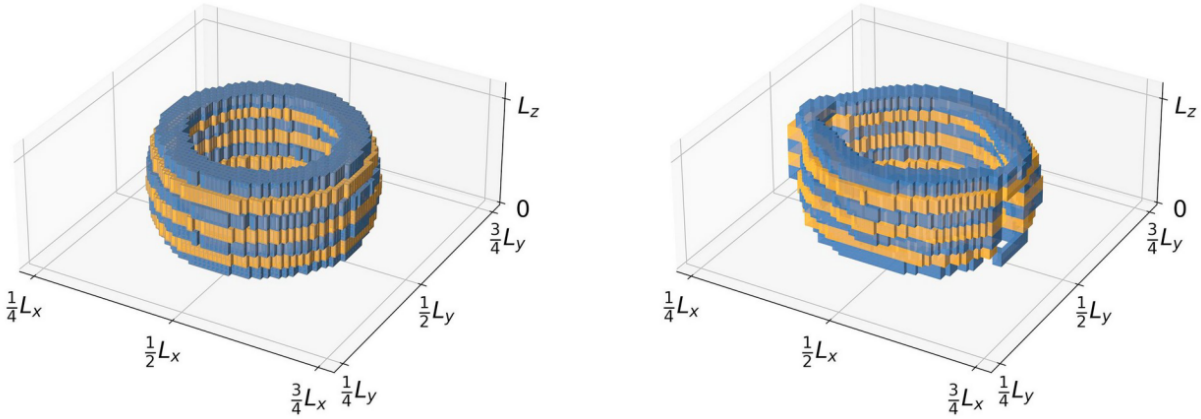

Fig. 2: Region of equal displacement in a single network with point force in the centre; left: non hierarchical structure, right: hierarchical structure

The non hierarchical network, shown on the left-hand side, behaves radially symmetric while the structuring in the hierarchical system leads to an anisotropy. This anisotropy is responsible for the differing behaviour between these two types of systems: In hierarchically structured materials, stresses are directed away from planar defects that intercept a propagating crack, which reduces the stress concentration that was driving crack growth.

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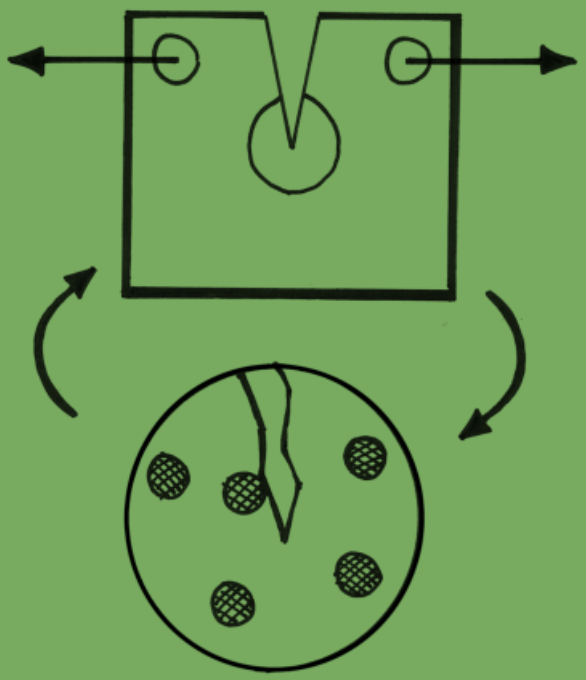

P8

FRACTURE IN POLYMER COMPOSITES: MESO TO MACRO

Maurice Rohracker

Paras Kumar

Lucie Spannraft

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Applied Mechanics
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P8: Performance Enhancements in Phase-Field Fracture Simulations

Maurice Rohracker and Julia Mergheim

Project P8 aims to study the influence of mesoscopic parameters on macroscopic fracture properties of nanoparticle-reinforced polymers using homogenization methods. Typical mesoscopic parameters are the volume fraction of these nanoparticle-reinforced structures. For the mesoscopic simulations, an efficient fracture simulation framework is a condition for a computationally feasible homogenization scheme. The phase-field fracture method is a suitable approach for simulating fractures in complex mesoscopic geometries. In this method, the crack is approximated by a smeared field, the crack phase-field, which is controlled by the length scale parameter l_c (see Figure 2) and requires appropriate mesh

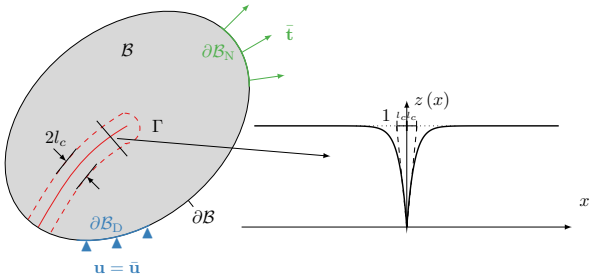

Fig 1: Smeared model of the phase-field fracture method.

sizes near the crack. Crack propagation
is only correctly captured with small time step sizes. Furthermore, a fully coupled problem of the displacement field and the crack phase-field is solved. Therefore, these simulations are computationally very expensive, especially for simulations of complex structures. Introducing and developing performance enhancing techniques is inevitable in our case. The phase-field model for brittle fracture is based on the Griffiths energy idea of fracture, the main developments of which are summarized in [1]. The solution of both fields can be obtained by finding $\mathbf{u} \in \mathcal{B} \rightarrow \mathrm{R}^{\mathrm{dim}}, \mathrm{z} \in \mathcal{B} \rightarrow [0,\,1]$, with $\mathrm{z} = 1 \;\Rightarrow$ intact and $\mathrm{z} = 0 \;\Rightarrow$ broken, s. t.

$$\mathcal{E}(\varepsilon, \mathrm{z}) = \int_{\mathcal{B}} \left[[z^2 + \mathrm{k}]\Psi^+ + \Psi^-\right] \mathrm{dV} + \int_{\mathcal{B}} \frac{\mathrm{G_c}}{\mathrm{c_\omega}} \left[\frac{[1-\mathrm{z}]^2}{l_c} + l_c |\mathrm{grad}\; z|^2\right] \mathrm{dV} - \mathcal{W}^{ext} \rightarrow \min$$

More details can be found in [2], where different methods of adaptive spatial refinement (ASR) are compared. ASR comprises the first performance enhancing technique, where the phase-field threshold refinement criterion is applied. Apart from that, a repeating time step scheme is employed. The residuum-based convergence criterion, which is often used as a convergence criterion in alternating minimization schemes, shows very slow convergence in the fracture time steps. Inspired by [3], a physically motivated ansatz for the convergence criterion based on the fracture energy - the core ingredient in these simulations - is embedded. Here, a time step converges if the relative change in the fracture energy is small compared to a tolerance value. Finally, adaptive temporal refinement and coarsening [4] complement the performance enhancing strategies. The large time step sizes are used at the beginning of the elastic loading regime, while the time step size is refined, and the time step is repeated if larger changes in the phase-field solution are observed. After the time step size is refined, coarsening is disabled until the initial time step is solved. The solution process of a time step is summarized in the scheme in Figure 2. This scheme ensures that crack propagation occurs only on the finest mesh with the

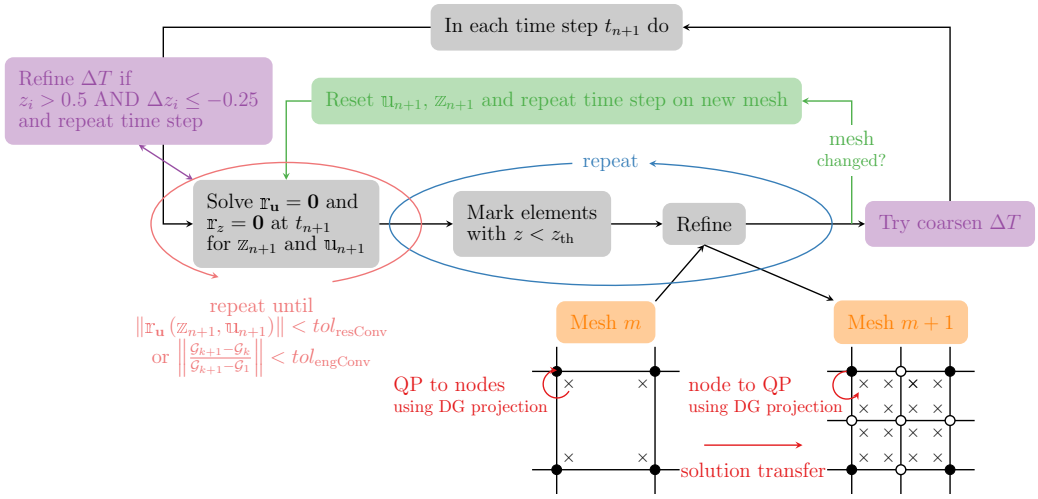

Fig 2: Staggered solution scheme with all performance enhancing techniques.

finest time step size. The parameters of the three strategies are calibrated independently of each other. A benchmark problem and a more complex fracture example are considered to evaluate the performance enhancing strategies. For the single edge notch shear (SENS) test, performance enhancements of the order of five are achieved with negligible loss of accuracy. The load-displacement curves in Figure 3 overlap, while the number of time steps (black stars) is much smaller when all performance enhancing strategies are applied, thus

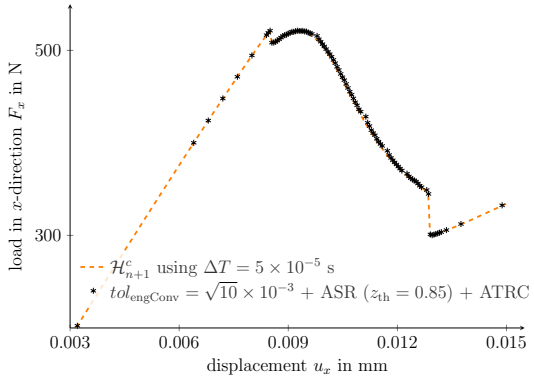

Fig 3: Load-displacement curves of the single edge notch shear test.

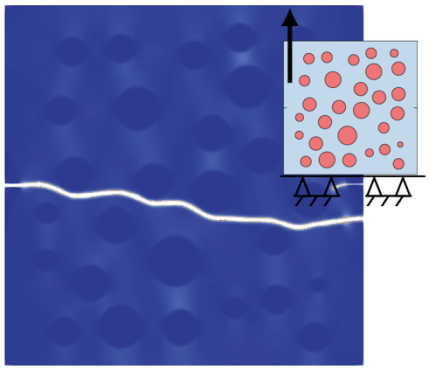

Fig 4: Phase-field contour of the tension test of the complex structure.

contributing to the performance improvement. Similar results are obtained for the simulation of the complex structure shown in Figure 4, where silica particles of different sizes are embedded in an epoxy matrix with two notches. A speedup of almost four times is achieved with a small loss of accuracy. The resulting crack path strongly depends on the configuration of the silica particles and the position (height) of the notches. The speedups are reached due to the reduced number of total time steps (97 instead of 300 for the SENS test), the reduced number of elements (9766 to 7186 for the SENS test), and the

reduced number of staggered iterations per time step. At the same time, accuracy is achieved with fine meshes and with small time step sizes in the vicinity of the crack and its propagation. In addition, the physically motivated convergence criterion based on the fracture energy ensures efficient and accurate phase-field fracture simulations. These three performance enhancements in phase-field fracture simulations allow for efficient and reliable fracture analysis.

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aPJ: Generalized mechanical interfaces modeling adhesive bonds

Lucie Spannraft, Paul Steinmann and Julia Mergheim

The application of adhesive bonds, e.g., for lightweight construction, aircraft production or convenience products, has been steadily increasing for decades. Finite-thickness adhesive layers can be approximated by zero-thickness interfaces for computational efficiency. Since adhesive layers show resistance and failure under tension, shear and in-plane stretch, a classical cohesive zone model is not sufficient to represent an adhesive. In contrast, generalized mechanical interfaces allow for displacement jumps under tension and shear loading, as well as, for traction jumps crucial for an in-plane response, cf. [1, 2]. Generalized interfaces at finite strains depend not only on the displacement jump $[\![\boldsymbol{\varphi}]\!]$ and interface deformation gradient $\bar{\boldsymbol{F}}$, but also on the spatial interface normal $\bar{\boldsymbol{m}}$ to account for anisotropic decohesion in a thermodynamically consistent model. Experiments in literature showed that the different failure modes affect each other, which justifies damage mode coupling between the cohesive normal (cm), cohesive tangential (ct) and the membrane in-plane (m) modes resulting in effective damage variables d_i^{eff}, i.e.,

$$\begin{aligned}\bar{\psi} \coloneqq\ & \bar{\psi}\big(\bar{\boldsymbol{F}}, \bar{\boldsymbol{m}}(\bar{\boldsymbol{F}}), [\![\boldsymbol{\varphi}]\!], d_i^{\mathrm{eff}}\big) \\ &= \big[1 - d_{\mathrm{m}}^{\mathrm{eff}}\big]\bar{\psi}^{\mathrm{m}}(\bar{\boldsymbol{F}}) + \big[1 - d_{\mathrm{cm}}^{\mathrm{eff}}\big]\bar{\psi}^{\mathrm{cm}}\big(\bar{\boldsymbol{m}}(\bar{\boldsymbol{F}}), [\![\boldsymbol{\varphi}]\!]\big) \\ &+ \big[1 - d_{\mathrm{ct}}^{\mathrm{eff}}\big]\bar{\psi}^{\mathrm{ct}}\big(\bar{\boldsymbol{m}}(\bar{\boldsymbol{F}}), [\![\boldsymbol{\varphi}]\!]\big).\end{aligned}$$

Soft adhesive bonds can undergo large in-plane deformations, e.g., 300% strain (Figure 1 b: time
t = 0.4s) during manufacture, unloading (c: t = 0.8s) and then compression by 25% (d: t = 0.8s) during the product life. A pure cohesive zone model shows no in-plane response to this large deformation. For comparison, the generalized interface model allows for significant in-plane failure during the stretch which may weaken the normal and shear modes via damage coupling and result in a more pronounced buckling during compression, cf. Case 2 in Figure 1 (e).

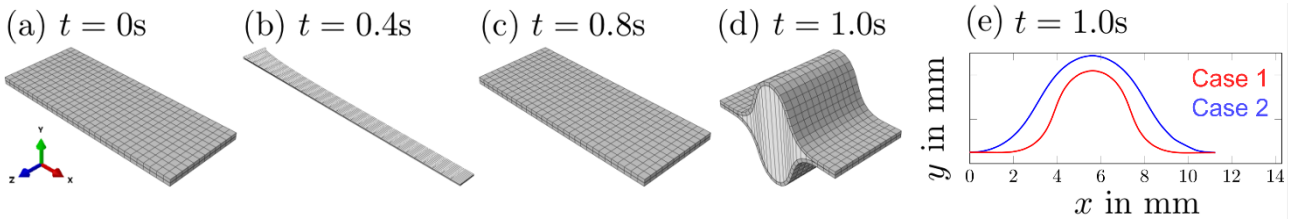

Fig 1: The deformation of a soft adhesive (modelled as a generalized interface) connecting two substrates undergoing (b) in-plane stretch, (c) unloading, (d) buckling, and thereby, (e) comparing Case 1 (no coupling of the damage variables) and Case 2 (coupling the damage variables of the different deformation modes), cf. [2].

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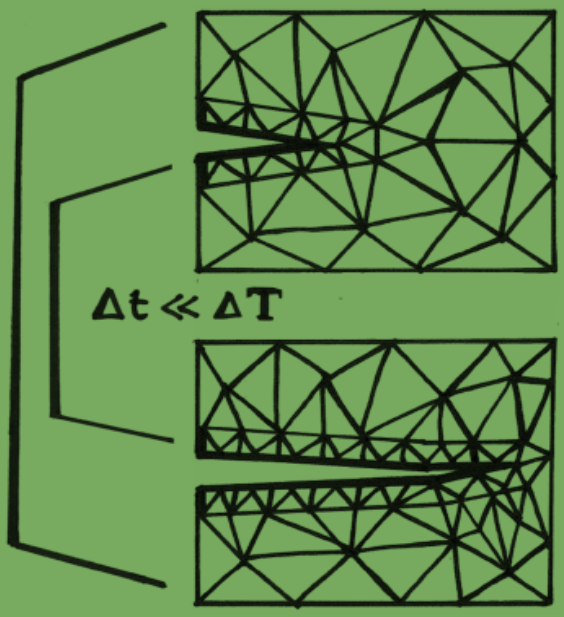

P9

ADAPTIVE DYNAMIC FRACTURE SIMULATION

Deepak Balasaheb Jadhav

Prof. Dr.-Ing. habil. Sigrid Leyendecker
Applied Dynamics
Department of Mechanical Engineering

P9: A modified asynchronous variational integrator for phase field modeling of dynamic fracture

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Phase-field modeling of fracture has gained attention as a relatively simple yet fundamental technique for predicting crack propagation. In this work, we present our newly developed asynchronous variational integrator (AVI) for phase-field modeling of

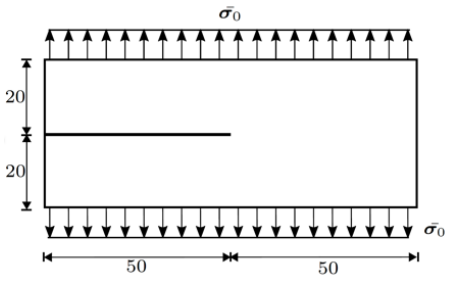

Fig 1: BTT specimen.

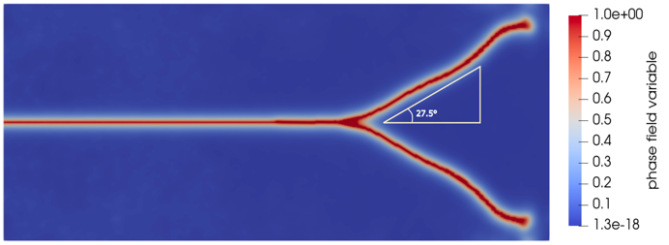

Fig 2: Phase field distribution of fully broken BTT specimen.

dynamic fractures. The AVI allows each mesh element to progress with its own time step [1].

In this new version named Globally Solved Asynchronous Variational Integrator (GSAVI), displacement updates occur as usual at each temporal update. However, instead of updating the phase field after every temporal update using an elemental patch [2], we solve for the phase field globally after the largest spatial element is updated. Figure 1 illustrates a boundary tension test (BTT) specimen along with its boundary conditions, used to investigate the characteristics of the new method. The distribution of the phase-field variable after the BTT specimen is fully broken is depicted in Figure 2. Significant

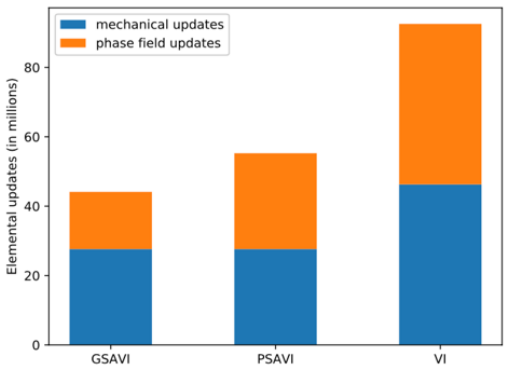

Fig 3: Comparison of elemental updates.

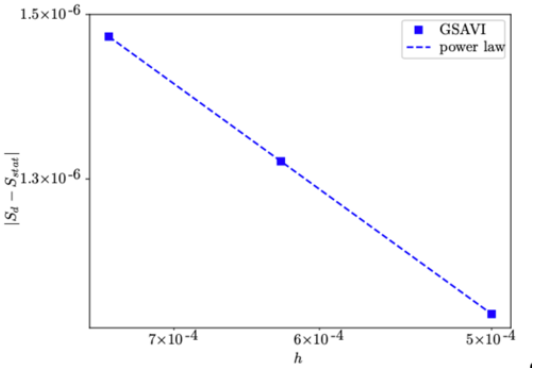

Fig 4: Convergence of discrete action sum.

computational savings achieved by the new method compared to its synchronous counterpart and the technique proposed by Niu et al. (2023) [2] are demonstrated in Figure 3. The convergence of the discrete action sum with spatial refinement, as depicted in Figure 4, signifies the reliability and robustness of the newly devised method.

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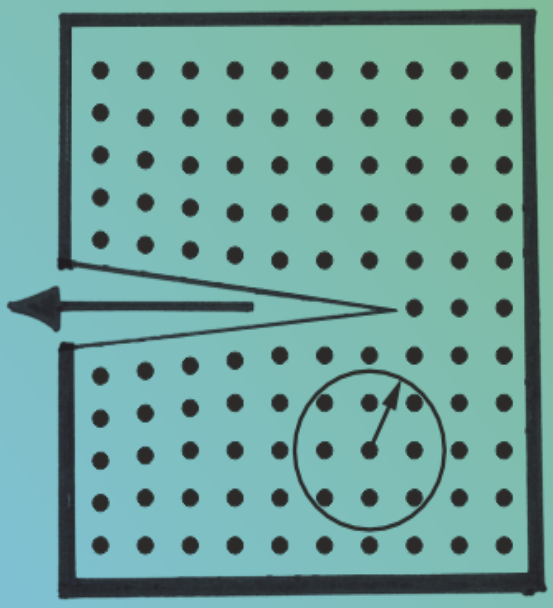

P10

CONFIGURATIONAL FRACTURE MECHANICS OF DISCRETE SYSTEMS

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Anna Titlbach

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Applied Mechanics
Department of Mechanical Engineering

P10 Damage in continuum-kinematics-inspired peridynamics

Marie Laurien, Ali Javili and Paul Steinmann

Peridynamics (PD) is a nonlocal continuum formulation that has become more and more established in the field of fracture mechanics [1]. The PD balance equations are governed by an integral term which computes the interactions between a continuum point and its neighboring points within a finite distance. This integral formulation readily allows for discontinuities, such as cracks. Recently, Javili et al. [2] developed an extended version of peridynamics, called continuum-kinematics-inspired peridynamics (CPD). The theory relies on capturing changes in length through one-neighbor interactions, changes in area through two-neighbor interactions and changes in volume through three-neighbor-interactions. In this work, we develop a damage formulation for CPD. For each type of interaction, we introduce a separate damage variable that depends on the length strain, area strain and volume strain, respectively. Brittle damage is modeled by considering an interaction as fully damaged once a strain threshold is exceeded.

We derive the CPD damage thresholds from the classical critical energy release rate that can be determined in experiments. For 2D, an analytical expression for the parameter conversion is obtained by comparing the critical energy release rate to the nonlocal energy required to break all one- and two-neighbor interactions across a fictitious crack surface.

The PD balance equations are numerically solved using a classical Newton—Raphson algorithm. In case of brittle damage, the sudden damage of a large number of bonds massively worsens the convergence behavior. Thus, we introduce a so-called sequential-damage-algorithm that is based on subiterations in which the bond breakages are limited to a predefined number. In this manner, the brittle damage behavior can be captured.

In order to validate the damage model, we compare experimental results of fracture benchmark problems to CPD results. This is exemplified by the brittle crack propagation in a notched cement mortar plate with a hole in Fig. 1. Moreover, in Fig. 2, experimentally observed cracks in diagonally loaded PMMA plates is shown. Here, the introduction of

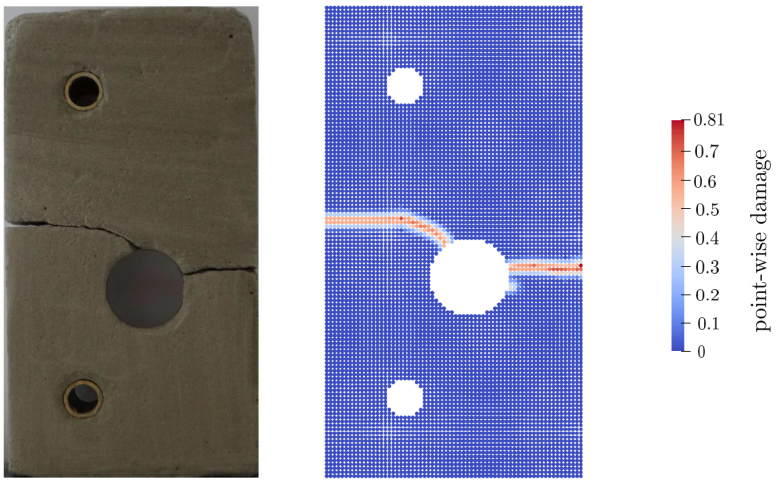
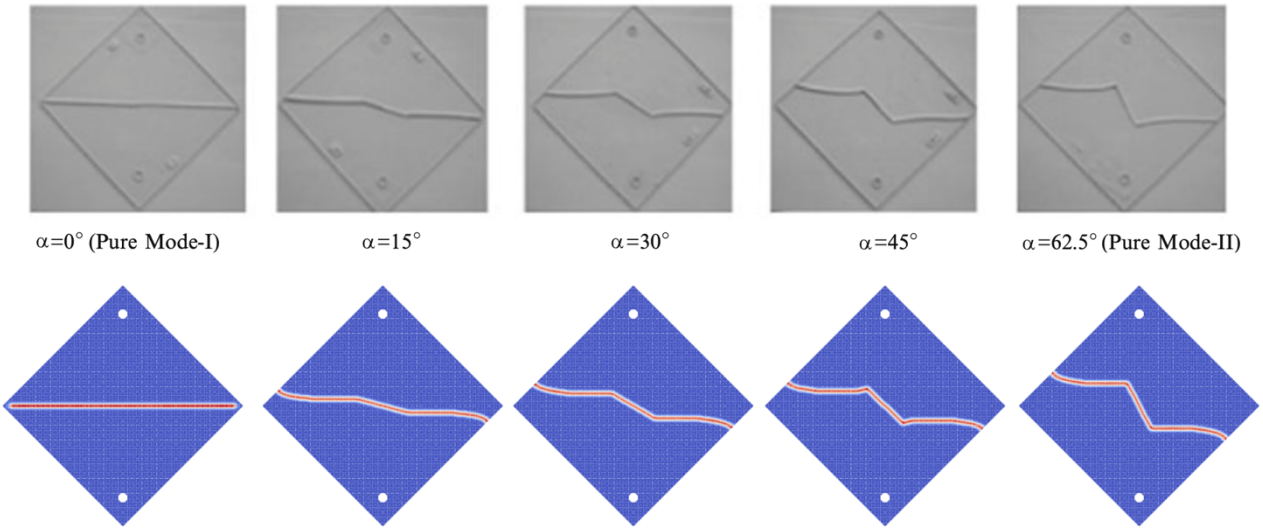


Figure 1: Comparison of an experimentally observed crack path in a cement mortar plate with a hole (left) to a numerically predicted crack path obtained by means of the CPD damage model (right).

precracks with varying inclination angles allows to capture pure mode I, pure mode II and mixed mode cases.

Subject of current work is the extension of the model to quasi-brittle damage. Here, the damage variables are obtained by evaluating damage functions that model a gradual



decrease of the interactions. Examples are linear, exponential and power law functions, as used in [3]. This requires additional CPD damage parameters. To this end, we, again, compare the critical energy release rate to the nonlocal energy required to break all one- and two-neighbor interactions across a

Figure 2: Comparison of the experimentally observed crack paths in a PMMA plate with varying crack angle α (top) to the numerically predicted crack paths obtained by means of the CPD damage model (bottom).

fictitious crack surface. In addition, the material's ultimate tensile strength is compared to the maximum nonlocal force normal to the fictitious crack surface.

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aP10: Simulation of the Flexoelectric Effect in Human Bone - A Micromorphic Modeling Approach

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Our bones are remarkable structures that constantly adapt to the physical stresses of daily life through a dynamic process called bone remodeling. This continuous renewal enables bones to maintain their mechanical stability and withstand changing loads over time. However, sudden increases in mechanical stress - such as during rapid escalations in exercise intensity or training - can disrupt the delicate balance of bone remodeling, leading to the formation of microcracks, which compromise the mechanical integrity of the bone [1]. Fortunately, the natural remodeling processes allow bones to self-repair such damage. Recent research [2,3] has shown that the ability of bone material to generate electric potential under inhomogeneous deformation plays a crucial role in coordinating the cellular mechanisms required for healing. A comprehensive understanding of these

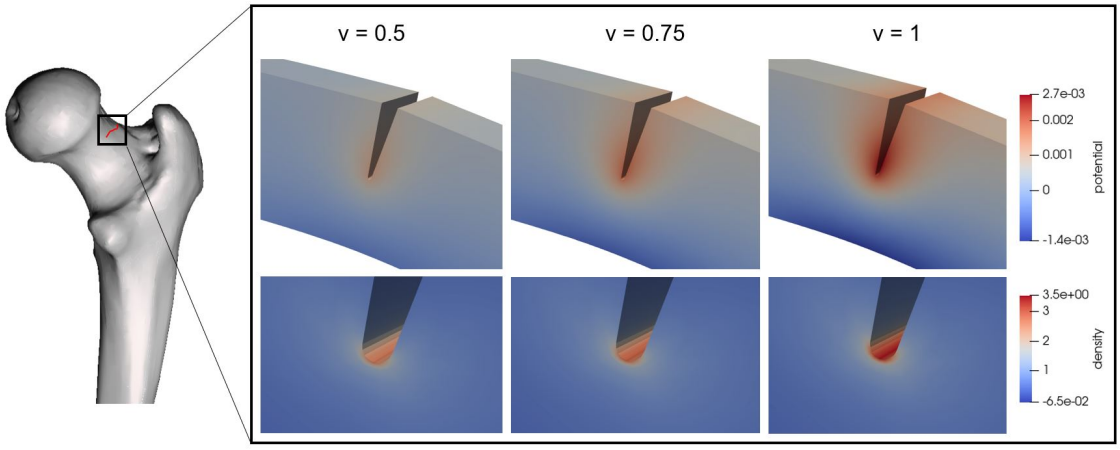

Fig 1: Analysis of the impact of flexoelectric coefficient variations on the electric potential magnitude and nominal density in the vicinity of a microcrack.

regenerative mechanisms, along with their modeling and simulation, is therefore essential for advancing effective medical treatment strategies and therapeutic approaches.

We propose a novel methodology that accounts for the trabecular microstructure of bone and size-dependent material effects using a micromorphic framework [4]. This framework has been extended to include nonlinear electro-elastic and flexoelectric energy contributions within the constitutive equations. To evaluate the approach, we utilize a cracked cantilever beam as a representative model, which approximates a bone sample affected by a microcrack, such as those that may occur, for example, in the femoral neck region. As illustrated in Figure 1, when a bone crack is observed, the so-called flexoelectric effect causes an electric field to be generated around the crack when asymmetric deformation (e.g., bending) is applied. The stress gradient is highest at the tip of the crack, creating the greatest possible electric polarization. The electric field is therefore most pronounced at the crack tip and decreases with further distance from the crack tip. This electric field acts as a biological trigger, activating the bone-building activities of osteoblasts [2,3], which in our case is captured by an increase in nominal bone density in the vicinity of the crack tip. The analysis presented in Figure 1 demonstrates the impact of the flexoelectric coefficient on the magnitude of the electric potential and, consequently,

Fig 2: Pictures taken during and after my presentation at the Queensland University of Technology during the seminar of the ARC Training Centre for Joint Biomechanics. Group Photo from left to right: Prof. Paul Steinmann, Prof. Peter Pivonka, Anna Titlbach, Prof. Areti Papastavrou.

on the nominal bone density. The finite element model is implemented using the open-source library deal.II. The highlight of this year was undoubtedly my research stay at the Queensland University of Technology (QUT) in Brisbane. Early in this year, I received an invitation from Prof. Peter Pivonka, the Head of the Department of Biomedical Engineering and Spinal Diseases at QUT in Brisbane, to undertake a research stay at his institute. The goal was to engage with local experts and address open questions to maximize the benefit of this opportunity. I began my work at QUT on July 10 at the Cube, the modern research facility on campus. During my stay, I worked closely with Prof. Papastavrou and Prof. Steinmann, who were also at QUT for a research semester. This collaboration significantly contributed to the progress of my doctoral project. In the following days, we made significant progress on the challenges of our modeling approach for the healing of microcracks in human bone, through daily exchange and intensive collaboration. One of the highlights was my lecture in the ARC Training Centre for Joint Biomechanics seminar series as shown in Figure 2, which led to valuable feedback and new insights.

Looking back, my research stay at QUT was an enriching experience, not only due to the excellent professional collaboration and the opportunity to present my work to a broader scientific audience but also for the numerous new contacts I made, expanding my academic network. I am grateful for this unique opportunity and I gratefully acknowledge the financial support I received from the International Visiting Scholarships of FAU, the Graduate School FRASCAL (GRK 2423), and the BayWiss Health Network, which were essential to making this research stay possible.

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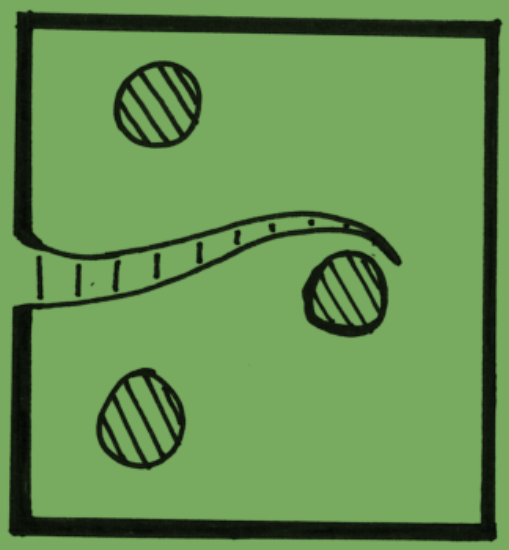

P11

FRACTURE CONTROL BY MATERIAL OPTIMIZATION

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(Continuous Optimization)
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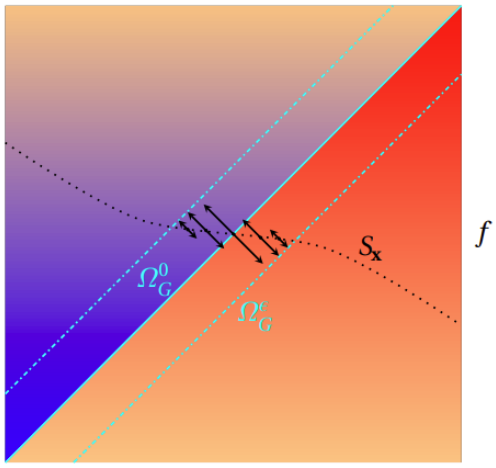
P11: Stochastic Optimization with high dimensional uncertainties with application to fracture control

Lennart Igel, Michael Stingl, Lukas Pflug and Julia Mergheim

Optimisation of fracture faces a significant challenge due to two major problems. On the one hand, the computational cost of evaluating each fracture simulation for a given design is high. Secondly, the landscape of the objective function is discontinuous. Thus, traditional methods for solving discontinuous optimization problems that require sampling the objective landscape, such as surrogate models like support vector machines[1] and Monte Carlo approaches [2], become infeasible for application in high dimensions. In addition, the curse of dimensionality means that the computational cost increases exponentially with increasing dimension [3]. However, regularisation is necessary to deal with the discontinuities in the objective and to transform the problem into a robust optimisation problem.



This difficulty in combining low computational cost with robustness motivates the new approach developed in our project. For this method, we exploit the special structure of the discontinuities that appear in such fracture optimization problems. In our observation, these are contained along lower

Fig 1: Visualization of each of the primary construction parts of the framework. The discontinuity set of the objective f is described by the zero set of the level set function G (Ω_G^0), a belt around the zero set (Ω_G^ε) denotes the set in which smoothing should be performed and scales the size of the smoothing set S_x with decreasing distance to the zero set. Outside the belt the size of S_x is zero and so it corresponds to the point x itself.

dimensional manifolds in the design space. In the rest of the domain, the objective function is continuously differentiable and simple gradient methods can be applied. Thus, our idea is to use an indicator function that encodes the location and orientation of the discontinuity in the domain. This indicator function can be a level set function determined from the structure of the problem, or a more complex function such as tracking the minimum eigenvalue of the state problem for each design point. Using this indicator function, it is now possible to dynamically determine the distance and orientation to the discontinuity during the optimisation process. The problem is made robust by applying smoothing in a zone around the discontinuity determined by the size of the function value of the indicator. In addition, smoothing is applied along the specified one-dimensional direction to the discontinuity set. The key elements of our method as a mathematical framework are outlined in Figure 1. smoothing only locally, in subsets where the discontinuity in the data exists. On the other hand, this smoothing is additionally restricted to the relevant direction in the design space, a one-dimensional line integral over the jump in the data, as opposed to integrating the entire domain in e.g. Monte Carlo methods. Over the past year, we have provided several results for this robust function, showing that it is continuously differentiable over the entire design domain, and that it satisfies an error estimate with respect to a globally smoothed robust function. Thus, the robust function produced by our

method can be treated as a computationally cheap approximation of a globally smoothed robust function. The quality of the approximation increases linearly with the size of the diameter of the smoothing region of the globally smoothed function.
We have also been working with project P14 to develop a new application for our

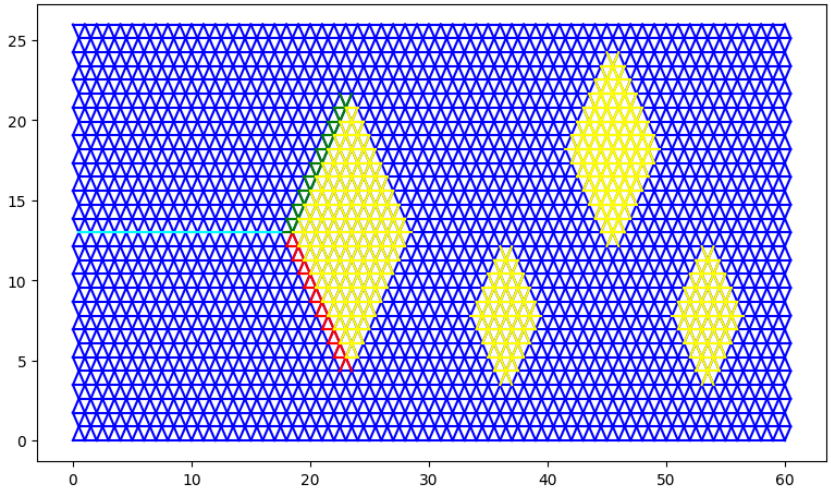


Fig 2: Visualization of the lattice. Tension is applied along the left side, split along the middle in opposing directions. This will generate the crack along the light blue interfaces. It will propagate towards the leftmost yellow diamond inclusion and either travel along the upwards (green) or downwards (red) edges, depending on which are structurally weaker. It then propagated parallel again and will either have to propagate around two small inclusions or one larger one.

optimisation method. We are working on adapting their atomistic model, as published in [4] and [5], to include design variables so that we can manipulate the stiffness and fracture toughness of edges between nodes in any region independently. We have constructed a suitable lattice design so that we obtain an interesting landscape for the work of fracture, which can be found in Figure 2. The lattice is designed with a matrix of a given fracture toughness, while the yellow diamond shaped inclusions have a much higher fracture toughness. The initial crack on the left (light blue) is much weaker than the matrix, suggesting fracture initiation. The green and red paths along the top and bottom of the left side of the leftmost inclusion can be manipulated in their fracture toughness. Depending on which is weaker, the crack will propagate upwards or downwards, and then must propagate around either one inclusion if propagating along the upward path, or 2 smaller inclusions, if propagating along the downward path. As these paths are different in length and fracture energy, the work of fracture will have a jump along the symmetric line, when passing from one path type to the other.

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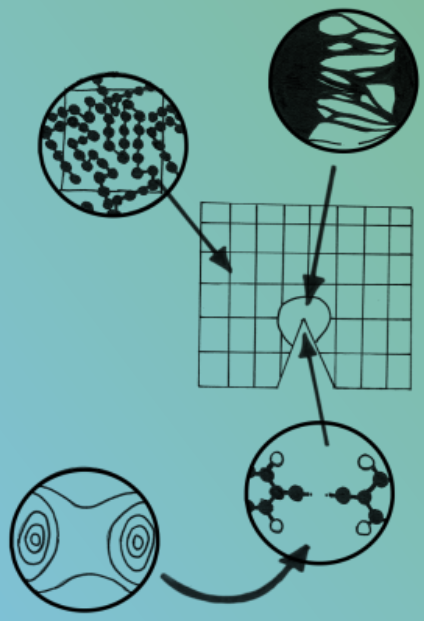

P12

QUANTUM-TO CONTINUUM MODEL OF THERMOSET FRACTURE

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P12: Quantum-to-Continuum Model of Thermoset Fracture

György Hantal, Bariscan Arican, Sebastian Pfaller and Ana- Sunčana Smith

Fracture is a complex phenomenon that spans multiple length scales. At the molecular level, fracture propagation occurs through a sequence of localized bond-breaking events, which are driven by far-field mechanical loading applied at macroscopic scales. The ultimate goal of Project P12 is to establish a simulation framework that seamlessly connects atomic-scale processes to the material's macroscopic behavior. Previously, a robust methodology, termed as "block chemistry" [1], was developed to construct cross-linked epoxy polymer networks. This approach leveraged a heuristic classical molecular simulation capable of dynamically modifying molecular topologies, complemented by quantum chemical data to accurately model the reactivity of various reaction pathways. This year, our efforts focused on two major objectives: (1) investigating the mechanisms of bond breakage in these cross-linked networks and (2) developing a coarse-grained model of the epoxy network. This coarse-graining approach aims to extend the effective length scale of simulations by systematically reducing the degrees of freedom while retaining the essential characteristics of the system.

Development of coarse-grained models (György Hantal)

The coarse-grained (CG) model must meet several key criteria: (1) it should retain the most relevant chemical information about the system's constituents, such as shape and connectivity; (2) it must accurately reflect the chemical structure and mechanical properties of the system, ensuring that it remains representative of the fully atomistic model; and (3) it should reduce the number of degrees of freedom to include only the essential ones, enabling simulations of larger systems. This is achieved by grouping clusters of atoms into single effective particles, each representing multiple atoms. Among the various well-established methods in the literature, we selected the Iterative Boltzmann Inversion (IBI) technique to develop the coarse-grained interaction potential. This method

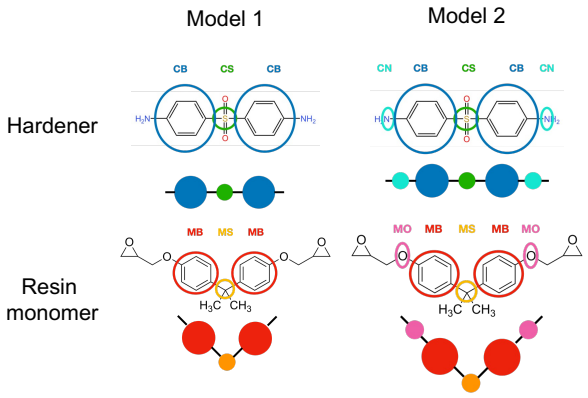

Fig 1: Comparison of the resolution (number of beads) of the two coarse-graining strategies currently tested. In model 2 (right) more chemical information is stored, which allows to develop a more refined potential at the price of an increasing number of non-bonded interactions (10 vs 21)

derives the CG interaction potential directly from the atomistic structure of the system. The objective is to create a CG potential that reproduces the same structural properties, defined in terms of radial distribution functions (RDFs), as the atomistic model being simplified. The IBI method is iterative: it begins with an initial guess for the CG potential,

followed by simulations using this potential to compute new RDFs. These RDFs are then used to refine the interaction potential, with the process repeated until the CG model accurately reproduces the atomistic structure. The key advantages of the IBI method are its straightforward automation and relatively fast convergence, typically achieved within 10–15 iterations.

While the method is well-defined, it leaves the determination of coarse-grained beads to the discretion of the modeler, requiring informed decision-making to balance accuracy and computational efficiency. In this project, we initiated the development of coarse-grained interaction potentials using IBI. This process was implemented via a custom Python script that interfaces seamlessly with the LAMMPS simulation software, which serves as the primary molecular simulation tool for this work. Concurrently, we are testing multiple coarse-graining strategies by varying the number of atoms grouped into each coarse-grained bead. These variations affect not only the structural representation but also the number and complexity of interaction potentials that need to be developed. Figure 1 illustrates a comparison of two such coarse-graining schemes, highlighting the differences in bead representation and interaction potentials.

Development of bond breakage simulation software (Barışcan Arican)

Our well-established block chemistry method incorporates essential quantum chemical information to capture the fine chemical details of bond formation reactions. Building on this foundation, we are developing an automated software tool within Project P12 to gain equivalent quantum chemical insights into bond breakage events in coarse-grained systems. This tool integrates detailed chemical information into our coarse-grained model.

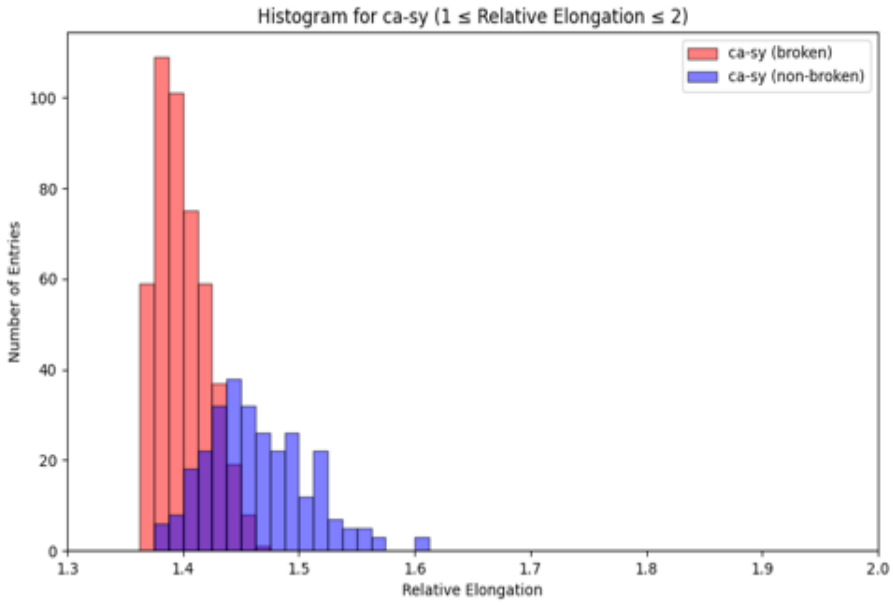

Fig 2: Occurrence of cases where a carbon-sulphur bond in cross-linkers is too elongated and found broken by QM/MM (blue histrograms) and where they are mistakenly flagged so (red histrograms) as a function of bond elongation. Clearly, this coordinate alone is not able to distinguish between the two cases (see the big overlap between the histograms).

As in our curing simulations, bond breakage is initially treated at the classical mechanics level. However, when a potentially broken bond is identified—typically due to excessive elongation—a quantum chemical calculation is performed on the relevant molecular

fragment to confirm whether the bond is truly broken. This hybrid approach ensures accuracy while maintaining computational efficiency. The primary objectives of this work are threefold: (1) to establish an automated partitioning scheme that identifies a quantum mechanically described region (QM) around the potentially broken bond, along with a sufficiently large classically described region (MM); (2) to couple the simulation codes, Gaussian (QM) and LAMMPS (MM), in an efficient, parallelized framework that minimizes communication overhead while maximizing resource utilization; and (3) to refine a classical, non-quantum indicator of bond breakage. This indicator aims to reduce reliance on computationally expensive QM calculations by accurately flagging bonds as broken based on classical criteria. The efficient coupling of the two software tools, Gaussian and LAMMPS, has been successfully achieved. Current efforts focus on rigorous testing to ensure the robustness of the framework and identify potential bugs or bond breakage scenarios that may not yet be adequately represented. To this end, hundreds of QM/MM calculations have been performed on potential bond breakage events. These simulations have also provided valuable data to evaluate and refine our primary bond breakage indicator, as illustrated in Figure 2.

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aPO: Investigating impact of curing dynamics on the microstructure and properties of epoxy thermosets

Sampanna Pahi, Christian Wick and Ana-Sunčana Smith

Objectives and status

The primary aim of the doctoral project titled "Molecular-Scale Fracture Modeling of Epoxy Resins" is to accurately model chemical bond dynamics in crosslinked polymers. In the current phase of the project, a robust and high-fidelity curing protocol is being optimized to generate models of epoxy thermoset. Prior research has shown that curing reaction dynamics intrinsically impact the morphological properties of epoxy resin[1]. Previously modeled using gas-phase calculations, we have updated the curing reaction protocol to incorporate explicit solvent effects. Discrepancies between QM gas-phase studies and experimental data necessitated considering environmental influences. ONIOM calculations were employed for this, analyzing a 30 Å radius around reaction sites as shown in Fig. 1 to obtain accurate energy barriers. Using Quantum Mechanics/Molecular Mechanics (QM/MM) techniques, we have included effects of the local environment by allowing

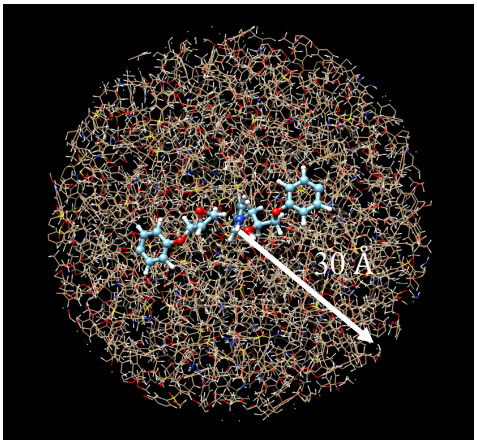

Fig 1: ONIOM system Stick model (QM) Wire model (MM).

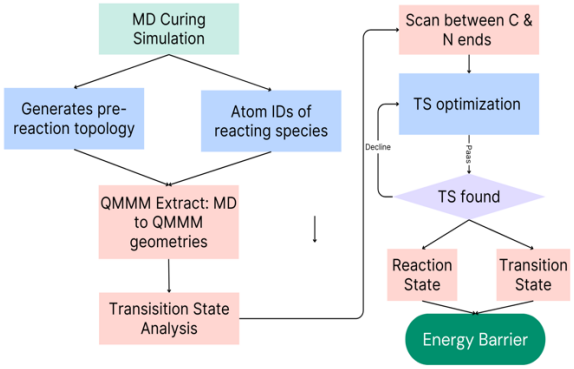

Fig 2: Automated workflow for post-a-priori QMMM analysis

incorporation of factors such as steric hindrance and hydrogen bonding. This approach enhances MD simulation accuracy for curing reactions, using parameters derived from QM/MM analysis.

Upon analyzing the initial results, we observed that activation energies were up to 100 kJ/mol higher than experimental values [2], with certain outliers exhibiting significantly lower energies. Further scrutiny revealed that these outliers coincided with the presence of hydrogen bonding, suggesting the stabilizing influence of hydrogen-bonded reaction sites as shown in Fig 3. As a result, we developed a modified curing protocol that constrains reaction events to occur only if a predefined hydrogen-bonding geometric criterion is satisfied. By systematically controlling hydrogen bonding interactions, we can now generate different hydrogen-bonded configurations and accurately assess their cumulative impact on the overall curing process.

An automated workflow was also developed and implemented to identify reaction sites and perform a posteriori QM/MM analysis with higher accuracy (Fig 2). The hydrogen-bonded results presented here are a direct outcome of this workflow, which facilitates

refined parametrization of MD curing simulations and ensures that environmental factors such as hydrogen bonding are consistently captured.

Conclusions, main achievements, and outlook

Our recent introduction of hydrogen bonding constraints into the curing protocol has addressed previously observed outliers in activation energies and brought computational results into closer alignment with experimental data (Fig 4). By linking reactive events to hydrogen-bonding criteria, the model now better reflects the stabilizing influence of hydrogen bonds in epoxy polymerization (Fig. 3). Preliminary evidence suggests that hydroxyl (OH) groups form more robust hydrogen bonds than amine (NH) groups, thereby altering both the reaction pathway and the isoconversional profile of the curing process.

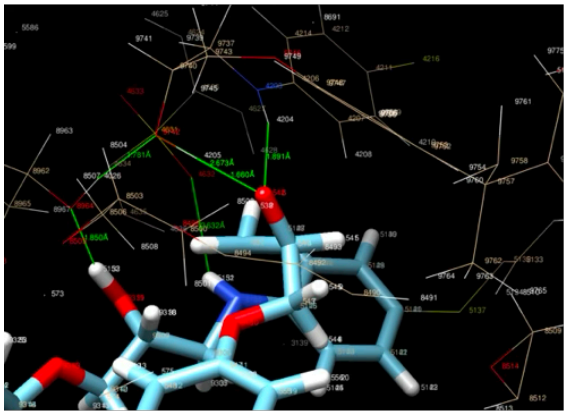

Fig 3: Hydrogen bonded stabilization of epoxy reactive ends.

Fig 4: Energetic barrier distribution for H-bonded interaction (orange) and non-H bonded interaction (blue) for Primary and Secondary crosslinking reactions.

We have developed and integrated an automated workflow to identify reaction sites and perform a posteriori QM/MM analysis, significantly improving the accuracy of MD curing simulations. Moving forward, we will employ graph theory to determine shortest loop sizes, providing insights into the rigidity of the cured network and enabling more detailed characterization of microstructural features for subsequent fracture modeling. By extending hydrogen-bonding considerations in both reaction site identification and subsequent QM/MM analysis, our approach will capture a broader range of intermolecular interactions critical to understanding epoxy polymer behavior at the molecular scale.

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P13

FRACTURE IN ROCKS: FROM SINGLE GRAINS TO SEISMIC SCALE

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P13: Modeling of fragmentation and fracturing processes in deformation bands

Bakul Mathur, Eric Solomon, Javad Karimi and Daniel Koehn

The main goal of this research is to establish a multiscale framework for investigating grain fragmentation and the formation of deformation bands in geological rock formations. Deformation bands are formed as a response to localized compression, shear and/or dilation stresses in porous rocks sandstones and sediments [1]. These bands are generally compactive in nature and lead to porosity and permeability reduction. They have a limited capacity for displacement accumulation, leading to the formation of numerous individual bands or clustered band structures[2]. We aim to model and simulate the formation of these compaction bands; capturing the (1) microstructural fragmentation of the individual grains, (2) formation of the mesoscale multiparticle fractured grain bands, followed by (3) the slippage driven large scale faulting.

Microscale modeling: In this part of the project, we aim to realistically model the splitting of the micro-sized rock particles. For a realistic model, polyhedral shaped grains are considered. The simulations are done using an extensible open-source framework focused on the Discrete Element Method [3]. We model the breakage of the particles in two manners:

(1) Mohr-Coulomb-Weibull split along the maximum shear plane: An earlier considered approach in this project involves splitting of particles following the Mohr-Coulomb-Weibull (MCW) criterion [4]. The MCW fracturing criterion was explained in my last report in detail. In the following section, the newly added splitting criterion is explained.

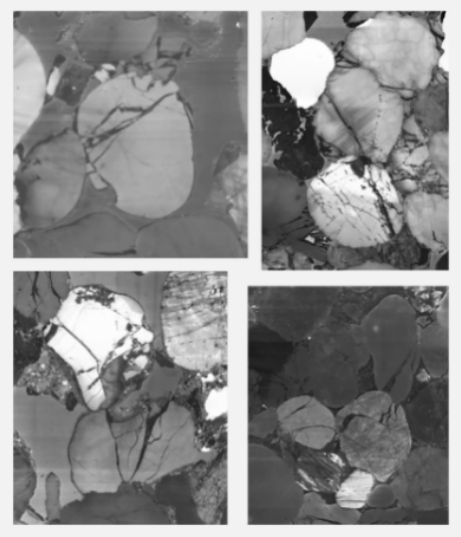

Figure 1: Thin-section images from sandstone rock samples showing fracturing along contact lines.

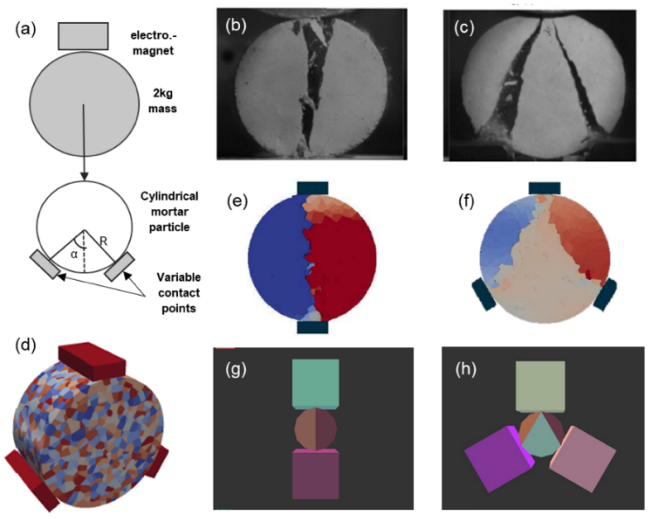

Figure 2: (a) sketch of the experimental setup of Neveu et al. Fracture pattern of the sample from high speed video recordings for (b) $\alpha = 0$ and (c) $\alpha = \pi/6$. (d) face view of the 3d Voronoi tessellation based model. (g),(h) fracturs along critically stressed contact lines from Yade

(2) Splitting along critically stressed contact lines: While observing the thin section images from rock samples collected from Namibia, we noticed that many grains were split along the lines joining the contact points. This observation inspired the development of the new splitting method for the polyhedral particles which split the particles along critically stressed contact lines. To avoid numerical instabilities, the model is restricted to maximum two splits in a body. The current

implementation is 2-dimensional. The model was validated with the results of experimental and numerical study by Neveu et al. (2017) [5]. The study by Neveu et al. investigates the effect of contact anisotropy on the crushing strength of granular materials through both experimental drop weight tests and numerical simulations using a Voronoi-based Discrete Element Method (DEM) model. In contrast to the Voronoi-based approach, our proposed model achieves similar fracturing behavior without requiring particle discretization. Each particle is treated as a single rigid polyhedron, avoiding internal subdivision into smaller Voronoi cells. Contact forces are projected onto the lines connecting contact points to determine stress distribution along these potential fracture paths. If the stress along any of these lines exceeds a predefined threshold, the particle fractures along that line. Once fracture occurs, DEM contact physics naturally separates the fragments, similar to the post-fracture behavior in the Voronoi model. This method retains the essential fracture physics without the need for additional degrees of freedom, reducing computational complexity while preserving the observed fracture patterns. Although the implementation differs, our model and the Voronoi-based approach are functionally equivalent. The Voronoi-based model breaks cohesive bonds when displacement thresholds are exceeded, while our model fractures the polyhedron when stress exceeds a threshold along projected contact lines. In both cases, the failure condition depends on contact-induced stress reaching a critical level. The Voronoi-based model and our model both predict a vertical crack for $\alpha = 0$ due to symmetric loading and two inclined cracks for $\alpha > 0$ due to contact anisotropy. Since the crack paths align with contact force transmission, our model naturally reproduces the same fracture patterns without additional tessellation. This demonstrates that our model is not just an approximation but a physically equivalent and more scalable implementation of the fracture process.

Mesoscale modeling: Traditional DEM focuses on simulating the mechanical behavior of granular assemblies by modeling individual particles and their interactions. However, when inter-particle cohesion is neglected, DEM may struggle to accurately capture the initiation and propagation of deformation bands. To address these challenges, we propose an enhanced modeling framework that incorporates local and global stress analysis to infer fracture probabilities and directions. Beyond analysing the fracturing particle, we compute the stress tensors within particles adjacent to the fracturing site. Based on the magnitude and direction of the principal stresses obtained from the neighbouring particles, and the global boundary stress state, we directionally adjust the fracture probability of particles surrounding the fractured body. By integrating the local stress directions, the model promotes anisotropic fracture propagation along paths that emerge naturally from particle-scale interactions while maintaining the overall orientation consistent with global stresses.

Large scale modeling: The extent, direction and pattern of large scale fractures mainly depend on the rock mechanical properties, heterogeneity, presence of planes of weakness, and their preferred orientation. Many a times the deformation bands precursor to large scale faults. We intend to employ a hierarchical or a volume coupling between the small scale and large scale models.

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aPM: Modelling Geothermal Systems in Faulted and Fractured Media Variation in outcrop-derived permeability tensors and influence on naturally fractured reservoirs

Ruaridh Smith & Daniel Koehn

General Motivation and Aims

Renewable energy is becoming an important alternative to fossil fuels and traditional forms of energy across the globe and a vital source of energy in reducing emissions and our carbon footprint. Whilst several forms of renewables can provide micro- to small-scale energy, other forms such as geothermal energy are increasing in popularity for providing large-scale energy production including in Germany (e.g., Weber et al., 2020). Major projects in areas such as Bavaria are primary focussed on areas in the Molasse Basin where increased heat flows are present in both high and low-permeable reservoirs (Schulz et al., 2013). Previous work has been undertaken in Northern Bavaria where low permeable reservoirs have been identified in the basement granite and overlying sedimentary sequences and the primary mechanism for fluid flow is fracture networks (e.g., Kämmlein et al., 2019; Freitag et al., 2022).

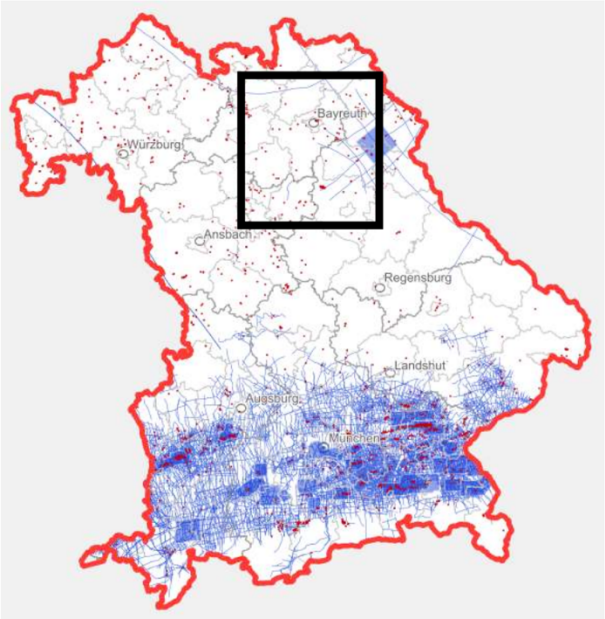

Figure 1: Map showing available subsurface data in Bavaria (Kühne *et al.*, 2006; GeotIS, 2014). Black box shows the general research area.

This research has mainly focused on the rock types and heat sources in the region however there have been few studies on the subsurface geology and fracture networks present in Northern Bavaria. Data collection for projects have also been constrained to the Molasse Basin to the south and as such there is limited subsurface data available in the north. Therefore, utilising surface data for fracture network interpretations and for modelling the subsurface is the vital. Outcrop analogues such as quarries and caves can be used to characterise fracture networks that are present in geological formations at depth and integrating these properties into models and simulations are useful for further understanding the fluid flow in reservoirs. The primary aims of this research is to integrate data from the surface and subsurface into a large-scale fractured model of the reservoirs and simulate geothermal fluid flow. Additionally, to better understand the effects of upscaling the interpretations in outcrop scale to reservoir scale we aim to investigate the spatial and scalar variability in the fracture networks.

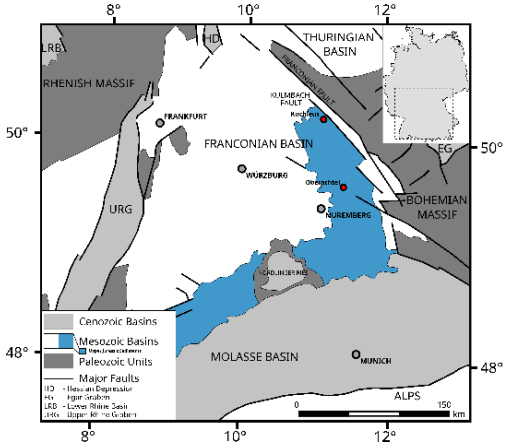

Figure 2: Structural map of Southern Germany showing the outcrop sites (modified after Smith *et al.*, 2022)

Methodology and Data Collection

We collected data from several sites across Northern Bavaria located along the Franconian Alb. Data collection comprised of structural measurements (fracture azimuth and dip angle; aperture) and imaging fractured quarry sections (2D photogrammetry and 3D LiDAR and drone capture). Using GIS software in combination with MATLAB and python packages, 2D geometric analysis from the photogrammetry provides additional fracture network properties, such as fracture density/intensity, connectivity, and variations in fracture orientation. This process includes fingerprinting networks as spatial graphs. The fingerprints are a combination of these block areas and block shape factors used to uniquely define the network. This is a method to characterise and represent fracture networks using the space between fractures rather than the fractures themselves and allows for the analysis of fracture networks without requiring fracture length (a difficult property to measure in the field). This therefore allows for an alternative method of visualising and interpreting network geometry and variability. The fingerprints are depicted as three bin area probability distributions plotted against shape factors that range from 0 to 1 approximating towards the circumscribing circular area. The fingerprint analysis is undertaken using a MATLAB script.

Fingerprint Analysis of Fractured Networks

The network fingerprints and geometrical analysis showed variation in the fracture networks within Oberachtel Quarry. We can see that shape size is quite consistent throughout the 4 samples with generally large box areas covering the network. We can see though that the shape factor does vary by sample which is likely caused by the faults through sample 3. Sample 4 has a consistent distribution likely due to being away from the fault damage zone to the right.

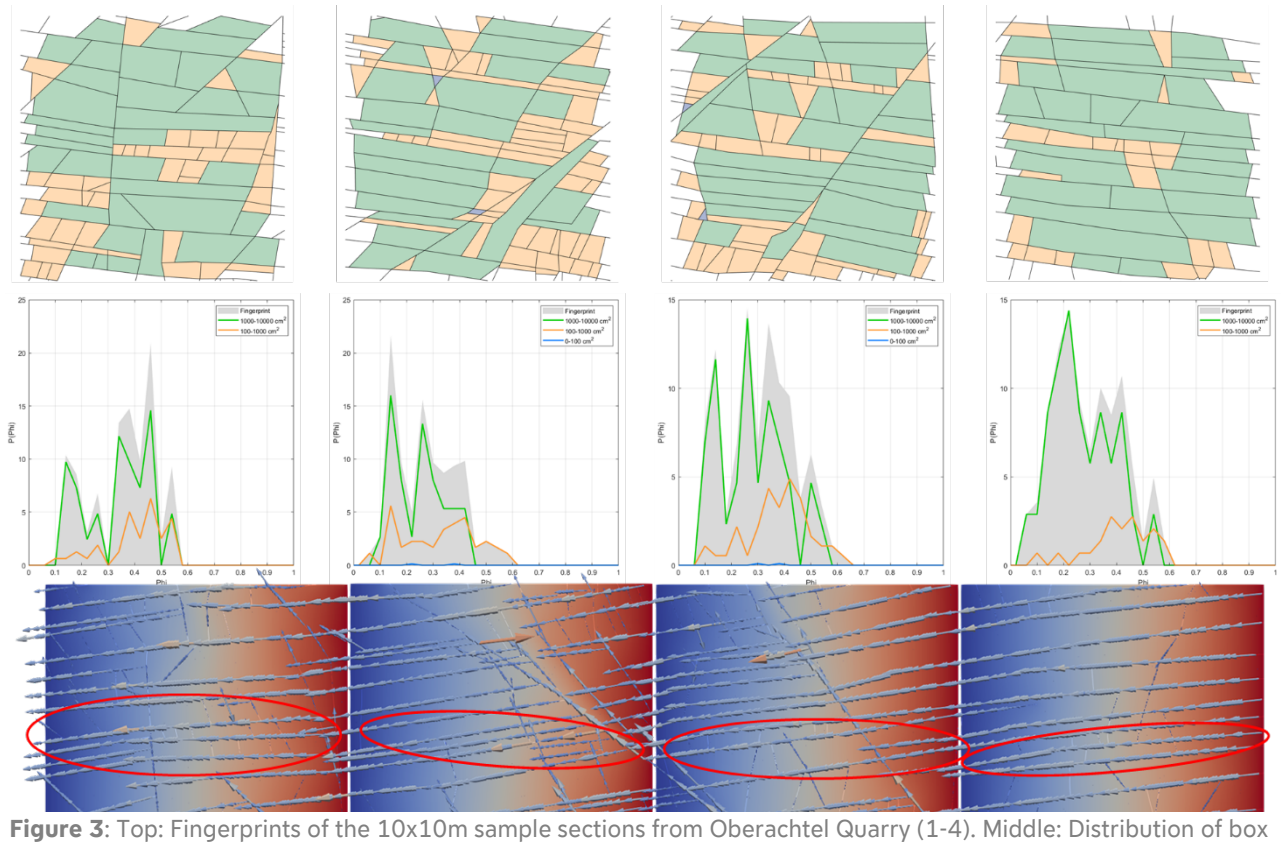

Figure 3: Top: Fingerprints of the 10x10m sample sections from Oberachtel Quarry (1-4). Middle: Distribution of box area plotted against shape factor of the sample sections showing the spatial variation. Bottom: Results from fluid flow simulations through each section showing the horizontal pressure gradient and resulting 2D permeability tensor.

Permeability Tensors Simulations

Permeability from the fractured traces can be obtained using 2D numerical fluid flow simulations using REDBACK (part of the MOOSE Framework) to calculate the average fluid velocities through the network which are then used to determine the overall permeability tensor. The results show a generally low orientation of the tensors due to dominant strike-slip faulting throughout the region and the strong influence of bedding parallel fractures. The faults are most prominent in sections 2 & 3. The resultant K-values for each section also show this control from the horizontal fractures and larger faults. Analysis in other quarry sections in Oberachtel also showed similar results however there was a presence of smaller angled fractures which connected the long horizontal lineations. These smaller features could be vital in improving vertical connectivity in the reservoirs and of the network as a whole.

Regional Modelling of Northern Bavaria

Current work is being undertaken to integrate the outcrop data into a large-scale regional model in Northern Bavaria. The fault model based on surface (drone, LiDAR, measurements), subsurface (seismic, wells) and previous interpretations can provide a basis on the large-scale structural systems in play. Integrating the field data within the modelled fault blocks will allow for a multiscale approach to the simulation of potential fluid flow in the region and to determine potential geothermal areas where increased subsurface heat flow is identified. These areas could be future exploration targets for geothermal projects.

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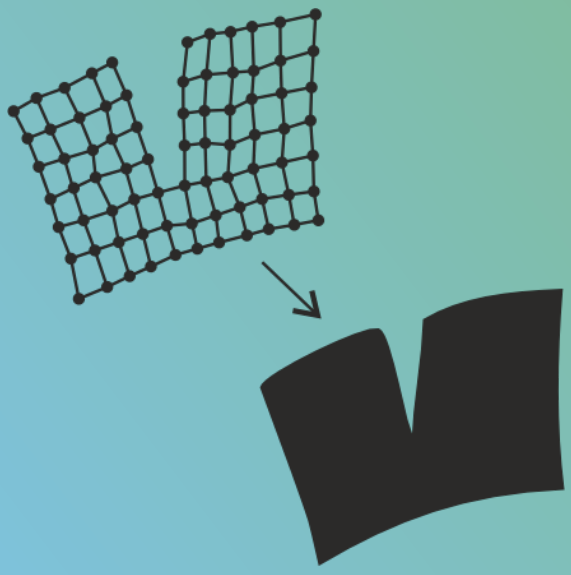

P14

PASSAGE FROM ATOMISTIC- TO CONTINUUM FOR QUASISTATIC AND DYNAMIC CRACK GROWTH

Joscha Seutter

Prof. Dr. Manuel Friedrich
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P14: Atomistic-to-Continuum Convergence for quasi-static crack growth in brittle materials

Joscha Seutter & Manuel Friedrich

Since the work of Francfort and Marigo, a natural mathematical framework for theoretical studies of fracture behavior is given by free discontinuity problems, where displacements and crack paths are determined from the minimization of the so-called Griffith energy. For the justification of these models on the continuum level one aims for rigorous results that relate the free discontinuity problem to minimization problems on the atomistic level. This is usually done by means of Gamma-convergence, which is a variational convergence that ensures convergence of minimizers of a series of energy-functionals to the minimizer of the limiting Griffith energy [7]. The first goal of our project was to extend this analysis to time-dependent crack growth and provide a rigorous analysis of the relation between atomistic and continuum models in the setting of quasi-static evolution. A further natural field of interest in this regard, is the inquiry of possible numerical approximation schemes for the minimization of Griffith-energies. The most prominent example is the Ambrosio-Tortorelli scheme, where the sharp jump-discontinuity is smoothed into a diffused crack, which leads to a further approximation parameter and thus gives rise to a multi-scale problem. However, there also exists a single-scale discrete approximation of Griffith-functionals, which relies on approximating functions that are piecewise linear on an implicitly optimized triangulation and was first introduced in [3]. In the second part of our project, we investigate this adaptive finite element approximation in the setting of irreversible quasi-static crack growth.

After the completion of the first step of our project, namely proving existence of a quasi-static evolution for a suitable variational model for atomistic crack growth [9], we focused on the atomistic-continuum passage in the quasi-static setting. Here, we slightly departed from the rather general modeling framework in [9] by making some additional assumptions such as restricting ourselves to the antiplane case, triangular lattices in 2D as well as nearest-neighbour interactions of Lennard-Jones type. By setting up a time-incremental energy-minimizing scheme and taking a diagonal sequence, we one obtains an evolution that is discrete in space and piecewise constant in time. The essential task was then, to prove the stability of the unilateral minimality property of the atomistic evolutions and an energy balance law. Our approach was to split the energy in an elastic part and a crack part by reformulating the energy in terms of triangles. More precisely, we wanted to define a notion of a ‘broken triangle’ and then, by an explicit construction, introduce a suitable interpolation that exhibits jumps exactly on these triangles. Such an interpolation would then enable us to reformulate the energy and view the minimizing displacements in terms of the suitable function spaces from the continuum theory that allow for discontinuities. Following this strategy, a major challenge was to to adjust the details of the ‘transfer of jump’ from [6] to the atomistic setting, because the energy contribution of a ‘broken’ interaction is not fixed but depends on its elongation, which gives rise to some further technical details in the proof. Moreover, we identified the continuum crack set by resorting to the notion of sigma-p-convergence introduced in [8]. Eventually, despite some temporary setbacks, we were able to complete the proof and submit the paper to the Journal “Mathematical Models and Methods in Applied Sciences” at the beginning of February 2024. We received the reviewers' reports at the beginning of November,

informing us that our work would be considered for publication if we addressed a number of suggestions for revision. Subsequently, we revised the manuscript accordingly and submitted our revision. Although the review process is not yet finalised, we are confident that the paper will be published soon.

After completing the planned investigation into atomistic-to-continuum convergence, we shifted focus to other potential research projects concerning the mathematical analysis of irreversible, quasi-static crack growth. Inspired by discussions within FRASCAL, particularly with P8, we aimed to explore the mathematical foundation of non-local fracture models, such as peridynamics. The objective was to study the quasi-static evolution of non-local models and prove their convergence to the quasi-static crack growth driven by the Griffith-functional, as formulated by Francfort and Larsen.

To this end, I spent February and March reviewing the literature on non-local variational models in fracture mechanics, as well as the associated mathematical results on existence and local limits. However, it became apparent that the problem was more analytically complex than initially anticipated. The primary challenge stemmed from the absence of a suitable irreversibility condition for the non-local model. In order to leverage our analytical framework based on sigma-convergence and 'jump-transfer' methods, it would have been necessary to define a concept of a 'non-local crack set', that gives rise to irreversibility in the limit. Since this seemed out of reach, we consequently decided to pivot away from non-local models and instead address a related but more tractable problem: the adaptive finite-element approximation of Griffith's energy.

Our investigation began with the works of [2] and [3], who introduced an approximation scheme for the Mumford-Shah functional with adaptive mesh refinement and suggested modifications for numerical implementation. Recently, Babadjian and Bonhomme extended this analysis to the Griffith functional from linearized elasticity, i.e., for functionals dependent only on the symmetric gradient of the deformation field u [1]. Since these results are static in nature, our aim was to provide a discrete-to-continuum passage for a quasi-static fracture evolution that accounts for the irreversible nature of crack growth. We sought to employ the Gamma-convergence results from [4] for a class of energies defined on pairs of function sets, thus taking a fundamentally different approach from [1]. Specifically, our strategy involved rewriting the discrete finite-element energy such that if features a bulk and surface terms. We then applied the lower-semicontinuity theorem from [4] to this displacement-void representation of the energy. This required introducing a notion of a 'discrete crack set' and relating its energy contribution to a surface energy by considering the boundary. The primary difficulty in this approach was proving that the surface energy provided a sharp lower bound for the original energy contribution. We were able to establish such a lower bound, up to an arbitrarily small error, by modifying the 'crack set'. It is worth noting that a similar approach was employed in [2] for the Mumford-Shah functional. In contrast to the scalar-valued problem, however, our proof of the modification did not only rely on extension results based on the Korn inequality, to 'heal' certain parts of the crack set, but also incorporated arguments from planar graph theory to estimate the number of triangles that could not be 'healed' in the Griffith case.

To demonstrate the stability of the unilateral minimality property, we intended to follow the approach outlined in [7]. Initially, we identified the need for a set-convergence notion suited for linearized elasticity, namely sigma-sym-convergence (see [4]), which controls

only the symmetric gradient. However, we later recognized that this notion is related to the original concept of sigma-convergence from [8], and it suffices to use this classical framework. Consequently, we could apply the 'jump-transfer' technique from [6] to ensure global stability and use well-established techniques to derive the energy balance law. Ultimately, this allowed us to identify the limiting evolution as a quasi-static crack growth in the sense of Francfort and Larsen. The paper is currently being finalized, with plans for submission at the beginning of the upcoming year.

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[6] G. A. Francfort, C. J. Larsen: *Existence and convergence for quasi-static evolution in brittle fracture* (2003) Comm. Pure Appl. Math. **56** 1465-1500

[7] M. Friedrich, J. Seutter: *Atomistic-to-Continuum convergence for quasi-static crack growth in brittle materials* (2024) Submitted to M3AS, https://arxiv.org/pdf/2402.02966

[8] A.Giacomini, M. Ponsiglione: *A Γ-Convergence Approach to Stability of Unilateral Minimality Properties in Fracture Mechanics and Applications*. (2006) Arch. Rational Mech. Anal. **180**, 399–447

[9] Rufat Badal, Manuel Friedrich, Joscha Seutter: Existence of quasi-static crack growth in atomistic systems (2022) FRASCAL Special Issue in Forces in Mechanics

3. Publications in peer-review journals, peer-reviewed contributions to conferences or anthology volumes, and book publications

The FRASCAL publications for 2024 are listed below with the corresponding abstract and the assignment to their respective projects. The acronyms in brackets behind the authors have the following meaning:

PhD: Doctoral Researcher
aPhD: Associated Doctoral Researcher
PDR: Postdoctoral Researcher
aPDR: Associated Postdoctoral Researcher
PA: Principal Advisor & Co-Principal Advisor
MF: Mercator Fellow

The FRASCAL community had a total of **11 publications** in 2024. Datasets can be published on the zenodo platform - with or without an associated text-based publication. A total of **4 datasets** were published here in 2024.

P1 | Chemistry at the crack tip

E. J. Schulze, C. L. Ritterhoff (PhD), E. Franz, O. Tavlui, O. Brummel, B. Meyer (PA) and A. Hirsch

Synthesis and Characterization of Bola-Amphiphilic Porphyrin-Perylenebisimide Architectures

In: Chemistry Europe (2024), Vol 30 (11)
DOI: 10.1002/chem.202303515

“We report on the synthesis and characterization of a family of three water-soluble bola-amphiphilic zinc-porphyrin-perylenebisimide triads containing oligo carboxylic-acid capped Newkome dendrons in the periphery. Variations of the perylenebisimide (PBI) core geometry and dendron size (G1 and G2 dendrons with 3- and 9-carboxylic acid groups respectively) allow for tuning the supramolecular aggregation behavior with respect to variation of the molecular architecture. The triads show good solubility in basic aqueous media and aggregation to supramolecular assemblies. Theoretical investigations at the DFT level of theory accompanied by electrochemical measurements unravel the geometric and electronic structure of the amphiphiles. UV/Vis and fluorescence titrations with varying amounts of THF demonstrate disaggregation.”

J. Kraus, L. Meinngast, J. Hald, S.B. Beil, J. Biskupek, C. L. Ritterhoff (PhD), S. Gsänger, J. Eisenkolb, B. Meyer (PA), U. Kaiser, J. Maultzsch, M. von Delius

Simultaneous Inside and Outside Functionalization of Single-Walled Carbon Nanotubes

In: Angewandte Chemie (2024), Vol. 63 (20)

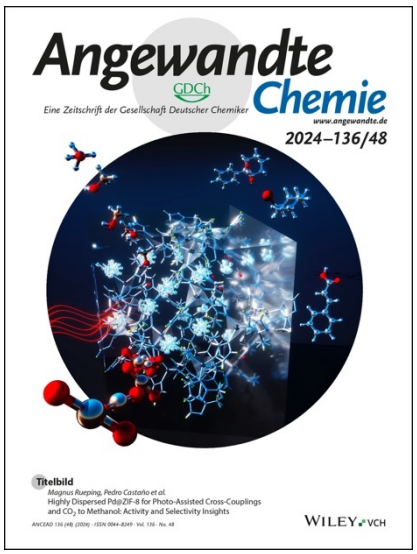
DOI: 10.1002/anie.202402417

„Functionalizing single-walled carbon nanotubes (SWCNTs) in a robust way that does not affect the sp2 carbon framework is a considerable research challenge. Here we describe how triiodide salts of positively charged macrocycles can be used not only to functionalize SWCNTs from the outside, but simultaneously from the inside. We employed disulfide exchange in aqueous solvent to maximize the solvophobic effect and therefore achieve a high degree of macrocycle immobilization. Characterization by Raman spectroscopy, EDX-STEM and HR-TEM clearly showed that serendipitously this wet-chemical functionalization procedure also led to the encapsulation of polyiodide chains inside the nanotubes. The resulting three-shell composite materials are redox-active and experience an intriguing interplay of electrostatic, solvophobic and mechanical effects that could be of interest for applications in energy storage.“

C. Oleszak, P.R. Schol, C.L. Ritterhoff (PhD), M. Krug, M.M. Martin, Y. Bo, B. Meyer (PA), T. Clark, D.M. Guldi, N. Jux

Fused Hexabenzocoronene-Porphyrin Conjugates with Tailorable Excited-State Lifetimes

In: Angewandte Chemie (2024), Vol 136 (48)
DOI: 10.1002/ange.202409363

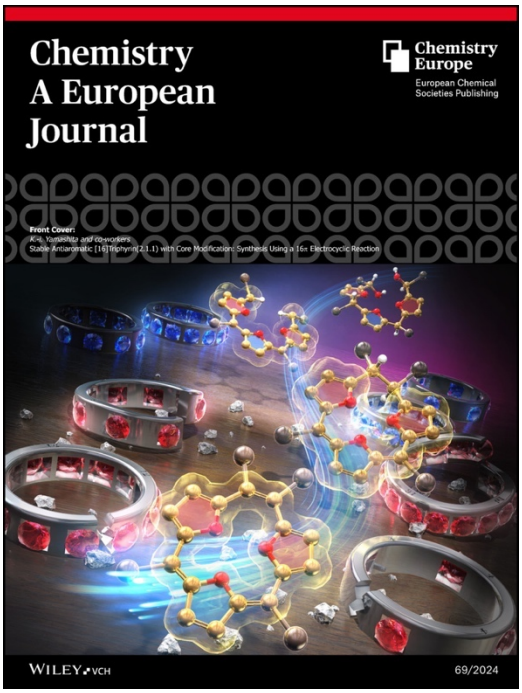


„A new clear-cut strategy for fusing N-heterocyclic and carbon-pure systems is introduced en route to a versatile platform of multi-purpose tetrapyrrolic chromophores. In particular, three novel C−C bond-fused porphyrin-hexabenzocoronene (HBC) conjugates were synthesized under oxidative cyclodehydrogenation conditions, starting from tailor-made nickel porphyrin precursors. The fusion of the individual aromatic systems via 5-membered rings led to highly soluble π-extended porphyrins in excellent yields. The resulting porphyrin-HBC conjugates exhibit absorption cross-sections that are of interdisciplinary interest in the ever-growing field of organic photovoltaics and near-infrared (NIR) dyes. Quantum chemical calculations show that the newly formed 5-membered rings induce biradicaloid character in the porphyrin core, which has a strong impact on excited state lifetimes. This is confirmed by a thorough optoelectronic and time-resolved characterization in order to understand these unique features better. Broadened absorption characteristics go hand-in-hand with short-lived excited states with up to six orders of magnitude faster decay rates.
“

C. Oleszak, C. L. Ritterhoff (PhD), M. M. Martin, B. Meyer (PA) and N. Jux

Manifold-Fused Porphyrin-Nanographene Conjugates

In: Chemistry Europe (2024), Vol. 30 (69)
DOI: 10.1002/chem.202403250



“A library of novel π-extended porphyrin-hexabenzocoronene (HBC) architectures is presented. Two distinct synthetic pathways were utilized to obtain either phenyl- or HBC-fused compounds. Absorption experiments reveal the species’ exciting photophysical and optoelectronic properties. Depending on the degree of π-extension, the number of porphyrins, and their relative position, a decisive change in shape, panchromatic broadening, and red-shifting of the absorption curves is observed. Theoretical studies give more profound insight into the molecule's electronic structures, showing vast decreases in HOMO-LUMO energy gaps.”
”

P3 | Fracture in polymer composites: nano to meso

Puhlmann P. (PhD), Zahn D. (PA):

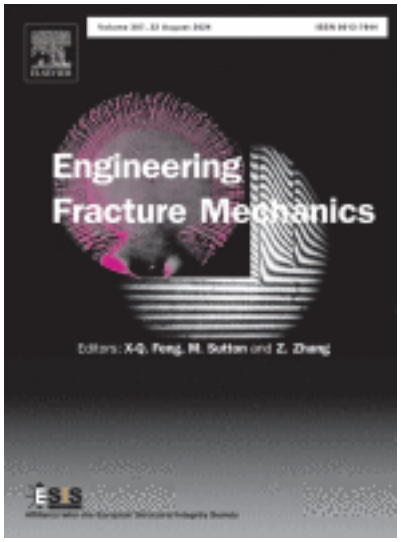
Molecular Dynamics Simulation of Silicone Oil Polymerization from Combined QM/MM Modelling

In: Polymers (2024), 16(12): 1755
DOI: 10.1007/s00894-023-05654-w

“We outline a molecular simulation protocol for elucidating the formation of silicone oil from trimethlyl- and dimethlysilanediole precursor mixtures. While the fundamental condensation reactions are effectively described by quantum mechanical calculations, this is combined with molecular mechanics models in order to assess the extended relaxation processes. Within a small series of different precursor mixtures used as starting points, we demonstrate the evolution of the curing degree and heat formation in the course of polymer chain growth. Despite the increasing complexity of the amorphous agglomerate of polymer chains, our approach shows an appealing performance for tackling both elastic and viscous relaxation. Indeed, the finally obtained polymer systems feature 99% curing and thus offer realistic insights into the growth mechanisms of coexisting/competing polymer strands.

P6 | Fracture in thermoplastics: discrete-to-continuum

Weber F. (PhD), Dötschel V., Steinmann P. (PA), Pfaller S. (PA) and Ries M. (PDR):
Evaluating the impact of filler size and filler content on the stiffness, strength, and toughness of polymer nanocomposites using coarse-grained molecular dynamics
In: Engineering Fracture Mechanics (2024), Vol. 307
DOI: 10.1016/j.engfracmech.2024.110270



“Their great versatility makes polymer nanocomposites an important class of engineering materials. In order to gain detailed insights into the nanoscale mechanisms underlying their macroscopic mechanical properties, molecular dynamics (MD) simulations are a valuable tool to complement experimental studies. In this work, we modify the analytical potential functions of an efficient bead–spring model representing a generic polymer nanocomposite to account for the breaking of covalent bonds. We perform uniaxial tensile simulations of double-notched specimens and validate the model using experimental trends for overall stiffness, strength, and toughness. First, we study the effects of sample size, notch geometry, strain rate, temperature, and molar mass for the pure thermoplastic matrix material. Second, we analyze the influence of filler size and filler content on the mechanical behavior of the polymer nanocomposite. With this study, we show that in both the development of new materials and the optimization of established materials, it is possible to gain important preliminary insights into the effects of pertinent material characteristics with a simple MD setup, which can then be further refined by increasing the complexity of the material description and the boundary conditions.

Ries M.(PDR), Laubert L. (aPhD), Steinmann P. (PA) and Pfaller S. (PA):

Impact of the unimodal molar mass distribution on the mechanical behavior of polymer nanocomposites below the glass transition temperature: A generic, coarse-grained molecular dynamics study

In: European Journal of Mechanics – A/Solids (2024), Vol. 107
DOI: 10.1016/j.euromechsol.2024.105379

“Polymer nanocomposites (PNCs) have shown great potential to meet the ever-growing requirements of modern engineering applications. Nowadays, molecular dynamics (MD) simulations are increasingly employed to complement experimental work and thereby gain a deeper understanding of the complex structure–property relations of PNCs. However, with respect to the thermoplastic’s mechanical behavior, the role of its average molar mass M_n is rarely addressed, and many MD studies only consider uniform (monodispersed) polymers. Therefore, this contribution investigates the impact that M_n and the dispersity Đ have on the stiffness and strength of PNCs through coarse-grained MD. To this end, we employed a Kremer–Grest bead–spring model and observed the expected increase in the mechanical performance of the neat polymer for larger . Our results indicated that the unimodal molar mass distribution does not impact the mechanical behavior in the investigated dispersity range $1.0<Đ<1.09$. For the PNC, we obtained the same - dependence and Đ-independence of the mechanical properties over a wide range of filler sizes and contents. This contribution proves that even simple MD models can reproduce the experimentally well researched effect of the molar mass. Hence, this work is an important step in understanding the complex structure–property relations of PNCs, which is essential to unlock their full potential.”

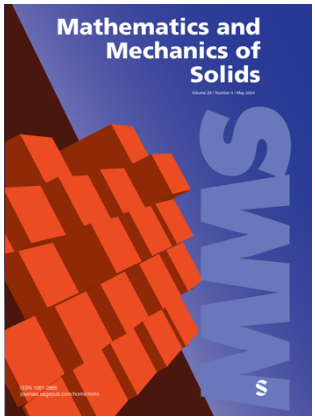
Richter E. M. (PhD), Possart G., Steinmann P. (PA), Pfaller S. (PA) and Ries M. (PDR):
Revealing the percolation-agglomeration transition in polymer nanocomposites via md-informed continuum RVEs with elastoplastic interphases
In: Composites Part B: Engineering (2024), Vol. 281
DOI: 10.1016/j.compositesb.2024.111477

“This contribution builds the concluding step of a multiscale approach to effectively capture the mechanical behavior of polymer nanocomposites (PNCs), in this case, silica-modified polystyrene. By introducing continuum-based representative volume elements (RVEs) that employ previously identified elastoplastic property gradients for the interphases surrounding the fillers, the effects of particle size, particle volume fraction, and agglomeration on the mechanical performance are investigated. Uniaxial tension tests are simulated with the respective finite-element RVEs, and stress–strain curves are derived. The elastic and plastic material properties of the RVE can then be extracted and analyzed quantitatively by fitting the stress–strain curves with a Voce-type elastoplasticity formulation.

At small degrees of agglomeration, i.e., good particle dispersion, in combination with sufficiently large particle volume fraction, percolation bands form, leading to improved elastic and plastic properties. Higher degrees of agglomeration or particle clusters behave like large single particles, which has an adverse effect, i.e., the nanoscale size effect is thereby neutralized. Therefore, the precise MD-informed elastoplastic interphase representation of our RVEs enables the investigation of the transition from beneficial percolation to unfavorable agglomeration. Ultimately, this contribution establishes a link between the effects of particle size, particle volume fraction, agglomeration, and percolation, which have so far only been discussed separately in the literature.

Our methodology offers new insights into the structure–property relations of PNCs and their resulting mechanical behavior. The underlying multiscale approach with a systematic transition from molecular to microscopic scales is required to complement experimental observations and exploit the full potential of PNCs.

Seibert J., Pfaller S. (PA) and Ries M. (PDR):
Investigation of the influence of nano-sized particles on the entanglement distribution of a generic polymer nanocomposite using molecular dynamics
In: Mathematics and Mechanics of Solids (2024), Vol. 29, Issue 3
DOI: 10.1177/108128652312065



“The addition of nano-sized filler particles to polymers leads to significant improvements in their mechanical properties. These can be traced back to the matrix–filler interactions of the interphase, which can be analyzed using molecular dynamic simulations. Usually, research in this context studies the general number of entanglements or the radius of gyration. However, this publication presents a novel approach by investigating the radial distribution of entanglements in an effort to characterize the interphase. To this end, we employ a coarse-grained model for a generic polymer composite and study multiple systems with varying particle radius and matrix–filler adhesion. Furthermore, the highly customizable and computationally efficient nanocomposite system developed during this research serves as a foundation for the further characterization of polymer nanocomposites and their interphases.

P7 | Collective phenomena in failure at complex interfaces

Greff C. (PhD), Moretti P. (PA) and Zaiser M. (PA):
Tuning load redistribution and damage near heterogeneous interfaces
In: Scientific Reports 14 (2024), Aticle Number: 29193
ISSN: 2666-3597
DOI: 10.1038/s41598-024-76681-7

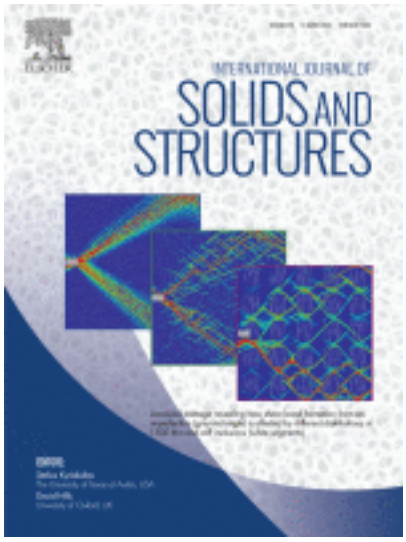
“We investigate interface failure of model materials representing architected thin films in contact with heterogeneous substrates. We find that, while systems with statistically isotropic distributions of impurities derive their fracture strength from the ability to develop rough detachment fronts, materials with hierarchical microstructures confine failure near a prescribed surface, where crack growth is arrested and crack surface correlations are suppressed. We develop a theory of network Green’s functions for the systems at hand, and we find that the ability of hierarchical microstructures to control failure mode and locations comes at no performance cost in terms of peak stress and specific work of failure and derives from the quenched local anistotropy of the elastic interaction kernel.”

P10 | Configurational Fracture | Surface Mechanics

Laurien M. (PhS), Javili A., Steinmann P. (PA):

Nonlocal interfaces accounting for progressive damage within continuum-kinematics-inspired peridynamics

In: International Journal of Solids and Structures (2024), Vol. 290
DOI: 10.1016/j.ijsolstr.2023.112641



“In this work, we present a modeling approach to nonlocal material interfaces in the framework of continuum-kinematics-inspired peridynamics. The nonlocal model accounts for progressive damage within a finite-thickness interface, as opposed to the more common practice of abrupt bond breakage across a zero-thickness interface. Our approach is based on an overlap of the constituents within the interface. Interfacial bonds between initially overlapping partner points are governed by a constitutive law reminiscent of a traction-separation-law. The governing equations for continuum-kinematics-inspired peridynamics in the presence of an interface are derived using a rate-variational principle. The damage formulation is established using the classical concept of internal variables. Following the notion of a standard dissipative material, thermodynamic consistency of the constitutive laws and the evolution of the internal variables is ensured. The latter results in a straightforward evaluation of a damage function. We give details about the computational implementation comprising a peridynamic discretization and a Newton–Raphson scheme. A sound approach to approximate the interface normal during deformation is presented, which allows to penalize material penetration across the interface. The proposed model is explored in a series of numerical examples, i.e., classical peeling and shearing tests, for a variety of damage functions. A key feature of our interface model are the nonlocal characteristics that are assumed to play a role especially at small scales. We, first, observe that an increasing thickness of the nonlocal interface leads to stronger interfacial bonding and less damage. Second, an increase in horizon size results in stiffer material behavior. When studying the wrinkling and delamination behavior of a compressed bilayer, it is found that an increase in interface stiffness leads to a smaller wrinkling wavelength. Moreover, delamination due to progressive damage of interfacial bonds in the post-wrinkling regime is observed, which, to the best of our knowledge, has not been studied in a nonlocal model before.”

3.1 Dataset publications on Zenodo

May 14

Ries M.(PDR), Richter E. M. (PhD), Pfaller S. (PA), Possart G. and Steinmann P.(PA):
Revealing the percolation-agglomeration transition in polymer nanocomposites via MD-informed continuum RVEs with elastoplastic interphases - dataset
In Composites Part B: Engineering, 281, 111477
ISSN: 1359-8368
DOI: 10.5281/zenodo.11190094

"This contribution builds the concluding step of a multiscale approach to effectively capture the mechanical behavior of polymer nanocomposites (PNCs), in this case, silica-modified polystyrene. By introducing continuum-based representative volume elements (RVEs) that employ previously identified elastoplastic property gradients for the interphases surrounding the fillers, the effects of particle size, particle volume fraction, and agglomeration on the mechanical performance are investigated. Uniaxial tension tests are simulated with the respective finite-element RVEs, and stress–strain curves are derived. The elastic and plastic material properties of the RVE can then be extracted and analyzed quantitatively by fitting the stress–strain curves with a Voce-type elastoplasticity formulation. At small degrees of agglomeration, i.e., good particle dispersion, in combination with sufficiently large particle volume fraction, percolation bands form, leading to improved elastic and plastic properties. Higher degrees of agglomeration or particle clusters behave like large single particles, which has an adverse effect, i.e., the nanoscale size effect is thereby neutralized. Therefore, the precise MD-informed elastoplastic interphase representation of our RVEs enables the investigation of the transition from beneficial percolation to unfavorable agglomeration. Ultimately, this contribution establishes a link between the effects of particle size, particle volume fraction, agglomeration, and percolation, which have so far only been discussed separately in the literature. Our methodology offers new insights into the structure–property relations of PNCs and their resulting mechanical behavior. The underlying multiscale approach with a systematic transition from molecular to microscopic scales is required to complement experimental observations and exploit the full potential of PNCs."

June 28

Weber F. (PhD), Dötschel V., Steinmann P. (PA) and Ries M. (PDR):
Evaluating the impact of filler size and filler content on the stiffness, strength, and toughness of polymer nanocomposites using coarse-grained molecular dynamics: dataset
DOI: 10.5281/zenodo.10473252

"Their great versatility makes polymer nanocomposites an important class of engineering materials. In order to gain detailed insights into the nanoscale mechanisms underlying their macroscopic mechanical properties, molecular dynamics (MD) simulations are a valuable tool to complement experimental studies. In this work, we modify the analytical potential functions of an efficient bead-spring model representing a generic polymer nanocomposite to account for the breaking of covalent bonds. We perform uniaxial tensile

simulations of double-notched specimens and validate the model using experimental trends for overall stiffness, strength, and toughness. First, we study the effects of sample size, notch geometry, strain rate, temperature, and molar mass for the pure thermoplastic matrix material. Second, we analyze the influence of filler size and filler content on the mechanical behavior of the polymer nanocomposite. With this study, we show that in both the development of new materials and the optimization of established materials, it is possible to gain important preliminary insights into the effects of pertinent material characteristics with a simple MD setup, which can then be further refined by increasing the complexity of the material description and the boundary conditions."

July 1

Pfaller S. (PA), Ries M. (PDR), Zhau W. (PDR), Bauer C. (PhD), Weber F. (PhD) and Laubert L. (aPhD):

CAPRICCIO – Tool to run concurrent Finite Element-Molecular Dynamics Simulations

DOI: 10.5281/zenodo.12606758

"The CAPRICCIO method is a framework to produce and analyse concurrent Finite Element (FE) - Molecular Dynamics (MD) calculations. It currently uses MATLAB R2022a (https://www.mathworks.com/) for the FE calculations and LAMMPS (2 Aug 2023 - Update 1) (https://doi.org/10.1016/j.cpc.2021.108171, https://www.lammps.org/) for the MD calculations.The FE meshes including the boundary conditions are created in ABAQUS/CAE 2021.HF7(https://www.3ds.com/products-services/simulia/products/abaqus/abaquscae/) and stored as .inp files. The following tools are included in CAPRICCIO:

- source/Capriccio_FEMD_main.m : Capriccio main routine calling the FE and MD functionalities
- source/preprocessing : Tools to create the non-periodic MD systems (00_PBC2HBC.sh) and the FE meshes (Python routines FE_mesh_*.py to be executed in ABAQUS)
- source/postprocessing : Tools to create an FEMD LAMMPS trajectory (FE2data) and to postprocess the FE and MD output

July 9

Ries M. (PDR), Laubert L. (aPhD), Steinmann P. (PA) and Pfaller S. (PA):

Impact of the unimodal molar mass distribution on the mechanical behavior of polymer nanocomposites below the glass transition temperature: A generic, coarse-grained molecular dynamics study – dataset

DOI: 10.5281/zenodo.8309118

"Polymer nanocomposites (PNCs) have shown great potential to meet the ever-growing requirements of modern engineering applications. Nowadays, molecular dynamics (MD) simulations are increasingly employed to complement experimental work and thereby gain a deeper understanding of the complex structure–property relations of PNCs. However, with respect to the thermoplastic's mechanical behavior, the role of its average molar mass

is rarely addressed, and many MD studies only consider uniform (monodispersed) polymers. Therefore, this contribution investigates the impact that and the dispersity Đ have on the stiffness and strength of PNCs through coarse-grained MD. To this end, we employed a Kremer–Grest bead–spring model and observed the expected increase in the mechanical performance of the neat polymer for larger . Our results indicated that the unimodal molar mass distribution does not impact the mechanical behavior in the investigated dispersity range Đ. For the PNC, we obtained the same -dependence and Đ-independence of the mechanical properties over a wide range of filler sizes and contents. This contribution proves that even simple MD models can reproduce the experimentally well researched effect of the molar mass. Hence, this work is an important step in understanding the complex structure–property relations of PNCs, which is essential to unlock their full potential."

3.2 Academic Activities: conferences, workshops & Co.(llaborations)

The following is a tabular list of academic activities that took place in 2024 and were attended by researchers of the FRASCAL community. In addition to conferences, these include summer and autumn schools, collaborations and the supervision of students.

P1 | Christian Ritterhoff

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
17.03.2024 22.03.2024	DPG	Berlin	**Poster**: Accelerating plane-wave-based ab initio molecular dynamics by optimization of Fast-Fourier Transforms for modern HPC architectures
22.07.2024 24.07.2024	Women in Science	Erlangen	**Poster**: Characterization of Novel Carbon-Rich Architectures by First-Principles Calculations.

Supervised Bachelor Student	Topic	Supervisor | Date
Tapio Juntunen	Bruchverhalten des polaren Perowskitoxids $KTaO_3$	Christian Ritterhoff, Bernd Meyer | 05.08.2024

Submitted publications

C.L. Ritterhoff, B. Meyer, Ab initio study of strain-induced polarization in $SrTiO_3$, $BaTiO_3$ and $KTaO_3$ during fracture, in preparation

C.L. Ritterhoff, T. Klöffel, S. Mandal, B. Meyer, Accelerating plane-wave-based *ab initio* molecular dynamics by optimization of Fast-Fourier Transforms for modern HPC architectures, in preparation

P3 | Pascal Franck

Name	Supported researcher	Course | field of study	Tasks relating to FRASCAL
Bakhmetau, Sviataslau	Pascal Frank, P3	Theoretical Chemistry	Simulation of Epoxy-Silica composites, tensile testing

P4 | Angel Santarossa

Collaborating Institution	Research topic	Researchers involved
Department of Physics, Universidad Nacional del Sur, IFISUR-CONICET, Argentinia	Hydraulic fractures under mixed mode I+III loading	Prof. Dr. Leopoldo Gòmez Dr. Anabella Abate Laureano Ortellado

P5 | Shucheta Shegufta

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
19.05.2024 23.05.2024	5th International Symposium on Phase-Field Modelling in Materials Science (PF24)	Hangzhou, China	**Talk:** Linking peridynamics, nonlocal elasticity and phase field models of damage and fracture
25.09.2024 27.09.2024	Advances in Peridynamic Material Modeling	Venice, Italy	**Talk:** Modeling damage of disordered porous material with homogenized microstructure using peridynamics

Name	Supported researcher	Course | field study	of Tasks relating to FRASCAL
Yuxin Luo	Shucheta Shegufta	Advanced materials and processes	Support in software maintenance, writing unit tests

P6 | Felix Weber

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
02.06.2024 07.06.2024	ECCOMAS CONGRESS	Lisbon	**Talk:** Fracture simulations of amorphous materials using a concurrent atomistic-to-continuum approach
22.09.2024 27.09.2024	11th ICMMM	Prague	**Talk:** Fracture simulations of amorphous materials across scales

Collaborating Institution	Research topic	Researchers involved
Institut de Physique de Rennes, Université de Rennes, CNRS	Multiscale fracture simulations of glasses	Vassaux, Maxime

Supervised Master Student	Topic	Supervisor | Date
Richter, Eva	A "Capriccio light" approach to study the capabilities of multiscale fracture simulations of thermoplastics	Felix Weber/ Maximilian Ries 26 Nov 24

P6 | Lukas Laubert

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
05.03.2024 02.06.2023	Journées Européennes des Composites	Paris	Participation only
18.03.2024 22.03.2024	94th Annual Meeting IAAMM	Magdeburg	**Talk:** Multistage parameter identification of a finite-strain viscoelastic-viscoplastic materialmodel for biobased thermosets

03.06.2024 07.06.2024	9th European Congress on Computational Methods in Applied Sciences	Lisbon	**Talk:** Sequential parameter calibration for a finite-strain viscoelastic-viscoplastic material model for biobased thermosets
26.08.2024 30.08.2024	26th ICTAM	Daegu	**Talk:** Multi-level parameter identification of a finite-strain viscoelastic-viscoplastic material model for bio-sourced epoxy

Collaborating Institution	**Research topic**	**Researchers involved**
Institut de Chimie et des Matériaux paris-Est at the Université paris-Est Créteil Val de Marne	BIO ART	Agustín Ríos De Anda Stephanie Chedid
Laboratoire Modélisation et Simulation Multi-Échelle at the Université Gustave Eiffel	BIO ART	Fabrice Detrez Moussa Lamamra
Department of Polymer Engineering at the Universität Bayreuth	BIO ART	Denise Schweser
Aerospace and Mechanical Engineering Department at the University of Liége	Continuum constitutive modeling	Ujwal Kishore Jinaga Mohib Syed Mustafa
PULS Group FAU	Molecular simulations	Christian Wick György Hantal Sampanna Pahi Bariscan Arican

P6 | Maximilian Ries

from | to	**Name of conference**	**Location**	**Title of own presentation / title of own poster presentation / participation only**
28.05.2024 31.05.2024	19th EMMC	Madrid	**Talk:** Identification of inelastic interphase properties in polymer nanocomposites based on molecular dynamics
03.06.2024 07.06.2024	ECCOMAS Congress	Lisbon	**Talk:** Identification of inelastic interphase properties in polymer nanocomposites based on molecular dynamics
03.06.2024 07.06.2024	ECCOMAS Congress – PhD Olympiad	Lisbon	**Talk:** Characterization and modelling of polymer nanocomposites across the scales
25.09.2024 27.09.2024	Fall meeting of ESIS TC4 on Polymers, Adhesives and Composites	Dublin	**Talk:** Investigating the mechanical behavior of epoxy-based thermosets via coarse-grained molecular dynamics
21.10.2024 25.10.2024	Lorentz workshop: Breaking barriers in polymer materials design	Leiden	**Poster:** Studying the mechanical performance of polymer nanocomposites with molecular dynamics-informed continuum model

Supervised Master Student	Topic	Supervisor | Date
Richter, Eva	A "Capriccio light" approach to study the capabilities of multiscale fracture simulations of thermoplastics	Felix Weber/ Maximilian Ries 26 Nov 24
Supervised Bachelor Student	**Topic**	**Supervisor | Date**
Roksvaag, Johannes	Improving the performance of the Capriccio Method by migrating to the open-source programming language Julia	Maximilian Ries/ Sebastian Pfaller 25 Oct 24
Supervised Project Thesis	**Topic**	**Supervisor | Date**
Richter, Eva	Modeling an Epoxy-based adhesive joint with coarse-grained molecular dynamics	Maximilian Ries 28 Mar 24
Dötschel, Vincent	Revealing the interphase in Epoxy-based adhesive joints via coarse-grained molecular dynamics	Maximilian Ries 25 Oct 24

P7 | Christian Greff

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
28.05.2024 31.05.2024	EMMC 19	Madrid	**Talk:** Controlling damage localization through hierarchical microstructure

Supervised Student	Topic	Supervisor | Date
Szalay, Peter (Bachelor thesis)	Statistische Analyse der Auswirkung von Variation der Struktur und Unordnung der lokalen Festigkeit auf das Bruchverhalten hierarchisch strukturierter Netzwerke	Christian Greff 21 Mar 24

Student assistant	Course/ field fo study	Funded Member of FRASCAL (from | to)	Tasks relating to FRASCAL
Taheri, Saba	Materials Science and Engineering	21.10.24 21.10.25	Design and implementation of unit tests for the in-house code used in simulations of the project

P8 | Maurice Rohracker

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
29.05.2024 31.05.2024	19th European Mechanics of Materials Conference	Madrid	**Talk:** Performance enhancements in phase-field fracture simulations

Supervised Student	Topic	Supervisor | Date
Krowiak, Martin (Bachelor thesis)	Phase-field modelling of fracture in rate dependent materials	Maurice Rohracker 18 Dez 2024

Student assistant	Course/ field fo study	Funded Member of FRASCAL (from | to)	Tasks relating to FRASCAL
Khanvilkar, Kaustubh	Computational Engineering	15.06.24 20.10.24	Parametrization of viscoplastic phase-field model for fracture using data from P3
Shastry, Aaniruddha P.	Computational Engineering	15.04.24 30.04.35	Extension and maintenance of the inhouse python toolbox RVEGen for generating geometry and meshes of RVEs

P8 | Lucie Spannraft

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
29.01.2024 02.02.2024	ELACTAM	Havana	**Talk:** generalized interfaces enabling macroscopic modelling of structural and soft adhesives and their failure

P9 | Deepak Jadhav

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
26.08.2024 30.08.2024	European Conference on Fracture	Zagreb	**Talk:** Phase field modelling of dynamic fracture using a modified asynchronous variational integrator
08.12.2024 12.12.2024	IUTAM Symposium in Computational Fracture Mechanics in Multi-field Problems	Bad Honnef	**Talk:** A spatially adaptive phase field model for static and dynamic fracture

Student assistant	Course/ field fo study	Funded Member of FRASCAL (from | to)	Tasks relating to FRASCAL
Setty, Prashanth	Mechanical Engineering	01.01.24 31.07.24	Implementation of implicit asynchronous variational integrators for elastodynamic problems
Poojari, Saurabh	Mechanical Engineering	01.10.24 30.04.2025	3D extension of new asynchronous variational integrator for phase field modelling of dynamic fracture

Submitted publications

D. B. Jadhav, D. Phansalkar, K. Weinberg, M. Ortiz, S. Leyendecker, "A new approach to asynchronous variational integrators for a phase field model of dynamic fracture," Submitted to International Journal of Numerical Methods in Engineering, Nov. 2024.

P10 | Marie Laurien

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
21.07.2024 25.07.2024	WCCM	Vancouver	**Talk:** Damage in continuum-kinematics-inspired peridynamics
16.09.2024 18.09.2024	SolMech	Wroclaw	**Talk:** Nonlocal interfaces in continuum-kinematics-inspired peridynamics

P10 | Anna Titlbach

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
23.07.2024	ARC Seminar	Brisbane	**Invited Talk:** A novel micromorpphic approach captures non-locality in continuum bone remodeling
29.10.2024	CMP Seminar	Nürnberg	**Invited Talk:** Modelling the Flexoelectric Effect in Bone - A micromorphic approach
from | to	**Institute visited**	**Local supervisor**	**Research activities performed and skills acquired during stay**
08.07.2024 04.08.2024	Queensland University of Technology	Peter Pivonka	Application-specific analyses on the FEM model for simulating the flexoelectric effect in human bone

P11 | Lennart Igel

Supervised Project Thesis	Topic	Supervisor | Date
Gupta, Manik	Peridynamics model for quasistatic fracture simulation	Lennart Igel 25 Sep 24

P12 | Sampanna Pahi

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
05.03.2024 08.03.2024	MMWS	Erlangen	**Talk:** Investigating the impact of Curing dynamics on the Microstructure and properties of epoxy
14.03.2024 19.03.2024	DPG	Berlin	**Talk:** Investigating the impact of Curing dynamics on the Microstructure and properties of epoxy
02.06.2024 08.06.2024	ALCHEMA	Frankfurt	**Participation only**
14.08.2024 19.08.2024	CESTC	Croatia	**Talk:** Investigating the impact of Curing dynamics on the Microstructure and properties of epoxy
14.11.2024 14.11.2024	Preparing the Disputation	online	**Participation only**

from | to	Institute visited	Local supervisor	Research activities performed and skills acquired during stay
01.11.2024 30.11.2024	ITER, India	K. Mahanta	DFT investigations on magnetic materials

P13 | Ruaridh Smith

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
14.05.2024 19.05.2024	EGU 2024	Vienna	**Poster:** Variations in fracture distribution across Northern Bavaria – Towards large-scale geothermal fracture models
06.10.2024 08.10.2024	EAGE Workshop on Naturally Fractured Reservoirs	Muscat	**Talk:** Characterising fracture network analogues for subsurface geothermal modelling - insights from Northern Bavaria

Supervised Master Thesis	Topic	Supervisor
Jakob, Fabian	Variations in fracture networks in Northern Bavaria	Daniel Köhn Rahul Prabhakaran Ruaridh Smith

P14 | Joscha Seutter

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
14.10.2024 18.10.2024	ICMS-Workshop: Mathematical Material Science	Edingburgh	**Participation only**

4. Qualification Concept

4.1 Qualification programme

The qualification programme comprises

- **“FRASCAL Qualification Days”,**
- **“FRASCAL Virtual Colloquia”,**
- **“FRASCAL Symposia”, and**
- **“FRASCAL Retreats**”

as basic activities. These are complemented by obligatory participation in international conferences and optional research stays abroad.

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 FRASCAL Mini Lectures including Special Seminars and Soft Skills Trainings. As most doctoral researchers of the second cohort have completed the largest part of their qualification program in 2024, the focus was more on the finishing of the doctoral theses and complementary lectures and visits by guest scientists, which allowed them to look beyond the everyday research field.

FRASCAL Mini Lectures

The Mini Lecture programme consists of four pillars addressing Mathematical Skills, Modelling Approaches, Computational Methods, as well as Material Sciences. 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, but occasionally also by FRASCAL doctoral researchers, scientists from the participating departments or external experts.

Picture @ Sebastian Pfaller

Prof. Ríos de Anda held a Mini Lecture series “Introduction on Polymers – from their synthesis to their applications” from 9th of December to 13th of December focussing on the relation between material chemistry and material properties relevant in engineering.

FRASCAL Special Seminars

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

Four special seminars were held in 2024. FRASCAL Mercator Fellows Prof. Anna Pandolfi and Prof. Erik Bitzek and the researchers Prof. Samit Roy (University of Alabama) and Prof. Jianbing Chen (Tongji University) could be engaged for the special seminar days.

Special seminars 2024

	Date	Title	Lecturer
01	2 February	A coupled approach for diffused fracturing in porous brittle materials	Prof. Anna Pandolfi
02	8 March	An atomistic perspective on fracture toughness of inorganic materials	Prof. Erik Bitzek
03	15 July	Predicting fracture in polymers using Capriccio-based atomistic-continuum concurrent coupling technique	Prof. Samit Roy
04	26 July	A new non-local macro-meso-scale damage model of quasi-brittle materials and reliability-based optimization of concrete strucutres	Prof. Jianbing Chen

FRASCAL Soft Skills Trainings

In 2024 the Soft Skills Seminar "Scientific presentation" was presented by PA Prof. Thorsten Pöschel on 11th of November.

Paul Gahmann's popular English courses were held on demand - for example, by providing advice on peer-reviewed papers. On the happy occasion of his successfully defended doctoral thesis, the FRASCALis met with Dr. Paul Gahmann for pizza, sparkling wine and Andrea`s Guacamole.

FRASCAL Seminars

In each lecture period one qualification day is reserved for a FRASCAL seminar, which is mandatory for the doctoral researchers. Within the framework of this seminar, recent developments in the doctoral and associated doctoral projects are presented as talks of 20 - 30 min duration, including a 5 - 10 min discussion. Based on these seminars, the doctoral and associated doctoral researchers can evaluate the progress of the doctoral project in comparison to the other projects together with the mentoring team.

The 9th FRASCAL Seminar was held at the IZNF, the 10th FRASCAL Seminar took place at the LTM.

The doctoral researchers and associated doctoral researchers of the second cohort had the opportunity to present the research results.

The second part of the FRASCAL Seminar 2024 was introduced by the spokesperson Prof. Steinmann with an entertaining and informative talk in which he gave insights into his time in Australia. Prof. Steinmann and doctoral researcher Anna Titlbach connected there both professionally and physically on the topic of biomechanics.

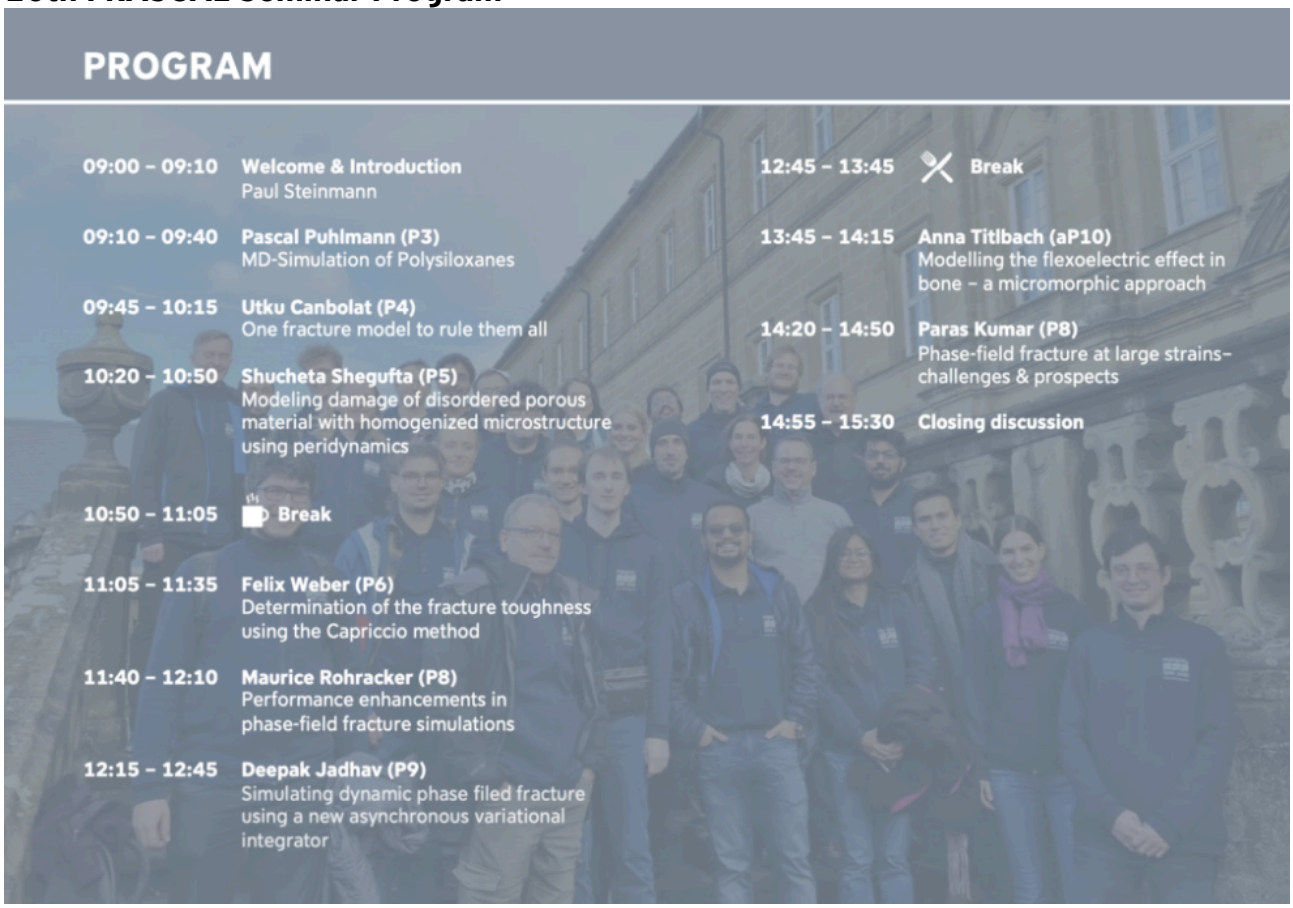
Prof. Steinmann about his research sabbatical down under in Australia

Pascal Puhlmann talked about his (linear) polysiloxanes, their simulation within the reaction of polycondensation and the potential influence of chain length on material properties. Utku Canbolat differentiated fracture models for the conception of the holy grail of fracture models. Shucheta Shegufta presented ideas of studying the effect of microstructure by artificially generated microstructures and the role of convergence. The Capriccio method and its use in simulating fracture toughness taking the example of SiO2glass was introduced by Felix Weber.

Maurice Rohracker then reports how to handle numerical difficulties in phase-field simulations by using performance enhancing techniques. A new asynchronous variational integrator for the simulation of dynamic phase field fracture was presented by Deepak Jadhav. After the lunch break Anna Titlbach compared micromorphic and flexo-micromorphic elasticity in bones and gave insights into the idea of the flexoelectric effect. Paras Kumar reported on the latest developments within his postdoc project on phase-field fracture at large strains and thus concluded the 10th FRASCAL seminar.

9th FRASCAL Seminar Program

10th FRASCAL Seminar Program



TOPZ

The digital format called FRASCAL TOPZ (Topical Overview Presentation Zoomposium), typically, once per week, was used for an informal get-together in ZOOM, where the PAs, the spokespersons, the doctoral and associated doctoral researchers, the postdoc, and the scientific coordinator were present. Typically, the latest scientific progress and open questions from one doctoral project were briefly presented and jointly discussed. Moreover, FRASCAL TOPZs provided an informal atmosphere to discuss any organisational, administrational, and topical issues related to FRASCAL in a relaxed manner. Active participation in the TOPZ was expected of every doctoral researcher. Unfortunately for late-rising DRs, our meeting time was moved to 9 a.m., as Prof. Steinmann would otherwise not have been able to attend from down under. Accordingly, the number of participants in 2024 was sadly reduced.

3rd FRASCAL Symposium

On November 21st, the FRASCAL community came together for an inspiring day of dialogue at the Wassersaal of the Orangerie in Erlangen. In total, the 3rd FRASCAL Symposium featured five speakers who shared their research with us. Professor Andrew McBride from Glasgow University started by talking about continuum-kinematics-inspired peridynamics. Dr. Sukhminder Singh from the Technical University of Denmark and still known to all as former FRASCALi gave insights into his research on two-dimensional periodic microstructures. Professor Julien Yvonnet from Université Gustave Eiffel talked about multiscale modelling of quasi-brittle fracture, focusing on machine learning. Professor Dorothee Knees from the University of Kassel discussed phase-field damage models. Professor Dirk Zahn from Friedrich-Alexander University Erlangen gave a talk on polymer fracture and, together with a spontaneous presentation by Spokesperson Professor Paul Steinmann, concluded our symposium. Each speaker offered valuable and engaging insights, contributing to a deeper understanding of fracture mechanics. We thank all the speakers and PhD students for making this event a success in that everyone contributed both physically and in terms of content!

Text & picture: Ann-Sophie Herzner & Anna Donhauser

4.2 Visiting researcher programme

We had the great pleasure to welcome Prof. Agustín Ríos from ICMPE (Institut de Chimie et des Matériaux Paris-Est) within the ERASMUS+ programme. Agustín Ríos gave a lecture series on polymers with particular focus on the relation between the chemistry of these materials and their properties relevant in engineering. Based on his long-standing expertise in the development of polymers from renewable resources, he gave detailed insights into the current challenges in the field of bio-based polymer materials. Agustín Ríos motiviated all participants to actively contribute, among others by using construction kits for long-chain molecules. We thank Agustín Ríos very much for sharing his knowledge and experience in the field of these fascinating materials!

Text & pictures: Sebastian Pfaller

Visiting researchers 2024

Date	Guest	Topic
April	Prof. Michael Ortiz | California Institute of Technology & Prof. Kerstin Weinberg | Universität Siegen	
July	Prof. Samit Roy | Director of Advanced Composite Materials Laboratory, University of Alabama	**Talk:** Predicting Fracture Toughness in Polymers using Capriccio-Based Atomistic-Continuum Concurrent Coupling Technique
December	Prof. Agustín Ríos | Institute de Chimie et des Matériaux Paris-Est, France	**Mini Lecture:** Introductory course on polymers

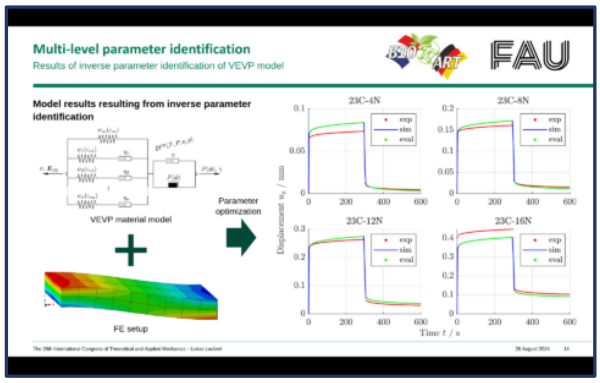
5. Selected Highlights

5.1 Anna`s PhD journey to Queensland University of Technology

Each year our PhD candidates have the opportunity to spend a research stay abroad.
For instance this summer, Anna Titlbach, a PhD candidate at Technische Hochschule Nürnberg Georg Simon Ohm in collaboration with FAU Erlangen-Nuremberg, spent her research stay at Queensland University of Technology (QUT) in Brisbane.
Near the end of her stay, Anna had the chance to present her research on bone biomechanics at a seminar held on Tuesday, July 23rd. The Australian ARC Training Centre for Joint Biomechanics described Anna's approach on LinkedIn as innovative and called her a leading researcher in her field. What a success! Indeed, what makes Anna's research so special is that she employs a micromorphic approach using the open-source finite element library deal.II.
Among the professors who joined Anna at her seminar were the FRASCAL spokesperson Prof. Paul Steinmann, Prof. Areti Papastavrou from Technische Hochschule Nürnberg Georg Simon Ohm and Prof. Peter Pivonka from Queensland University of Technology.

Text: Ann-Sophie Herzner, Picture: Anna Titlbach

5.2 Lukas`visit at ICTAM 2024 in Deagu



From August 26th to 30th, Lukas Laubert attended the International Congress of Theoretical and Applied Mechanics (ICTAM) 2024 held in Daegu, South Korea. This international event offered him a chance to connect with researchers from around the world, which was indeed a valuable opportunity for Lukas. His week centered around sessions on "Nonlinear Mechanical Models for Biological and Bioinspired Materials", where he took on the moderator role and presented his research on "Multi-level Parameter Identification of a Finite-strain Viscoelastic-viscoplastic Material Model for Bio-sourced Epoxy" on the first day of the conference. In addition to his contributions, Lukas participated in lectures and presentations on various topics, such as composites and damage mechanics, each providing valuable insights for his own research. The conference also featured numerous networking events, including a welcome reception and congress banquet, allowing him to exchange ideas with fellow researchers from around the globe.

Text & pictures: Lukas Laubert

5.3 Symposium at MMM11 in Prague

Felix and Sebastian organised together with Fabrice Detrez (Paris), Andrea Giuntoli (Groningen), Matej Praprotnik (Ljubljana), and Maxime Vassaux (Rennes) the symposium "Multiscale simulations of polymers and polymer composites" at the 11th International Conference on Multiscale Materials Modeling (MMM 11) in Prague. It was a pleasure to welcome 30 speakers, including 5 keynote lecturers, addressing various aspects of polymer and polymer composite simulations across different time and length scales. In addition, there were many occasions for highly fruitful scientific exchange. Overall, MMM 11 was a great experience and benefited a lot from the excellent local organisation team.

Aside from the scientific part, we had the chance to explore the exciting capital of the Czech Republic together with its traditional cuisine and beer culture. A specific highlight was certainly our joint visit of an excellent performance of Verdi's Otello in the State Opera. We thank all co-organisers for this outstanding scientific and personal experience in Prague!

Text & picture: Sebastian Pfaller

5.4 Wuyang Zhao receives DFG individual research grant

We are delighted to announce that Wuyang Zhao received a DFG individual research grant for his project "Investigating brittle-to-ductile transition in glassy polymers by multiscale modeling across atomistic and continuum scales". In this project, he will investigate the mechanisms of toughness in glassy polymers based on molecular simulations. Using the Capriccio framework, the molecular descriptions will be embedded into a continuum domain to apply loading conditions that are not feasible in pure molecular approaches as, e.g., those typically arising in fracture problems. Beyond this, Wuyang is also going to study the effect of nanoparticles added to the polymer matrix.

The first funding period will last for 2 years and start from February 2025. We sincerely congratulate Wuyang for this great success and wish him a very good start!

Text: Sebastian Pfaller, picture: Giulia Ianicelli

5.5 Research stay at the Institute de Physique in Rennes

Felix Weber visited Dr. Maxime Vassaux at the Institut de Physique de Rennes (IPR) for five weeks. During this research visit, Maxime and Felix discussed and performed multiscale fracture simulations of silica glass using the Capriccio method. The focus was on analyzing the structural (e.g., radial/angular distribution function and ring sizes) and mechanical (e.g., critical stress intensity factor) properties of oxide glasses during crack propagation and on suitable virtual experimental setups that are comparable to real experiments. For Felix, it was very valuable to visit the laboratories and see real fracture mechanics experiments on glasses that are carried out at the IPR. During Felix' stay, Sebastian Pfaller visited Maxime and Felix in Rennes to hold a joint seminar and to have fruitful discussions with the scientists conducting research at IPR. Sebastian and Felix were able to experience the culture of Rennes first hand by visiting one of the city's impressive markets and a church service, which culminated in a course on preparing and eating oysters taught by Maxime. During a visit to the historic French port city of Saint-Malo, Maxime, Sebastian and Felix reflected on the topics they had been working on in the previous weeks. Two highlights of the scientific activities in Rennes for Felix were attending the PhDay at IPR, where PhD students gave talks on their research topics, and his own presentation of the current state of the collaboration with Maxime at the IPR's non-permanent seminar. In summary, the research stay in Rennes was a great success and has intensified the collaboration between the Capriccio group and IPR.

Text & pictures: Felix Weber

5.4 Doctoral degree

We are pleased to announce one successfully completed FRASCAL dissertation project in 2024:

Dr. Tarakeshwar Lakshmipathy

We are delighted to announce that Tara successfully defended his dissertation on January 29, 2024.

Pictures: Andrea Dakkouri-Baldauf

Dr. Tobias Müller

On December 16, Tobias defended his doctoral thesis on "Ab-initio investigation of the impact of structural motifs on the fracture toughness of silicon".

The examination committee was made up of the three PAs Dirk Zahn, Julia Mergheim and Bernd Meyer.

Congratulations, Tobias!

Picture: Nico van Eikema Hommes

5.5 FRASCAL recruitment symposium and 3rd FRASCAL cohort

„At FRASCAL, we break things – but only in theory," explains the FRASCAL spokesperson with a wink, as the graduate college warmly welcomes prospective PhD candidates. Indeed, FRASCAL will soon have the pleasure of welcoming a new cohort of PhD students from January onward. On September 12th, shortlisted candidates had the opportunity to present their master thesis to the FRASCAL research team. Presentations covered a broad field from „Cracks & Growth: Fracture Mechanics and Life" to „Fracture in Rocks: From Single Grains to Seismic Scale". Throughout the day, engaging discussions followed each presentation, and continued during networking coffee and lunch breaks. As a preview of what's ahead, Felix Weber, Marie Laurien, and Paras Kumar introduced the incoming PhD students to the projects of previous cohorts. They not only shared key findings from past research but also highlighted some of the gaps the new cohort will have to resolve. How exciting!

Text & pictures: Ann-Sophie Herzner & Anna Donhauser