Friedrich-Alexander-Universität
Erlangen-Nürnberg

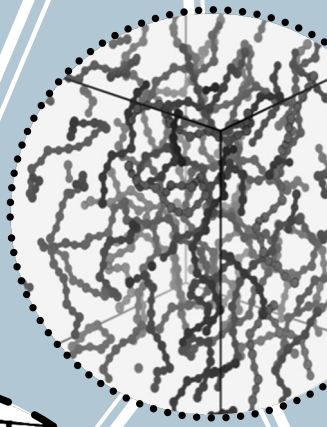
FRACTURE ACROSS SCALES

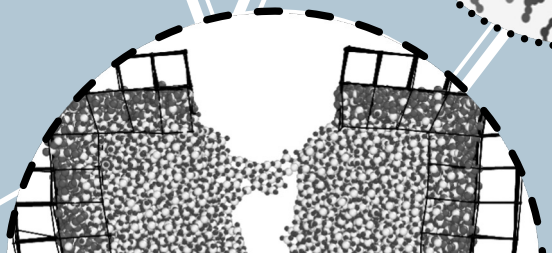
Integrating Mechanics, Materials Science, Mathematics, Chemistry and Physics

ANNUAL REPORT 2023

FRASCAL

GRK 2423





Annual Report

of the Research Training Group GRK 2423

FRASCAL

Fracture across Scales

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

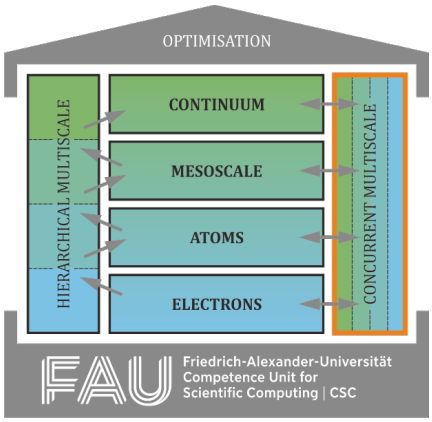
at the

Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

Prof. Dr.-Ing. Paul Steinmann (spokesperson)

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

2023



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IMPRESSUM

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Preface

As we present our FRASCAL annual report for the year 2023, we are filled with immense pride and gratitude for the remarkable achievements we have collectively attained. The highlight of this year undoubtedly revolves around the successful attainment of our primary objective: securing a second funding period. This milestone stands as a testament to the dedication, collaboration, and unwavering enthusiasm of all involved.

We extend our heartfelt appreciation to the whole FRASCAL team - our doctoral researchers, postdocs, and principal advisers - who have played pivotal roles in making this year a resounding success. Their tireless efforts, commitment to excellence, and harmonious collaboration have laid the foundation for our achievements and propelled us toward our shared goals. The harmonious atmosphere among our FRASCAL team members has been instrumental in fostering creativity, innovation, and productivity.

In addition to securing funding, 2023 has been marked by a series of exciting publications and significant milestones in the form of submitted dissertations and successful defenses. These accomplishments are a testament to the intellectual rigor and scholarly contributions of our community.

We extend our deepest gratitude to each and every member of our team for their dedication, passion, and hard work. Without their enthusiasm and unwavering commitment, our achievements would not have been possible.

As we reflect on the year gone by and look ahead to the opportunities that lie ahead, let us continue to uphold the values of collaboration, excellence, and integrity that define FRASCAL.

Erlangen, May 2024

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:
Christian Greff

Doctoral researchers' gender representative:
Deepak Balasaheb Jadhav

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.	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**

Doctoral Researchers	Chair, Department, Work Address	Contact Data	Research Area
[1]**Canbolat**, Utku	Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraβe 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**

[1] 2nd cohort of FRASCAL

Doctoral Researchers	Chair, Department, Work Address	Contact Data	Research Area
[1]**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**
[1]**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**
[1]**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**
Kumar, Paras	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-20 323 / -503, paras.kumar@fau.de, www.ltm.tf.fau.eu	**Fracture in Polymer Composites: Meso to Macro**
[1]**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**
[1]**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**
[1]**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**
[1]**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**
[1]**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**
[1]**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**
Singh, Sukhminder	Mathematical Optimisation, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen	+49 9131 85-67 048 / -20785, sukhminder.singh@fau.de, www.mso.math.fau.de	**Fracture Control by Material Optimisation**
[1]**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
Hiemer, Stefan	Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65 062 / -066, stefan.hiemer@fau.de, www.matsim.techfak.uni-erlangen.de	**Machine Learning of Failure of Disordered Materials**
Ries, Maximilian	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-67 619/ -503, maximilian.ries@fau.de, www.ltm.tf.fau.eu	**Multiscale Simulation of Amorphous Polymers**
Santarossa, Angel	Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraße 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**
Schmidt, Ina, Dr.-Ing.	Faculty of Mechanical Engineering Kesslerplatz 12, 90489 Nürnberg	ina.schmidt@th-nuernberg.de	**Computational Bone Remodelling**
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**
Zhao, Wuyang	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-28 511/ -503, wuyang.zhao@fau.de, www.ltm.tf.fau.eu	**Small-Scale Informed Constitutive Modelling**

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

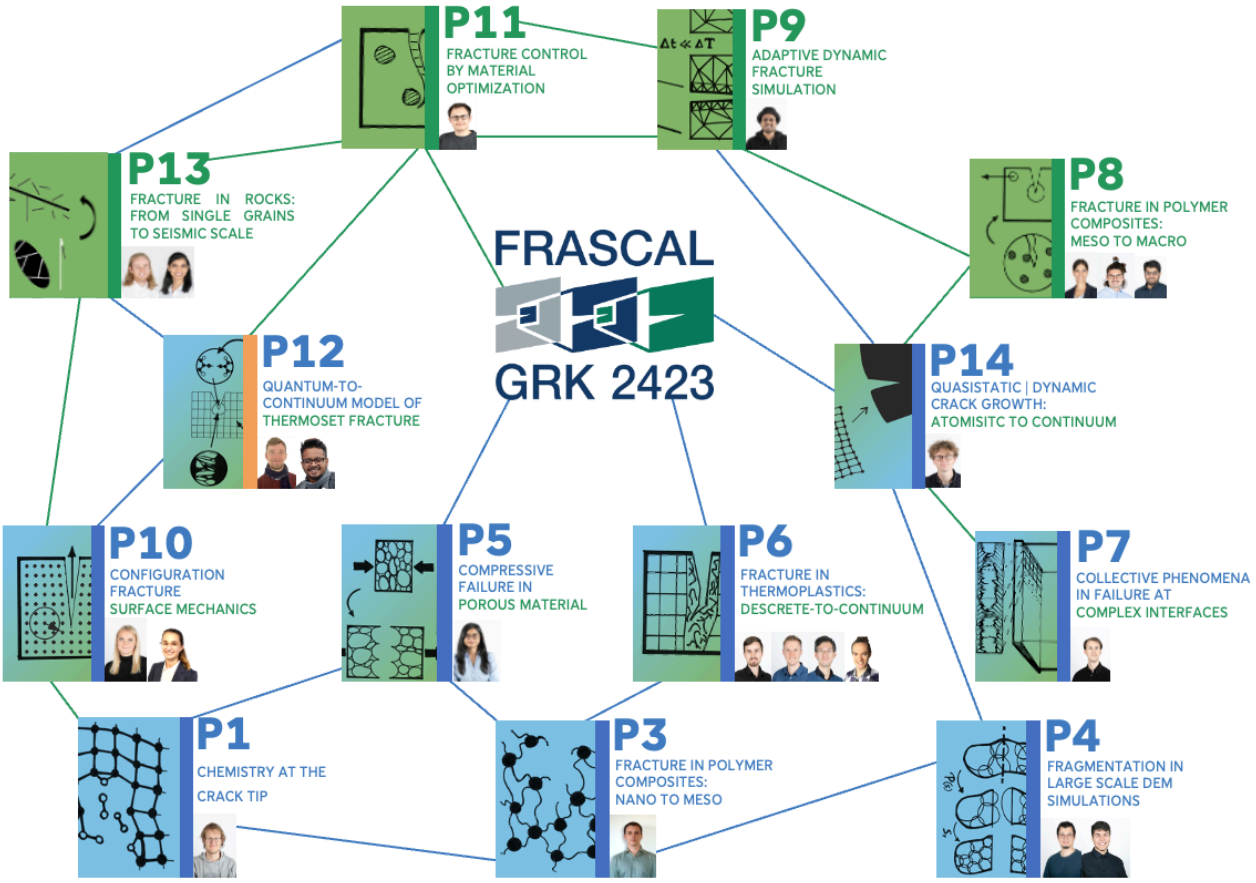
Coordination and administration of GRK 2423 FRASCAL

	Work Address	Contact Data	Work Area
Zinser, Heidi, Dr.	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**
Pflug, Lukas, Dr. rer. nat.	Department of Mathematics Chair of Applied Mathematics, Cauerstraße 11, 91058 Erlangen	+49 9131 85 67139 / -67134, lukas.pflug@fau.de, www.csc.fau.eu	**CSC Managing Director**

1.4 Reporting period

01 January 2023 to 31 December 2023

2 Research Programme



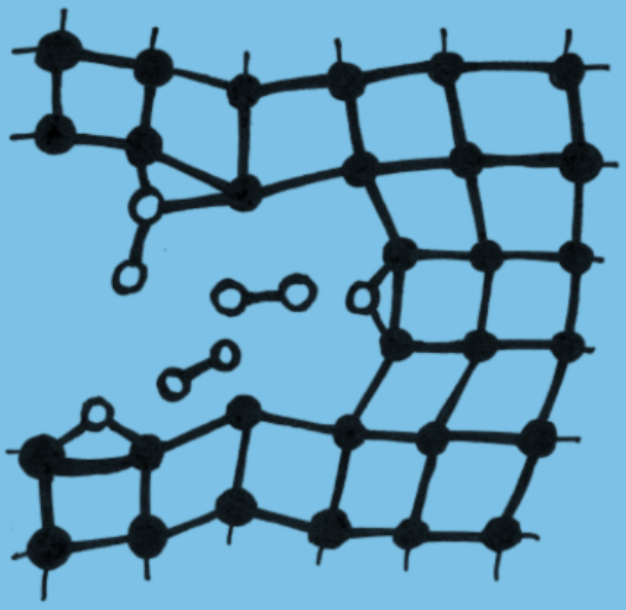
2.1 Research projects

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



P1

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 will 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, I'm improving in a first step the performance and scalability of our DFT code to speed-up the calculation of larger cutouts and extend the time scale of molecular dynamics (MD) simulations. This is done by optimizing the existing 3D Fast-Fourier Transformation (3D-FFT) routines,[1-3] which take up to 90% of the CPU time in a plane-wave DFT calculation. With larger cutouts, the problem of continuously readjusting the boundary conditions becomes less severe so that it can be done by more approximate and computationally cheaper methods.

Last year I began with the FFTX library of the Quantum Espresso software package and adapted it to the CPMD code.[3] Using a 1D+1D+1D decomposition of the 3D-FFT, I implemented several "tricks" such as the batching of multiple states and write/read-consecutive loop structures. The goal was always to build a code which runs as fast as possible on modern multicore CPUs while it is left to the user to decide the distribution of MPI tasks and OMP threads. This leads to the highest degree of flexibility on today's HPC clusters, with more and more nodes, having an increasing number of cores, and it allows to extent significantly the scalability of the 3D-FFT routines to make use of the vastly increasing compute resources.

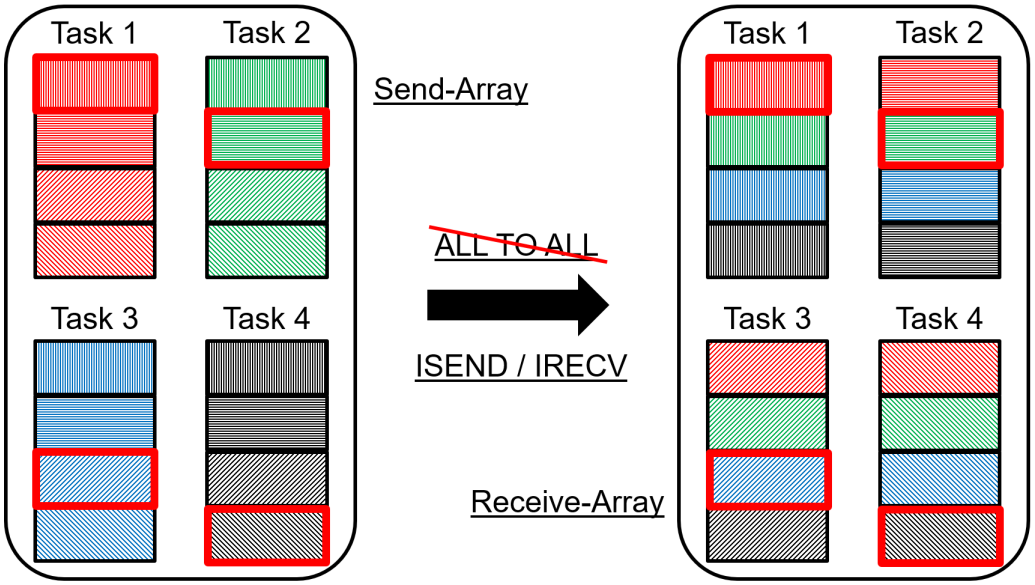


Figure 1: Illustration of the workflow of the ALL-TO-ALL MPI communication routine as well as the Point-to-Point communications ISEND and IRECV. Data in the red boxes remains on the initial MPI task.

One crucial step in this process was the change of the MPI routines for communication. Outlined in Figure 1 is the general workflow of how an ALL-TO-ALL MPI routine for transposing an array works. Each MPI task has to swap a part of the array with all other MPI tasks. This is done in such a way that the first array part of each MPI task goes to the first task, each second part goes to the second task, and so on. In doing so, the number of the task where the specific part of the array comes from represents the location where it is located afterwards. This approach is very straight forward and

therefore often used, however, its efficiency is lacking. As pointed out by the red boxes in Figure 1, certain parts of the arrays, specifically the n^{th} part of the n^{th} MPI task, are communicated needlessly since they remain on the same task at the same position in the array. As such, using an expensive MPI communication routine rather than a simple copy operation is inefficient. Therefore, in the present code I use the Point-to-Point MPI communication routines ISEND/IRECV to facilitate many direct communications between two specific tasks rather than the complex ALL-TO-ALL routine where all tasks take part. This change comes with the benefit that tasks, which finished their own communication early, can continue since they need not to wait on all communication to complete.

Even after this improvement, communication still represents a bottleneck since its speed depends entirely on the memory bus. Increasing the number of tasks does not reduce the time for communication. Thus, in a last optimisation step I increased the scalability of the routine by overlapping the communication and calculation parts. This is done by separating off one core on each node, which is then only responsible for the communication while all other cores do the calculation.

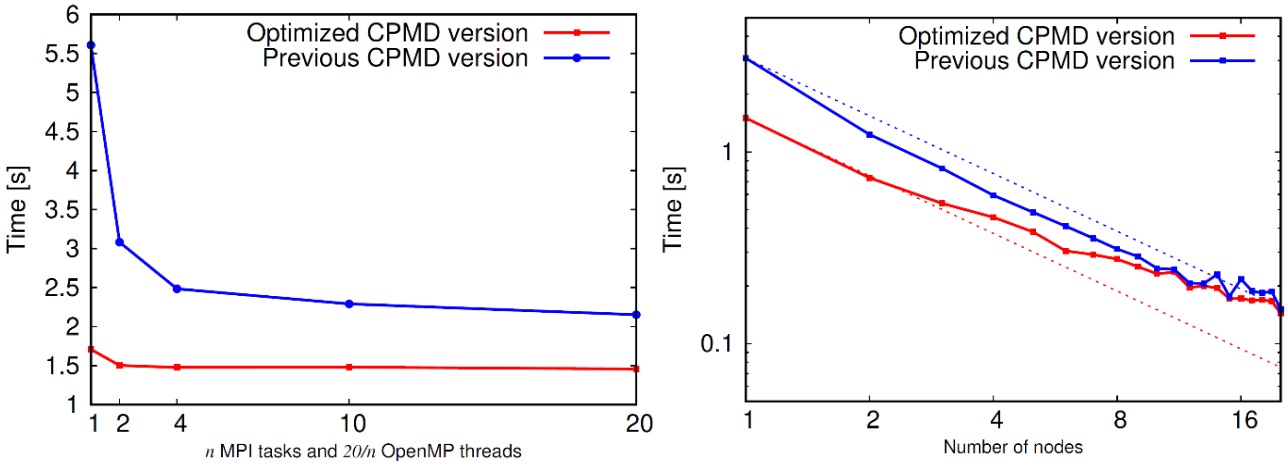


Figure 2: Performance improvements of the new optimized CPMD code shown for calculations with 256 water molecules. Left: Timings using a varying ratio of MPI tasks and OMP threads on a single node. The desired outcome is a straight line parallel to the *x*-axis. Right: Comparison of old and new code with multiple nodes using 2 MPI tasks and 10 OMP threads per node. The dotted lines represent ideal scaling.

The left graph in Figure 2 shows the improvements on the single-node level. The pure OMP implementation (only one MPI task) is now multiple times faster with the new code, and the execution time is at least reduced by 40% for any MPI task/OpenMP thread distribution. However, the multi-node scaling of the optimized new code, shown in the right graph of Figure 2, is still not as good as for the old code, even though the overall execution time is always faster due to the improvements on the single-node level. To solve this problem, I'm currently working on refactoring loop structures further in order to make better use of the OpenMP parallelisation, which seems to break down rather quickly with increasing number of nodes in the new implementation.

An additional, somewhat invisible yet enormous task was the harmonization of the code. Since a large part of the PW code was transferred to and adapted in CPMD, a program which had already its own FFT routines, many code segments became redundant. Since it is no option to leave the code as such a patchwork for the next generation of code developers, I spend significant time unifying and standardising the code. This was almost completed this year but will be continued in the first months of the next year.

In parallel to the code development, I started using the faster code for the investigation of perovskite oxides. Perovskite oxides have a cubic unit cell with ABO_3 composition and are used in a wide range of applications due to their variety of chemical, mechanical and electronic properties. Consequently, perovskite oxides are the topic of many experimental and theoretical studies. Recently, Sokolović *et al.*[4] reported results of cleavage experiments on $SrTiO_3$. Even though they are more interested in preparing ideal, clean surfaces for their surface science experiments rather than fracture mechanics, their setup presents a unique opportunity to study the process of uniaxial cleavage on the level of atomic resolution. Rather than finding perfectly cleaved surfaces, Atom Force Microscopy (AFM) imaging reveals a constant fraction of 14% of adatoms on one, and the same amount of holes on the other cleaved surface, independent of experimental conditions. However, simple charge equilibration condition implies that the surfaces should be defect-free. Atomistic simulations of the cleavage process can provide new insights, which may help to understand this unexpected fracture behavior.

To reduce the computational effort for such a study, we decided to turn to a machine-learned (ML) interatomic potential trained on DFT data instead of approaching the problem directly by DFT calculations. Specifically, we use a recently proposed new ML approach based on the atomic cluster expansion (ACE),[5] which is very promising due to its speed and accuracy. It comes along with the PACE maker tool for potential fitting and many tools for potential testing.[6] The dataset required for the ML training of the potential is generated using our improved CPMD code. Short MD runs at different temperatures are performed and snapshots are taken from the trajectories at regular intervals. They are gathered and send to the PACE maker, which uses the atomic positions, the total energies, and the atomic forces of the snapshots to learn a ready-to-use interatomic ACE potential. The ACE potentials are implemented in the LAMMPS software package so that all functionalities of LAMMPS can readily be used together with ACE.

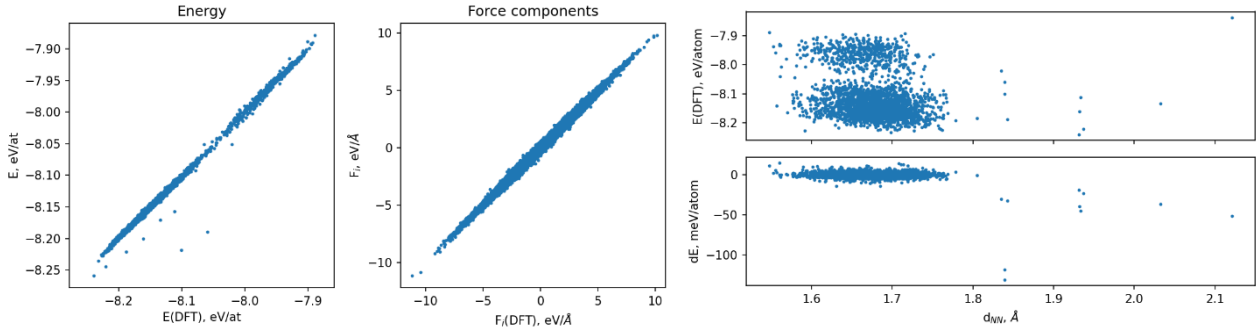


Figure 3: Results from the PACE maker fit of the interatomic ACE potential for $SrTiO_3$. Left: The energies and forces of the reference structures from the DFT calculation and the fitted ACE potential are plotted against each other. Right: The next neighbour distance of the atoms in the reference structures is plotted against their DFT energy (top) and the energy error of the ACE potential (bottom).

The result of one of the potential fitting attempts is shown in Figure 3. For a perfect ACE potential, all data points in the two graphs on the left side should lay on the diagonal. However, there are a few outliers from the ideal line. The analysis of the energy and the next neighbour distances in the training structures (graphs on the right side of Figure 3) reveals a bimodal energy distribution and outliers at large distances. This demonstrates that the training data set has "holes" and has to be extended by additional structures, which cover the underrepresented range of energies and atomic distances. The preparation of a more complete data set for the training of the potential is currently in progress. This is done by using an active learning strategy: LAMMPS provides a so-called "trust parameter" which indicates if a structure is outside the interpolation range of the training data set.

This allows us to identify problematic structures in new MD runs, which are then added to the training data set for refitting the potential.

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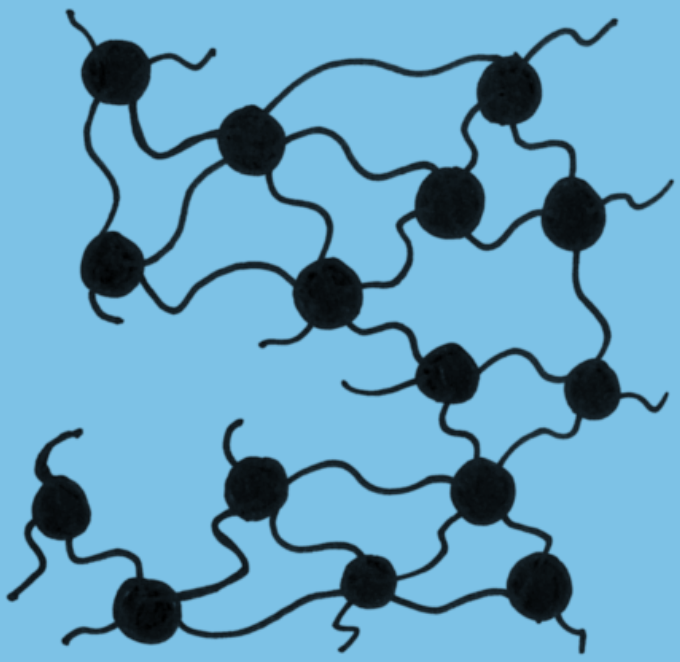

P3

FRACTURE IN POLYMER COMPOSITES: NANO TO MESO

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P3: Fracture in polymer composites: nano to meso

Pascal Frank and Dirk Zahn

Polysiloxanes are mainly known as silicones. Silicone is a term for various classes of liquids, resins and elastomers made from polymerised siloxanes. These are substances whose molecules have in common that they consist of chains of alternating silicon and oxygen atoms. This distinguishes them from conventional organic polymers such as polystyrene, whose backbone consists exclusively of carbon atoms. The absence of carbon atoms in the backbone makes polysiloxanes rather unusual inorganic polymers, even though an organic functional groups, which is usually methyl (-CH3), is attached to each silicon atom in the chain.

It is precisely this composition of inorganic main chain and organic functional groups that gives this class of materials 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. 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.

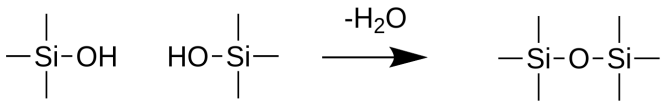

Figure 4: Example reaction for a condensation reaction. Two trimethylsilanol react to hexamethyldisilane by splitting off water.

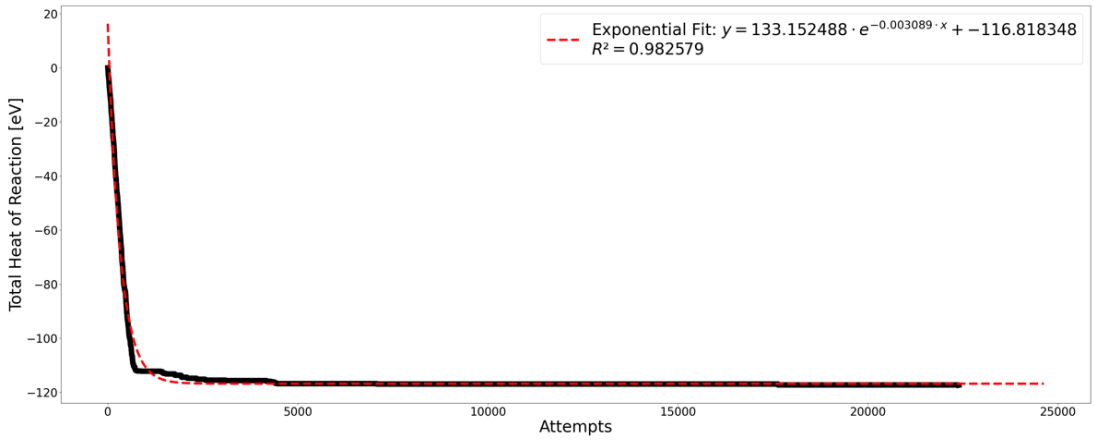

Figure 5: Sum of total energy released for each attempt. The first attempts at reactions are successful, later fewer and fewer reaction attempts are successful, which leads to less and less energy being released over time/attempts. The behaviour can be clearly described by an exponential function.

For the MD simulation of the polymerisation, a distance-angle criterion was implemented to find potential reaction partners in order 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 (Only the backbones are shown).

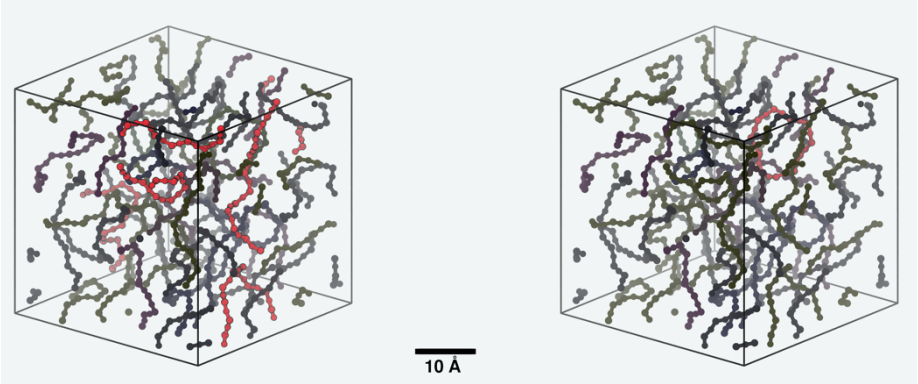

Figure 6: Final product of polymerised dimethylsilandiol monomer units. On the left a long silicone polymer chain is highlighted in red. On the right in the same box a big silicone ring is highlighted in red. (Only backbones)

This product is already an elastomer, although cross-linkers such as orthosilicic acid (Si(OH)4) are missing. Initial deformation tests show that although the linear products unthread when the box is pulled, no bond is broken. This is partly due to the lack of cross-linkers, but also to the fact that no chains have yet hooked/knotted together in this box or even formed concatenated rings (Hopf link).

In our future research, we will continue to focus on the polymerisation of more complex silicones with different weights of crosslinkers, terminators etc. in order to subsequently test the mechanical properties of the newly formed silicones.

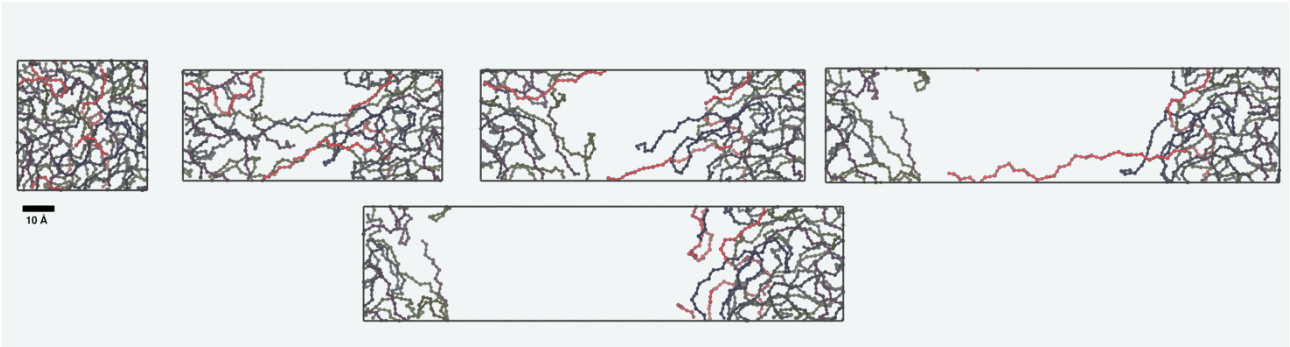

Figure 7: The deformation process of the box of polymerised products shows the unentangling of the polymer chains for the fastest pulling rate (39 m/s).

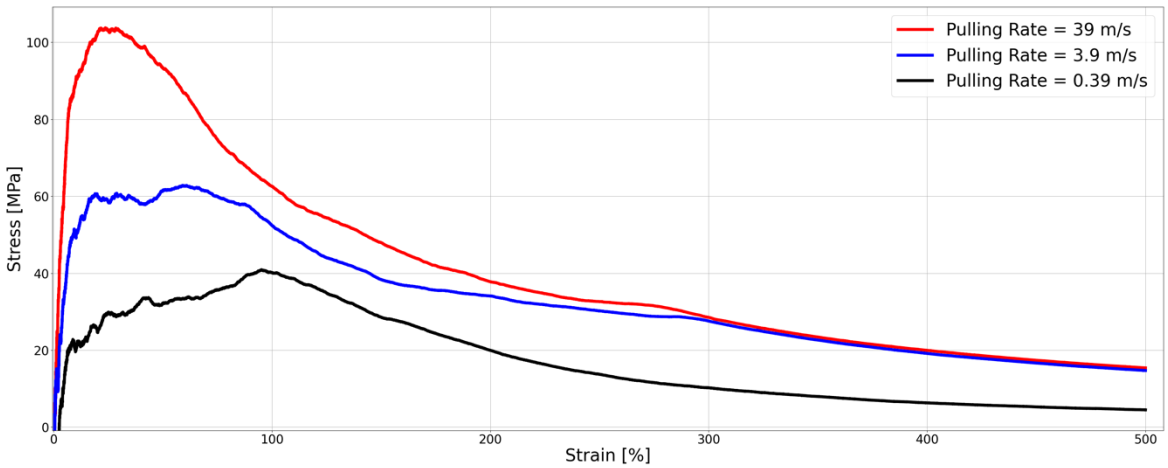

Figure 8: Stress-Strain diagram of the deformation process for different pulling rates with the maximum stresses of 104 MPa, 63 MPa and 41 MPa respectively and therefore shows well a pulling rate dependence.

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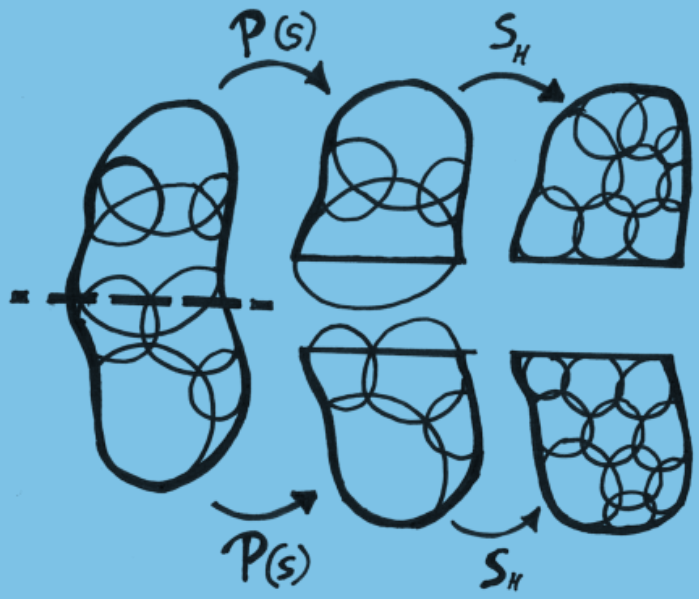

P4

FRAGMENTATION IN LARGE SCALE DEM SIMULATIONS

Utku Canbolat

Angel Santarossa

Prof. Dr. Thorsten Pöschel

Multiscale Simulation

Department Chemical and Biological Engineering

P4: Modelling Fragmentation in Large Scale DEM Simulations

Ahmet Utku Canbolat, Thorsten Pöschel and Michael Zaiser

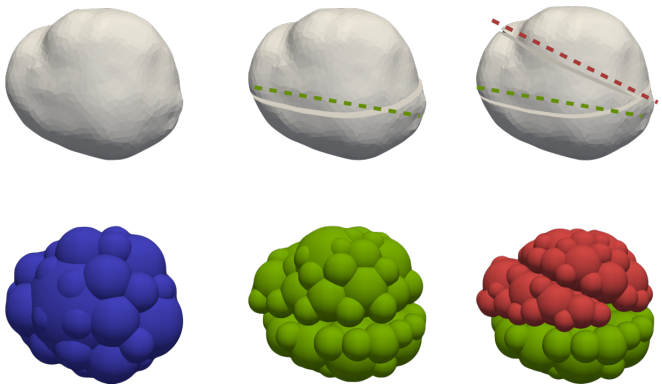

Figure 8: The upper images show the STL data, the the bottom images are their corresponding multisphere representation. The dashed lines indicate the fracture planes.

In the granular material fracture analysis, two main particle-based approaches stand out in the literature: the particle replacement method and the bond-breaking method. Each of these approaches harbors its own set of advantages and drawbacks, primarily balancing between computational cost and accuracy. Addressing these challenges, our research introduces a novel particle-breaking algorithm designed to enhance accuracy while reducing computational cost. This is achieved by concurrent consideration of multisphere representation and image data (such as STL files) of the particles throughout the simulation process (see Figure 8). Upon the occurrence of a fracture, our model splits the image data, enabling reconstruction of multispheres from the resultant fragments. This approach yields significant advantages: 1) It inherently preserves the volume and mass of the particles, 2) retains the morphological information of the particles, and 3) allows for multiple fractures of the particles without compromising on accuracy.

The primary aim of our research is the implementation of this novel model. We have designed it for scalability, making it suitable for extensive applications, such as handling over 100,000 complex-shaped particles in scientific and industrial applications, while maintaining a reasonable timeframe for processing. To achieve this, we have selected YADE, an open-source discrete element method software, as our platform of choice. Codes in YADE are written in Python, which are then seamlessly translated to C++ using the Boost library. This integration harnesses C++'s speed, ensuring that our implementation is both swift and efficient without sacrificing performance.

YADE already supports clump dynamics meaning that inertia tensor calculations and the motion integration for clumps are automatically done. However, the multisphere generation feature is not included in YADE. For this purpose, the CLUMP2 code, available for MATLAB, was used. The aim of the CLUMP codebase is to collect various multisphere creation methods into a singular package. The selection of this package was influenced by its inclusion of a robust multisphere creation method known as the Euclidean Distance Transform. This method is deemed suitable for the project on account of two specific criteria:

1) The method assures that the created multispheres remain confined within the image data, a critical factor to prevent artificial overlap of spheres after fragmentation.

2) It offers the ability to fully control the number of spheres constituting the multispheres, an aspect vital for adjusting the fidelity of multispheres to optimize simulation performance.

The initial implementation involved integrating the clump code for multisphere generation, executed externally from Python via MATLAB. However, this approach was found to be inefficient,

as each instance of multisphere generation required approximately 15 seconds, attributable to the obligatory import of unused modules with each MATLAB execution. This inefficiency necessitated the development of a native multisphere creation implementation in Python. Consequently, the CLUMP code was translated into Python. After translation, the time required to create multispheres was significantly reduced from 15 seconds to approximately 100 milliseconds. This substantial increase in speed facilitates continued advancements in the project.

The translated codebase is slated for submission to the journal SoftwareX as an update to a previously published paper. Given the considerable impact of the original publication, evidenced by 19 citations within two years, the forthcoming open-source version is anticipated to exert an even greater influence in the field. The code can be found on https://github.com/utkucanbolat/PyCLUMP.

With the implementation of multisphere generation, the generation of complex-shaped particles within a reasonable timeframe in YADE has now been enabled. The subsequent step involves synchronizing the image data with the clumps in YADE. To accomplish this, the initial orientation and position of the image data are kept in the memory. Then the current orientation and positions of the clumps, as derived from YADE, are obtained to update their corresponding STLs (image data). This process is essential to ensure that the multispheres are generated in the correct position and orientation after fragmentation, thereby accurately replacing the parent clump.

For the purpose of simulating fracture, the combined Mohr-Coulomb-Weibull criterion has been employed. This criterion was selected due to its computational efficiency and reasonable accuracy. The calculation of the fracture probability involves iterating through all the clumps in the system to find the forces acting upon them. Subsequently, the average stress tensor for each clump is calculated. If the stress exceeds the Mohr-Coulomb curve threshold, the decision to split the clump is made. The fracture plane is presumed to pass through the centroid of the clump, with its orientation determined by the maximum shear stress present in the clumps.

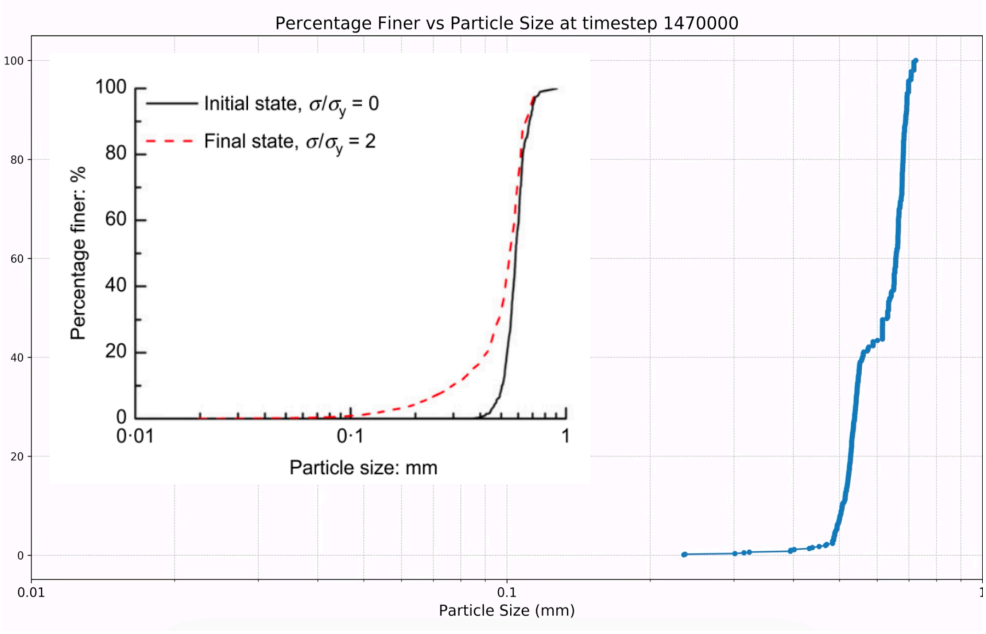

Figure 9: The inner and outer images are from the experiment and simulation results, respectively. The discrepancy in the particle size distribution can be seen in the middle of the curve.

In order to ascertain the functionality of the model and code, tests were conducted on both single and multi-particle systems. In the case of single particle systems, the code executed flawlessly. For

multi-particle systems, an experiment3 from existing literature was replicated. An identical system to that of the experiment was prepared, mirroring material properties, particle count, and packing density. Although the Particle Size Distribution (PSD) trend was consistent, a discrepancy was observed (see Figure 9), attributed to the employed splitting method. The method, which solely traverses through the centroid, fails to capture the chipping mechanism of fragmentation - a process where small fragments split from the material. To address this, the fracture plane was adjusted based on the weighted average of the forces acting on the clump. Tests for this modified approach are currently ongoing. In the near future, enhancements including a refined mesh splitter, which will also process the image data of the fractured plane using spherical harmonics, are planned to be added. Furthermore, the inclusion of dynamical fracture feature will enable the application of the code to dynamic fracture scenarios such as ball-milling processes, in addition to static or quasi-static applications.

This year, the integration of wear effects into the model is projected for completion. Subsequently, in the following year, the addition of heat transfer mechanisms, encompassing conduction and radiation, is planned. These incorporations are expected to conclude the second funding period, thereby achieving a comprehensive model encompassing all pertinent multiphysical correlations.

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

Angel Santarossa and Thorsten Pöschel

Leopoldo R. Gómez, Achim Sack, Laureano Ortellado, Anabella Abate

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 that are inclined respective to the mother planar crack [2]. Unfortunately, the underlying physical mechanisms responsible for this phenomenon remain 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 in fluid-driven fractures under mixed loading. In particular, we aim to study with a combination of experiments, X-ray imaging, and FEM simulations mix-mode I+III fractures in hydro-gels in 3D. To that aim, this project is divided into three stages. Parts one and two are developed and implemented by the Frascal team in collaboration with researchers of Universidad Nacional del Sur, Argentina, while the collaborators perform the numerical simulations.

The initial goal was to design and develop a novel experimental setup to produce such mix-mode I+III fractures when fluid is injected into a gel at a predefined fluid rate. Part one was successfully achieved. We designed, developed, and built a novel experimental setup for investigating fluid-induced fractures under a combination of uniaxial tension and shear stress (as illustrated in Fig. 10). The apparatus is specially designed to be used in X-ray scanners, allowing the non-invasive reconstruction of complex fracture morphologies in 3D, which are often challenging to observe and analyze using traditional methods. The device includes sensors for measuring tension, torque, and fluid pressure. Furthermore, the apparatus is made of 3D-printed components, making it affordable and adaptable. A detailed description of its parts, functioning, and examples demonstrating its capabilities are published in an open-access research article [5].

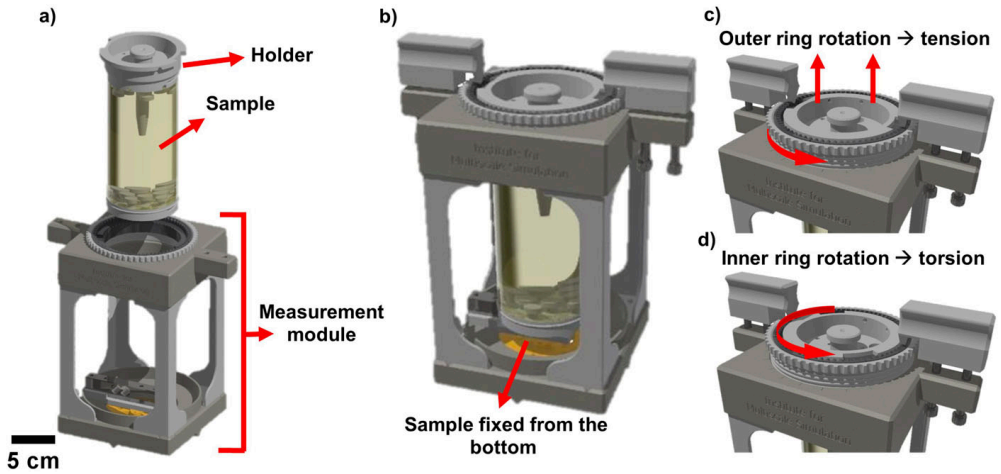

Figure 10: Experimental setup. The sample is mounted to the measurement module (a) and is fixed at the base (b). Two modes of loading can be applied: tension (c), by elongating the sample through the rotation of an outer ring, and shear stress (d), by rotating an inner ring that induces torsion. From: Rev. Sci. Instrum.. 2023;94(7). doi:10.1063/5.0145709.

In the second stage, the developed setup is used to analyze the geometry of mixed-mode I+III fluid-driven fractures for different tensile and shear stress values. Examples of different crack geometries obtained for different combinations of tension and shear stress are shown in Fig. 11. In addition to reconstructing a 3D image when the crack arrests, the device can also be utilized for in situ measurements. In this approach, the sample is scanned sequentially after injecting small amounts of fluid, 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. 12.

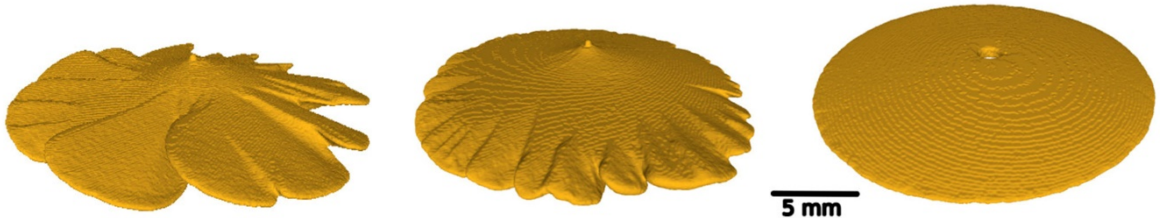

Figure 11: Visualization of crack geometries in mixed modes I+III fractures using air and an 8 mm elongation of the gel. Cracks were obtained for different values of the torsion angle: 50°(left), 30° (middle), a zero torsion (a mode I driven fracture) (right). From: Rev. Sci. Instrum.. 2023;94(7). doi:10.1063/5.0145709.

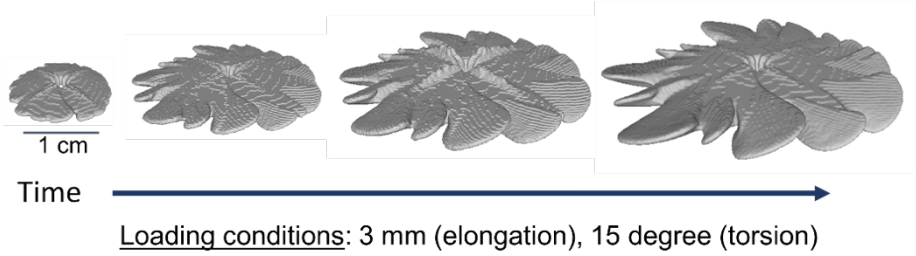

Figure 12: Reconstructions of a crack geometries under mixed mode I+III loading and using air as fracturing fluid in different steps of the crack propagation. Loading conditions are described in the image.

In the third step, the obtained reconstructed geometry of the cracks in combination with the experimental conditions (angle of torsion, gel's elongation) are used to develop FEM simulations and to infer fracture mechanics parameters that otherwise will be inaccessible by experimental methods (such as stress intensity factors at the crack tip, as shown in Fig. 13). Preliminary results show that in a mixed mode I-III fracture, the stress intensity factors corresponding to shear modes (KII and KIII) vanish at the crack tip, suggesting that facets grow in the direction of pure tension mode (mode I), as predicted by the principle of local symmetry.

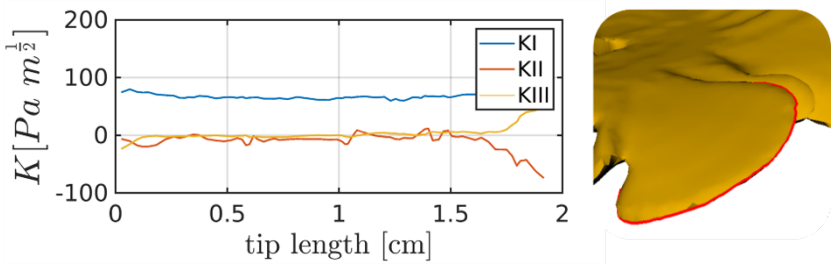

Figure 13: Stress intensity factors (KI, KII, and KIII) as a function of the tip length (left), calculated at the crack tip of a facet of a mixed-mode I+III fractured, obtained under the conditions described in Fig.3. Illustration of a segmented crack tip on a facet. The distributions of stresses were obtained by finite element analysis and the stress intensity factors through stress matching.

By combining the experimental data with numerical simulations, we aim to shed light on the complex behavior exhibited by mixed-mode I+III cracks front in brittle materials.

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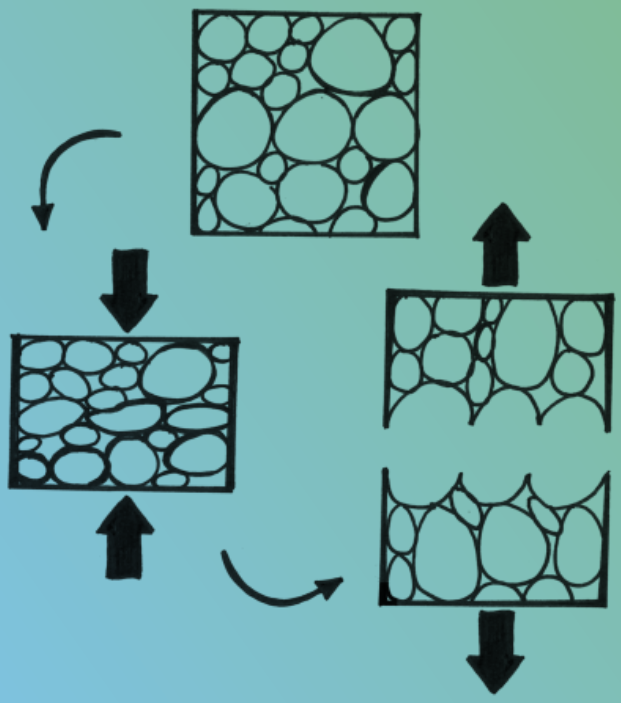

P5

COMPRESSIVE FAILURE IN POROUS MATERIAL

Shucheta Shegufta

Prof. Dr. Michael Zaiser

Materials Simulations

Department Material Science and Engineering

P5: Deformation and Failure of Disordered Porous Material

Shucheta Shegufta and Michael Zaiser

Microstructure geometry plays a crucial role in determining the mechanical behaviour of porous materials. In addition to porosity, the distribution of pores is also a significant factor for these materials. We use artificially generated two dimensional porous microstructure to study the combined effect of porosity and disorder on the elastic and failure properties of the material [1]. Both quasi-static and dynamic loading conditions have been considered, as well as brittle and quasi-brittle damage properties.

The 2D geometries are generated using a Voronoi tessellation like algorithm where the circular pores are arranged with various degrees of randomness for a prescribed porosity and a fixed number of pores. Width of pores size distribution increases with increasing porosity and disorder.

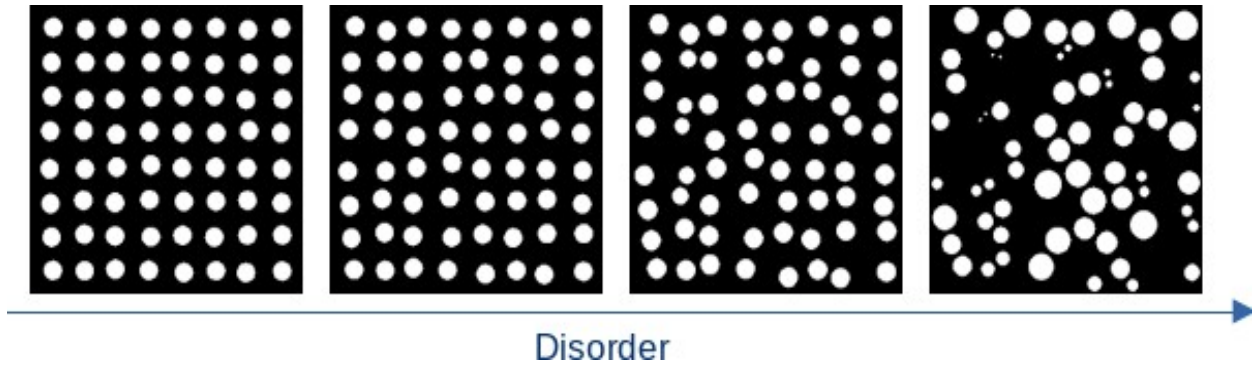

Figure 14: Microstructures with same porosity and number of pores with increasing disorder.

Three different structure sizes, 50mm X 50mm, 100mm X 100mm and 200mm x 200mm, with five different porosities ranging from 5% to 45% and four disorder values are chosen for this study. Bond-based peridynamics model is used for the simulations. We first focus on an elastic-brittle material behaviour. We can compare the elastic stiffness of the structures with the Hashin-Shrikman limit, and notice that for higher porosities, elastic modulus of the disordered systems fall significantly below the lower bound. Similarly, peak stress and work of failure obtained from the simulations can be compared with finding's by Kirsch [3], and considering multiple voids as

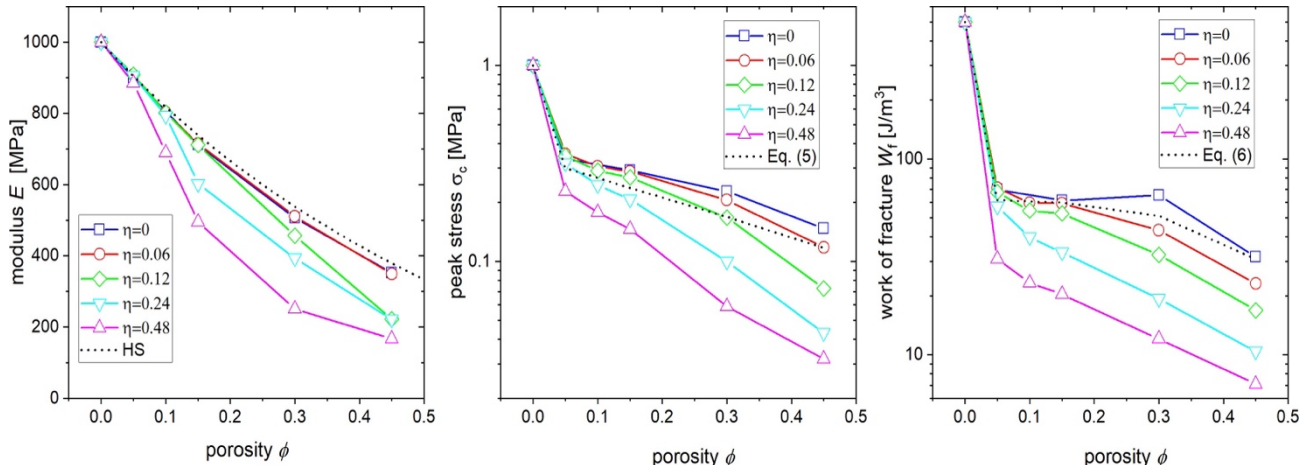

Figure 15: Effect of disorder and porosity on mechanical properties for quasi-static tension simulations.

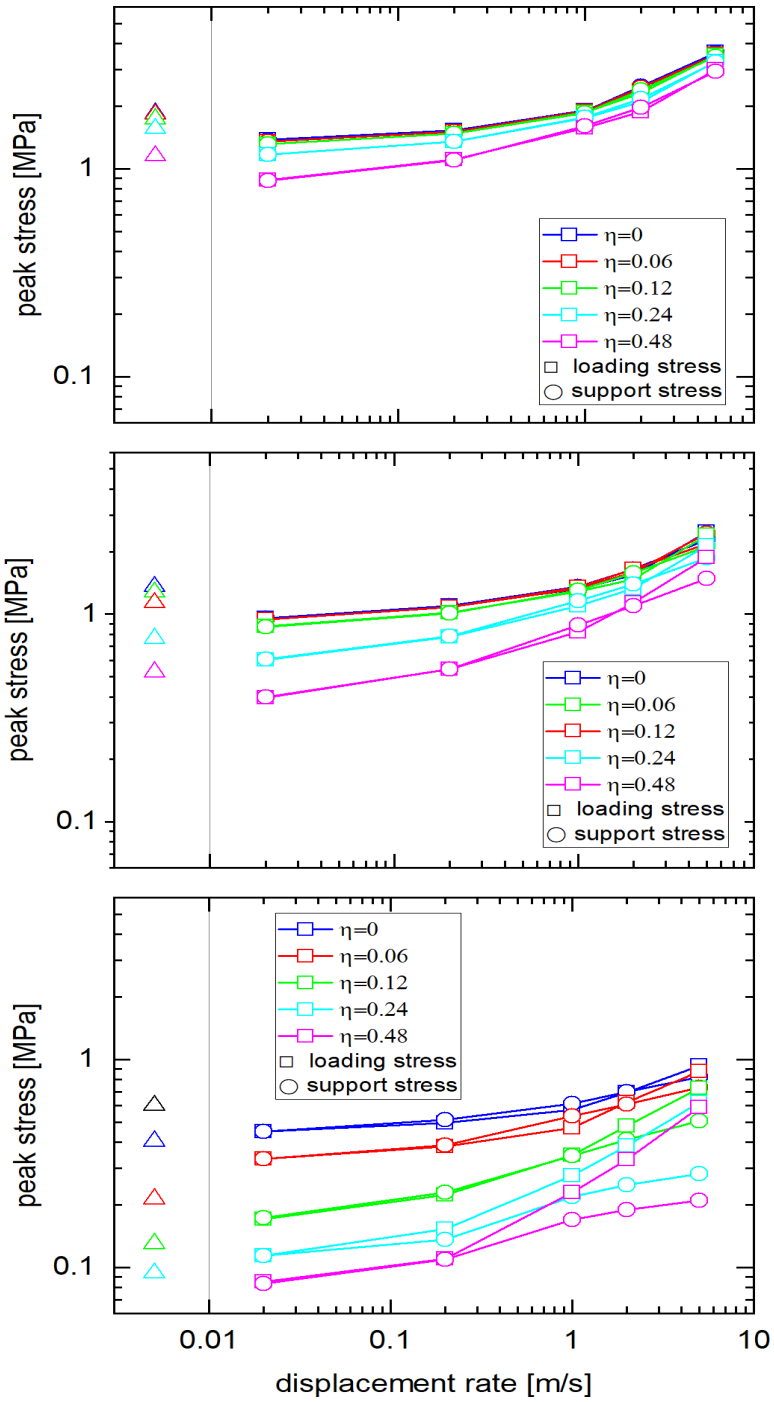

Figure 16: Results of dynamic simulation for different displacement rates.

equivalent to a single void. It is observed that for peak stress and work of failure, effect of disorder is even more pronounced than elastic modulus and for high disorder these values are much lower than as predicted by the mean field approach. At higher disorder and porosity, probability of existence of weak spots with high stress concentration increases, which causes a knock-down effect. Similar trends can be observed in dynamic compression simulations, however, as displacement rate increases, effect of disorder tends to diminish. We make two interesting observations from the dynamic simulations. First one is that for high porosity and high disorder, peak stress at the support layer is significantly lower than he displaced layer, because the weak spots near the displaced layer fractures and hinders the transmission of stress waves to other part of the structure, thereby working as a shock absorber. The second observation is that even with very low displacement rate, the peak stress for quasi-static simulation are higher than dynamic simulations, indicating that quasi-static is not the limit case of dynamic simulations.

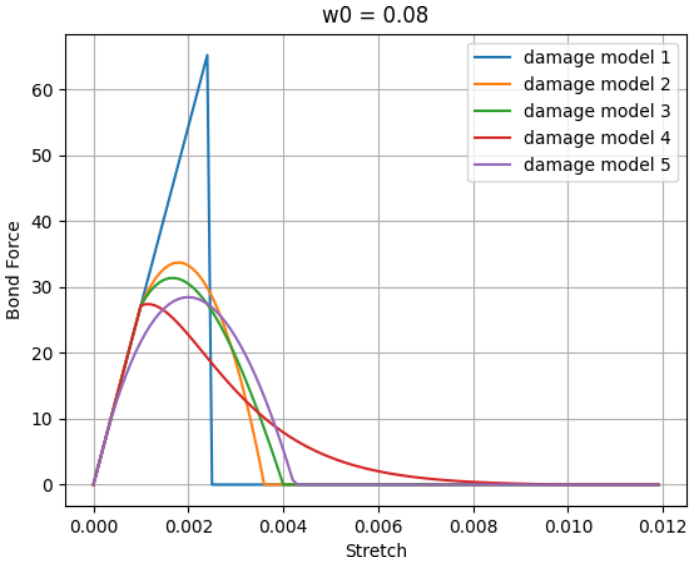

Figure 17: Different damage models with work of failure.

Next, we focus on the effect of different damage models on failure behaviour of porous microstructures by expanding the damage model to include a softening branch, which should give us a quasi-brittle type failure in global sense. We consider five damage models that have the same work of fracture but different softening behaviours. We conduct both quasi-static tension and dynamic tension tests as before. For quasi-static simulations, the failure behaviour is dominated by peak bond force, but for dynamic simulations, minimal effect of the different softening models is

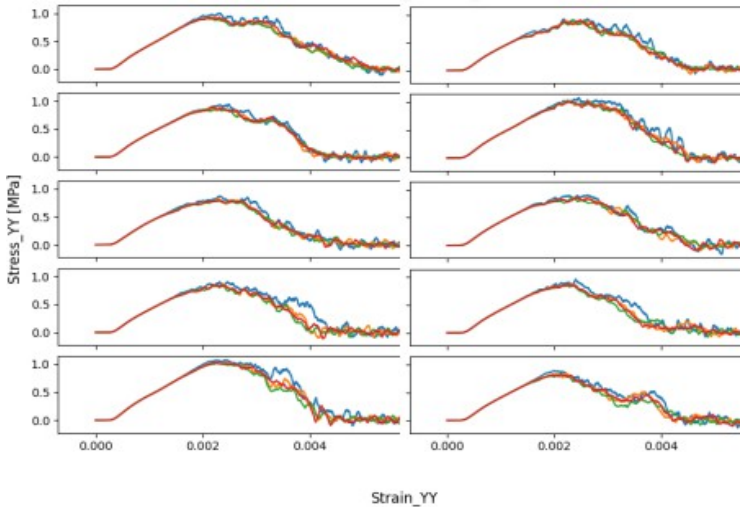

Figure 18: Results of dynamic compression on different microstructures with same porosity and disorder.

noticed for different porosity and disorder.

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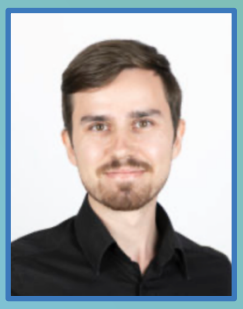
P6

FRACTURE IN THERMOPLASTICS: DISCRETE-TO-CONTINUUM

Felix Weber

Lukas Laubert

Wuyang Zhao



Maximilian Ries

PD Dr.-Ing. habil. Sebastian Pfaller

Applied Mechanics

Department of Mechanical Engineering

P6.2: Single and Multi-Scale Fracture Simulations of Glassy Materials

Felix Weber and Sebastian Pfaller

Studying Failure of Polymer Nanocomposites with a Generic MD Model

Their great versatility makes polymer nanocomposites (PNCs) an important class of engineering materials. To gain detailed insights into the nanoscale mechanisms underlying their macroscopic mechanical properties, molecular dynamics (MD) simulations have become a valuable tool to complement experimental studies. In [1], we modify the analytical potential functions of an efficient bead-spring model representing a generic polymer nanocomposite [2] to allow for breakage of covalent bonds. We then perform uniaxial tensile simulations of double-notched samples, see Figure 19. Here, we replace the classical periodic boundary conditions with nonperiodic ones on the precracked surfaces and apply Dirichlet boundary conditions in the x direction to regions of width L_d (plane strain condition in the z direction).

Validation of the model against experimental trends in stiffness, strength and toughness measurements is performed in two stages: First, we investigate the effects of specimen size, pre-crack geometry, strain rate, temperature, and degree of polymerization for the pure polymer. In a further step, we analyze the influence of filler size and filler content on the behavior of the PNCs. With this study, we show that when developing new materials or optimizing established ones, it is possible to use a simple MD setup to gain initial valuable insights into the effects of key parameters, which can then be extended by increasing the complexity of both the material description and the boundary conditions.

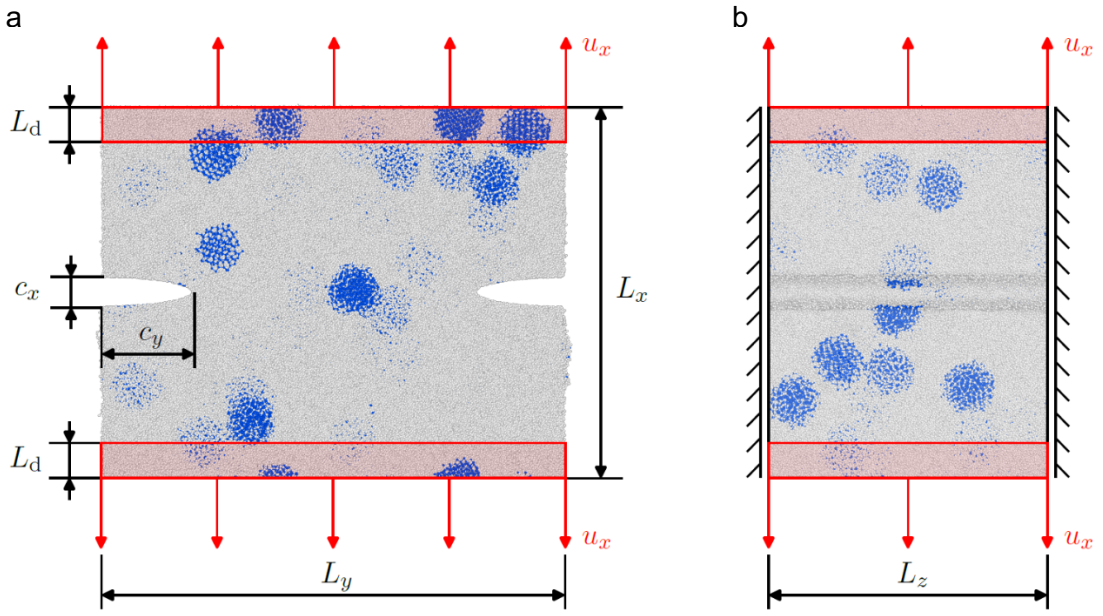


Figure 19: Setup of the double-notched samples of polymer nanocomposites subjected to uniaxial tension: Exemplary specimen in a) x-y-plane and b) x-z-plane [1].

FE-MD Fracture Simulations of Silica Glass using the Capriccio Method

Recently, together with Dr. Maxime Vassaux (Institut de Physique de Rennes, Université de Rennes, CNRS), first multi-scale fracture simulations of SiO_2 glass were performed using the Capriccio method [3], a concurrent approach coupling molecular dynamics (MD) with the finite element (FE) method based on the concept of anchor points. Already in these first tests, where we used an atomistic MD model of SiO_2 [4] and subjected the linear-elastic FE domain to Dirichlet or Neumann boundary conditions (see Figure 20), we obtained virial stresses within the MD region as well as

reaction stresses at the Dirichlet boundary of the FE domain that quantitatively match experimental findings. In the coming months, we plan to perform simulations comparable to established, standardized tests (e.g. from ASTM standards) to evaluate fracture mechanical parameters such as crack opening displacement, J-integral or energy release rate and compare them with experimental data. Important issues to be addressed are: i) the investigation of the influence of the boundary conditions, the FE-MD coupling and the sample size (especially in the direction of crack propagation), ii) the calculation of stresses in the fractured MD region, iii) the treatment of long-range electrostatic interactions, especially at the free surface of the MD domain in the coupling region, and iv) the evaluation of dipole moments possibly introduced by the system setup. For these purposes, our previous studies on the FE-MD coupling by means of the Capriccio method for amorphous thermoplastics with respect to the treatment of surface effects [5] and the FE-MD equilibration [6] provide an important basis. To investigate the influence of different factors, we currently use an FE-MD setup that couples a particle system to a continuum in only one direction (quasi-1D configuration).

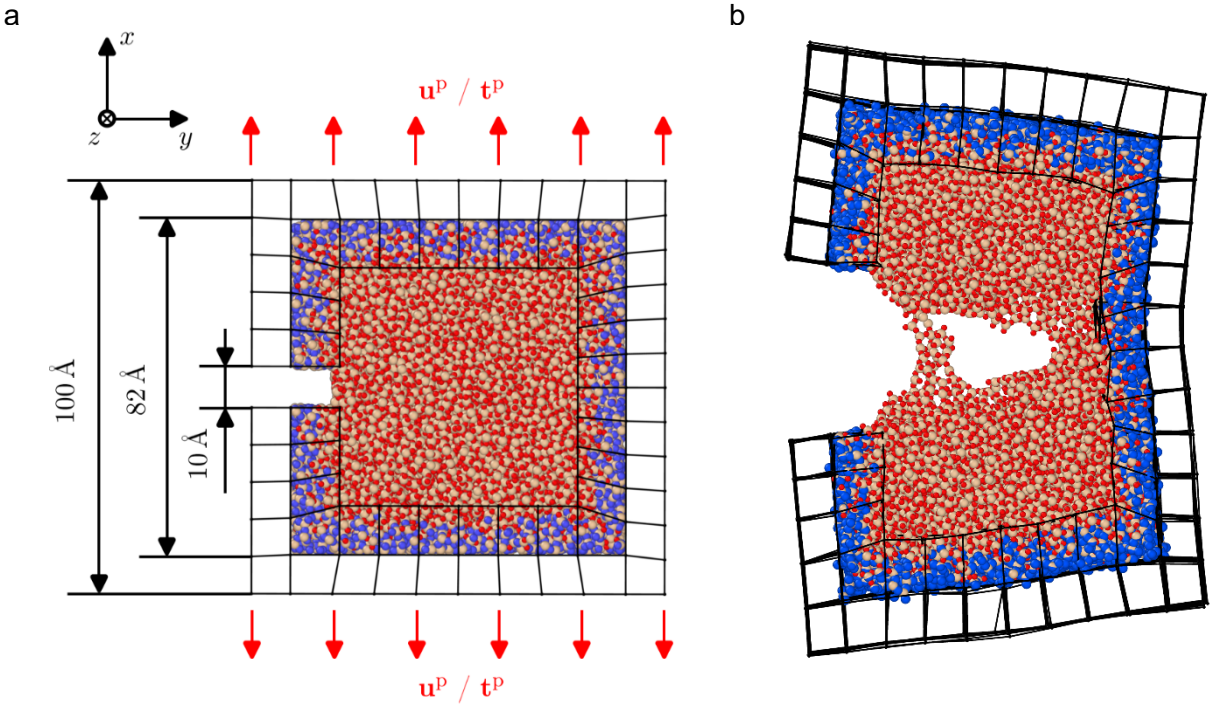


Figure 20: Setup of the FE-MD simulations: a) Exemplary atomistic molecular dynamics system of silica glass containing 35 000 atoms and approximately 8 000 anchor points subjected to Dirichlet boundary conditions (prescribed displacement $\mathbf{u}^\mathrm{p}$) or Neumann boundary conditions (prescribed surface traction $\mathbf{t}^\mathrm{p}$) by means of the finite element method and b) crack opening under Neumann boundary conditions.

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P6: Characterization and modeling of polymer nanocomposites across the scales

Maximilian Ries

Polymers represent a highly versatile material class and can be further enhanced to meet the requirements of highly demanding applications by adding filler particles. Particularly with nano-sized fillers, remarkable improvements in polymer nanocomposites' (PNCs') mechanical performance could be achieved experimentally. The outstanding mechanical properties of PNCs are mainly attributed to the matrix-filler interphase, which has a major impact, especially for nano-sized fillers. Therefore, a detailed understanding of the interphase and its impact on the overall behavior is necessary to exploit the full potential of PNCs.

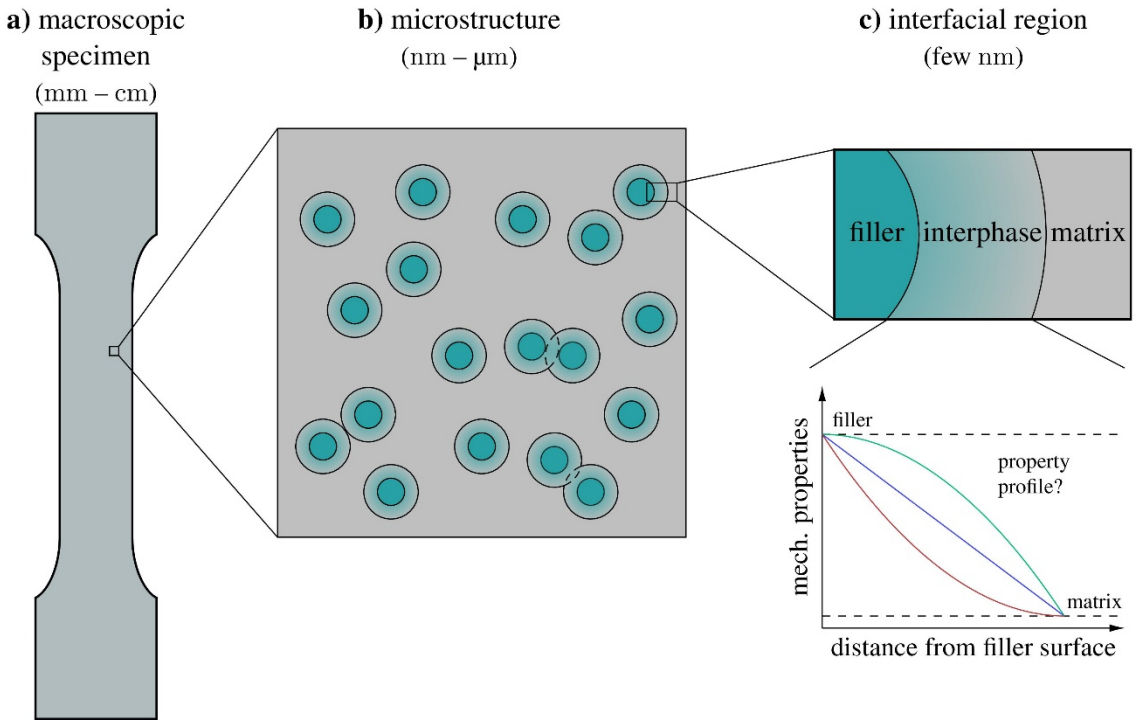

Figure 21: Multiscale setup of polymer nanocomposites: **a)** macroscopic specimen with dimensions of nm to cm, **b)** representative microstructure with filler, matrix, and interphase, and **c)** unknown property profiles in the filler-matrix-interphase spanning only a few nanometers; from [1].

For this purpose, precise numerical models are required, to complement the challenging experimental investigation at the nano-scale. Particle-based methods such as molecular dynamics (MD) provide a detailed resolution of the microstructure, but are too expensive to solve problems at the engineering scale. To this end, computationally more efficient continuum approaches like the finite element (FE) method are commonly employed. However, these methods require accurate constitutive laws that capture the impact of the interphase and are usually not available.

To this end, the present work introduces a methodology to derive continuum mechanical models for PNCs based on molecular dynamics and thus combines the advantages of particle-based and continuum approaches.

Although we use nano-silica-reinforced polystyrene as an example for our investigations, the methods can be easily transferred to other material pairings. First, we present a strategy to characterize the mechanical behavior of neat polymer and filler based on MD simulations. These

insights enable us to subsequently calibrate appropriate continuum mechanical constitutive laws for the viscoplastic polymer and the anisotropic, elastic filler.

Since the interphase cannot be investigated separately, we consider polystyrene-silica samples with two nanofillers at different filler distances. In order to realize comparable simulation setups, we employ an MD-FE coupling method to perform uniaxial tension simulations. The resulting overall force response and interparticle strain facilitate the identification of the inelastic property profiles within the interphase. This continuum mechanical interphase model reproduces the characteristic size effect of PNCs. Furthermore, the obtained constitutive descriptions for matrix, filler, and interphase form the prerequisite for analyzing representative volume elements (RVEs). Using these RVEs, we evaluate the influence of filler content and distribution on the nanocomposite's overall stiffness.

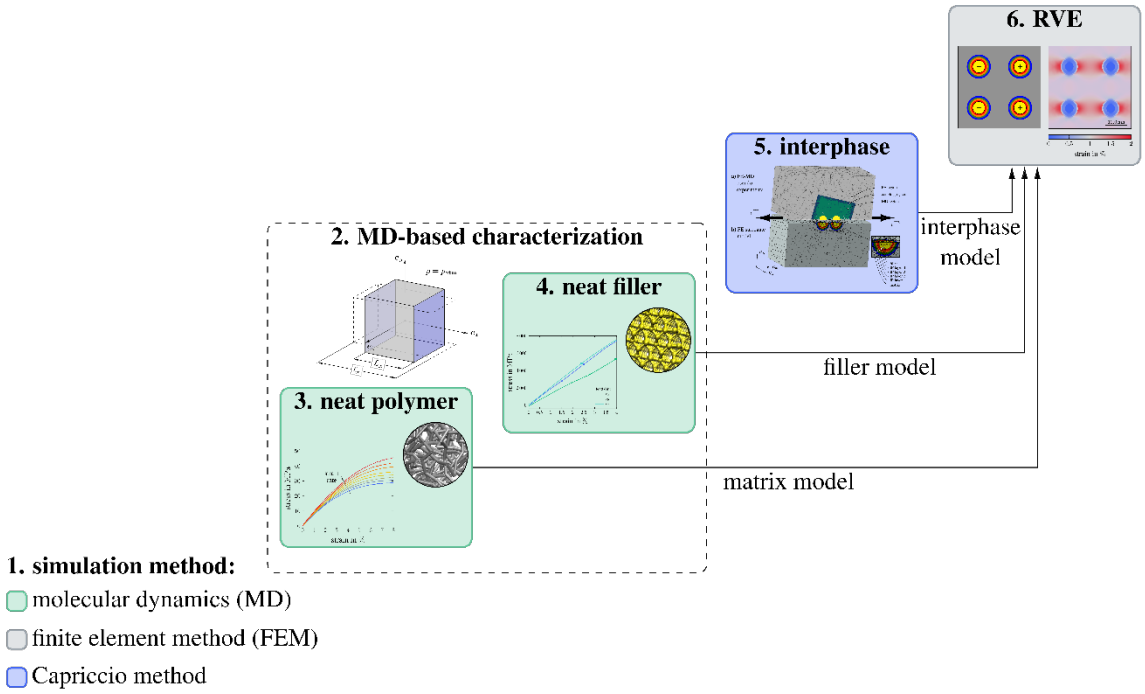

Figure 22: Graphical abstract: molecular dynamics (MD)-based characterization of the mechanical behavior of neat polymer, and neat filler together with the inverse parameter identification for the filler-matrix interphase provide the constitutive models required for the analysis of representative volume elements (RVEs); from [1].

Consequently, this interdisciplinary work contributes significantly to understanding polymer nanocomposites, especially the crucial matrix-filler interphase, and thus complements experimental insights. Moreover, the transfer of molecular-scale insights into continuum mechanical models forms an essential link between the chemistry and engineering communities for the numerical modeling of polymer nanocomposites [1].

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aPH: A visco-hyperelastic-viscoplastic constitutive model for rate- and temperature-dependent strain hardening behavior of glassy polymers

Wuyang Zhao, Paul Steinmann and Sebastian Pfaller

Glassy polymers typically exhibit elastic, intrinsic strain softening, and intrinsic strain hardening behavior with increasing uniaxial deformation. While softening could cause strain localization that is related to brittle fracture, the strain hardening behavior plays an important role in increasing the toughness of glassy polymers by inhibiting this localized failure. It is widely accepted that strain hardening originates from chain orientation accompanied by chain sliding, which is associated with dissipative behavior [1]. Therefore, strain hardening exhibits rate- and temperature-dependent behavior. Various constitutive models have been developed to account for this behavior, e.g. by incorporating a deformation-dependent viscosity [2], considering dissipative orientation-induced back stress [1], or assuming a rate-dependent effective shear modulus [3], etc. In contrast to these models, which represent the strain hardening using internal variables, we use the rate of the total strain to account for its rate-dependence. Using the viscous potential $\Psi^{\mathrm{v}} = \Psi^{\mathrm{v}}(\boldsymbol{C}, \dot{\boldsymbol{C}})$ with the right Cauchy Green tensor $\boldsymbol{C}$ and its rate $\dot{\boldsymbol{C}}$ proposed in [4], and adding it to an elasto-viscoplastic (EVP) model, we propose a thermo-dynamically consistent visco-hyperelastic-viscoplastic (V-EVP) model [5] as schematically illustrated in Figure 1. In conventional EVP models, the second Piola-Kirchhoff stress tensor $\boldsymbol{S}$ is defined by assuming

$$\left[\boldsymbol{S} - 2\frac{\partial \Psi}{\partial \boldsymbol{C}}\right] : \dot{\boldsymbol{C}} = 0$$

with Ψ being Helmholtz free energy density. $\boldsymbol{S}$ usually contains an equilibrium part $\boldsymbol{S}^{\mathrm{e}}$ representing the elastic response and a non-equilibrium part $\boldsymbol{S}^{\mathrm{vp}}$ for the viscoplastic flow. In contrast, the approach developed in [4] introduces a viscous stress term $\boldsymbol{S}^{\mathrm{v}}$ by assuming the existence of the viscous potential Ψ^{v}, s.t.

$$\left[\boldsymbol{S} - 2\frac{\partial \Psi}{\partial \boldsymbol{C}}\right] : \dot{\boldsymbol{C}} = \frac{\partial \Psi^{\mathrm{v}}}{\partial \dot{\boldsymbol{C}}} : \dot{\boldsymbol{C}} \geq 0,$$

where the viscous stress tensor is defined as $\boldsymbol{S}^{\mathrm{v}} = \frac{\partial \Psi^{\mathrm{v}}}{\partial \dot{\boldsymbol{C}}}$. Combining the viscous term and the conventional EVP model, the total stress tensor of the V-EVP model is given by

$$\boldsymbol{S} = \boldsymbol{S}^{\mathrm{v}} + \boldsymbol{S}^{\mathrm{e}} + \boldsymbol{S}^{\mathrm{vp}}.$$

The second Piole-Kirchhoff stress can be pushed forward to the deformed configuration as $\boldsymbol{\sigma} = \frac{1}{J}\boldsymbol{F}\boldsymbol{S}\boldsymbol{F}^{\mathrm{T}} = \boldsymbol{\sigma}^{\mathrm{v}} + \boldsymbol{\sigma}^{\mathrm{e}} + \boldsymbol{\sigma}^{\mathrm{vp}}$, where $\boldsymbol{F}$ denotes the deformation gradient and $J = \det \boldsymbol{F}$ is the Jacobian determinant. The individual terms $\boldsymbol{\sigma}^{\mathrm{v}}$, $\boldsymbol{\sigma}^{\mathrm{e}}$, and $\boldsymbol{\sigma}^{\mathrm{vp}}$ are schematically represented by different branches in Figure 23.

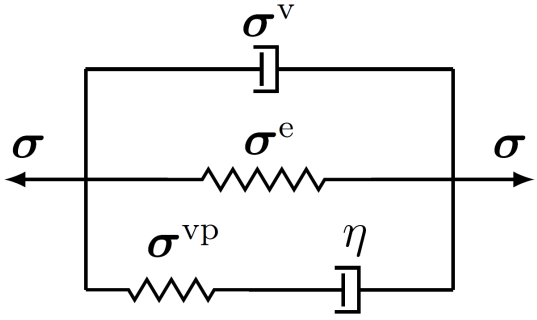

Figure 23: Rheological representation of the constitutive model.

With appropriate definition of the viscous potential Ψ^{v} and after calibration of the parameters, the V-EVP model can well reproduce the rate- and temperature- dependent hardening behavior in molecular dynamics (MD) simulations of coarse-grained polystyrene in uniaxial tension simulations as shown in Figure 24, where strain rates of $\dot{\varepsilon} = 1\%/\mathrm{ns}$ and $\dot{\varepsilon} = 100\%/\mathrm{ns}$ at temperatures across a wide range of $T = 10\mathrm{K} - 170\mathrm{K}$ below the glass transition temperature $T_g = 171.5\mathrm{K}$ have been considered. As this work currently focuses on modeling the hardening behavior, the strain softening is not yet considered.

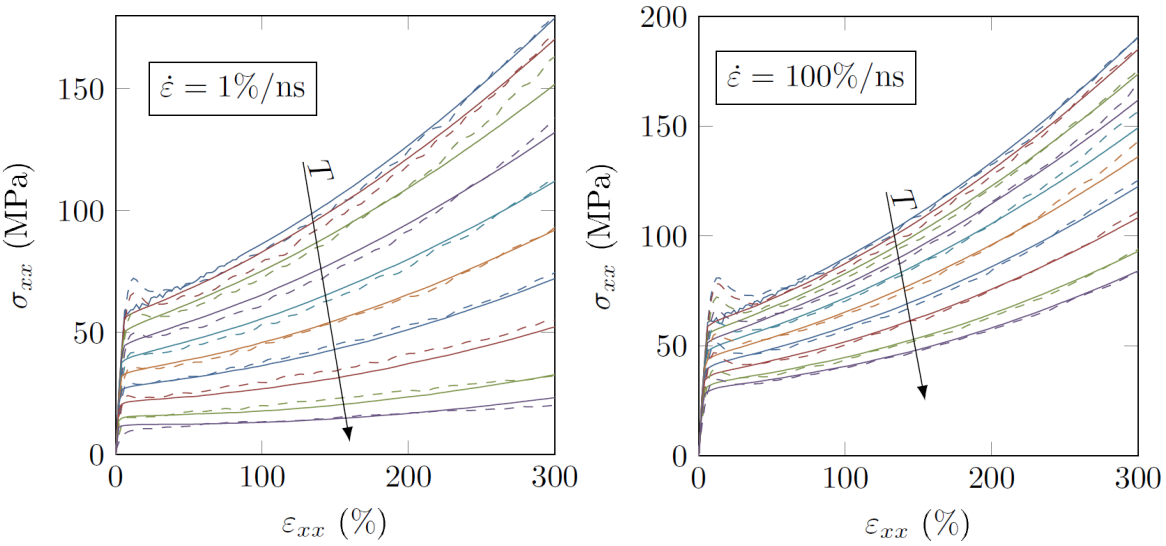

Figure 24: Comparison between the constitutive model and the MD simulations in uniaxial tension at the temperatures of $T = 10K - 170K$ with different strain rates.

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Franco-German Research Project BIO ART

Lukas Laubert, Sebastian Pfaller

BIO ART (Optimization of the mechanical properties of BIO-sourced epoxy resins through ARTificial intelligence) is a DFG and ANR funded joint research project of four institutes, namely the Institut de Chimie et des Matériaux Paris-Est (ICMPE) at the Université Paris-Est Créteil Val de Marne (UPEC), the Laboratoire Modélisation et Simulation Multi-Échelle (MSME) at the Université Gustave Eiffel (UGE), the Department of Polymer Engineering (PE) at the University of Bayreuth (UBT), and the Capriccio group at the Institute of Applied Mechanics (LTM), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU).

BIO ART's main goal is to develop a fully bio-based epoxy-fibre composite at a competitive price with thermal and mechanical properties comparable or even superior to classical petro-sourced epoxy composites. The work package designated to the LTM is mainly concerned with multiscale modeling of the epoxies and related composites developed by the ICMPE and PE. This task covers two domains, namely the "rheological properties of the continuum", which develops and calibrates a continuum mechanical constitutive law that establishes a link between the network structure of the epoxy formulations and their mechanical properties at larger scales as well as "Multiscale simulations of fracture", which develops a multiscale simulation tool that couples a fine-scale network model capable of polymer fracture at the network level with the coarse-scale continuum model providing realistic boundary conditions.

In order to enable the MSME to train an epoxy network model based on the mechanical properties of biobased epoxy synthesized by the ICMPE in a next step, a continuum mechanical model has been selected and calibrated during Lukas Laubert's master thesis, where the mechanical properties of the bio-sourced epoxy ER/A-LIM, synthesized from the resin epoxidized resorcinal (ER) and the hardener diaminelimonene (A-LIM), is analyzed with respect to its elastic, viscous, and plastic characteristics. Subsequently, the material's creep response under external loading at 23 °C as well as its recovery behavior is modeled via a finite element (FE) simulation. To this end, an elaborate viscoelastic-viscoplastic (VEVP) phenomenological material model is deployed, whose parameters are determined following two

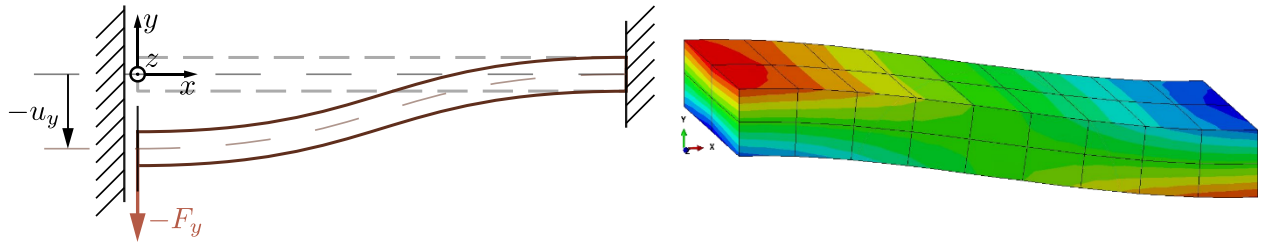

Figure 25: Schematical setup representation and deformed FE visualization.

consecutive steps: First, master curves are fit to available data from dynamic mechanical thermal analysis (DMTA) and time-temperature superposition (TTS) in a specified frequency range in order to determine the elastoviscoelastic parameter values. Next, parameter optimization is performed to inversely identify a set of remaining viscoplastic parameter values able to approximate the material behavior in the creep recovery experiments reasonably well across various load levels.

Analysis of the available experimental data provided by the ICMPE revealed a strong temperature dependence of the mechanical properties and, in particular, a decreasing overall stiffness under increasing temperature. The glass transition temperature is found to be in a range between 55 °C and 110 °C. Creep recovery tests performed under a single cantilever setup demonstrate viscoelastic behavior as well as significant plastic behavior when a certain load threshold is

surpassed. In addition, these investigations revealed nonlinear elastic behavior under loads high enough to result in significant plastic deformation. Furthermore, from examining the DMTA-TTS derived data, the material turns out to exhibit viscoelastic behavior with the viscous portion increasing relatively to the rate-independent one with increasing temperature.

A three-dimensional geometric model replicating the specimen used in the single cantilever creep recovery setup and its settings, specified to conduct a parameter optimization under application of the VEVP material model, is set up and run within the commercial FEM package Abaqus. A corresponding 2D representation of the experimental creep recovery setup is depicted in Figure 25, showing a schematical representation including the boundary conditions on the left and a deformed FE representation on the right side. A study to determine an efficient model structure is conducted, resulting in a model setup with a simplified FE mesh. The accuracy of this setup is validated by comparing it to an analytical model following Euler-Bernoulli beam theory for small deflections as well as to a more elaborately meshed model for higher loads.

A Prony series based on a linear elastic Maxwell formulation including eight viscoelastic and one elastic branches is calibrated by fitting master curves to DMTA-TTS obtained storage and loss modulus data. Based on this, the parameters of the elaborate VEVP model are calibrated. This material model's Fortran implementation as a UMAT subroutine was made publicly available by researchers of the project Multi-scale Optimisation for Additive Manufacturing of fatigue resistant shock-absorbing MetaMaterials (MOAMMM). The VEVP model connects a hyperelastic bi-

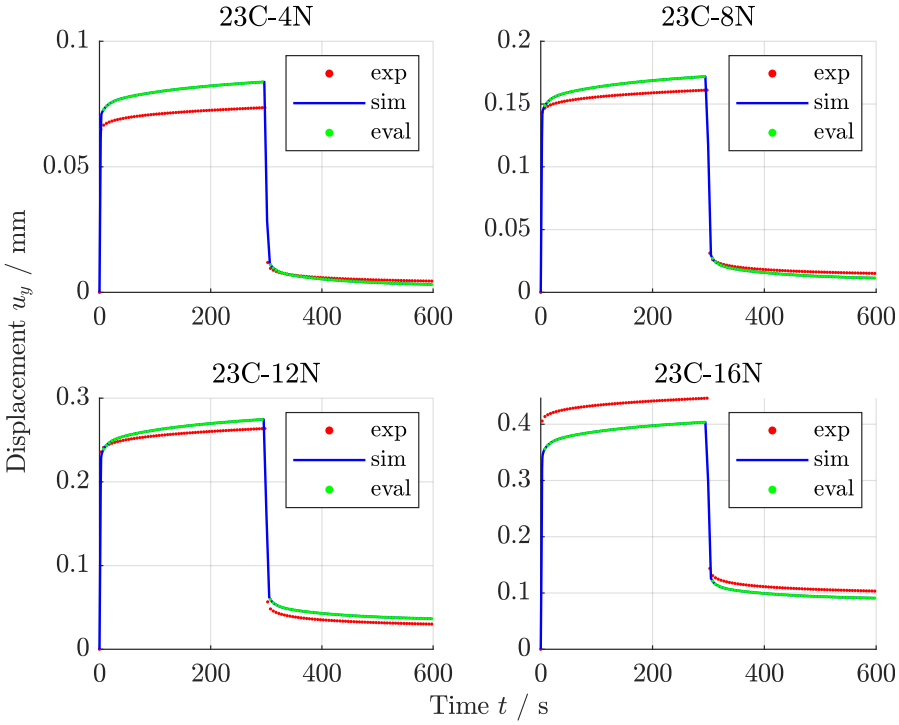

Figure 26: Comparison between experimental (exp) and simulation (sim/eval) results.

logarithmic elastic potential function and quadratic dissipation terms in the viscoelastic part in series to a viscoplastic rheological formulation capable of capturing compression-tension flow asymmetry as well as isotropic and kinematic hardening effects. The optimization is carried out using a self-implemented script consortium written in MATLAB and Python using the Abaqus' Python library, which exhibit certain advantages over commercially available material optimization toolboxes and more flexibility.

For the calibration, the linear viscoelastic parameter values obtained for the Prony series turn out to fit equally well for the viscoelastic part of the VEVP model and are therefore fixedly adopted for the calibration of the viscoplastic parameters. Under assumption of certain relations between the

respective tension and compression hardening mechanisms, the optimization is conducted using a particle swarm optimization technique. The calibration leads to parameter values of the VEVP model which reproduce the experimental results fairly well, especially with regard to plastic behavior, with some shortcomings for nonlinear elastic effects. The results of the four comparisons at 23 °C and different force levels during the creep phase are displayed in Figure 26. The model is finally successfully validated using the more elaborately meshed model. As the simulation results revealed certain shortcomings with regard to the hyperelastic law of the VEVP model employed, this area will be addressed in the follow-up work.

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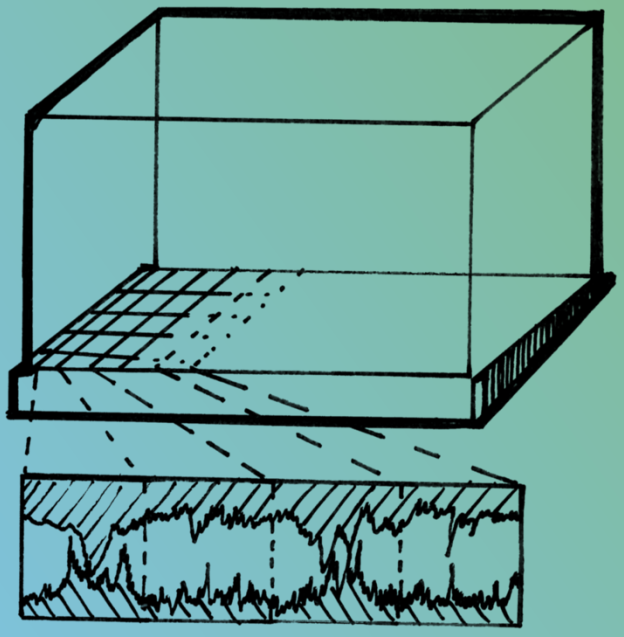

P7

COLLECTIVE PHENOMENA IN FAILURE AT COMPLEX INTERFACES

Christian Greff

PD Dr. Paolo Moretti

Materials Simulations

Department Material Science and Engineering

P7: Tuning adhesion properties of hierarchical materials

Christian Greff and Paolo Moretti

The research of this project uses network-based models to investigate the failure and detachment of hierarchically structured materials in thin films under tension. Understanding of such systems would be of interest for example in the context of dry adhesives [1]. Forces are treated as scalar, so that the model functions as an electric analogue and local strength of the material is incorporated into the model by assigning randomly distributed failure thresholds to the edges of the network. A scaling parameter t defines the ratio between the adhesion connections at the lower interface to the cohesion connections within the network, thereby controlling whether the interface is a weak layer. The focus of this research is directed to how structuring, by removal of edges, can be used to tune the failure behavior of such systems.

Hierarchical structuring of the thin film, using vertical 'gaps' of missing edges, localizes failure under tension towards the interface of the film, independent of whether the interface is a weak layer or not. A reference system with the same number of removed cross-links at random positions in the network only localizes damage at the interface in the case of it being a weak layer and shows

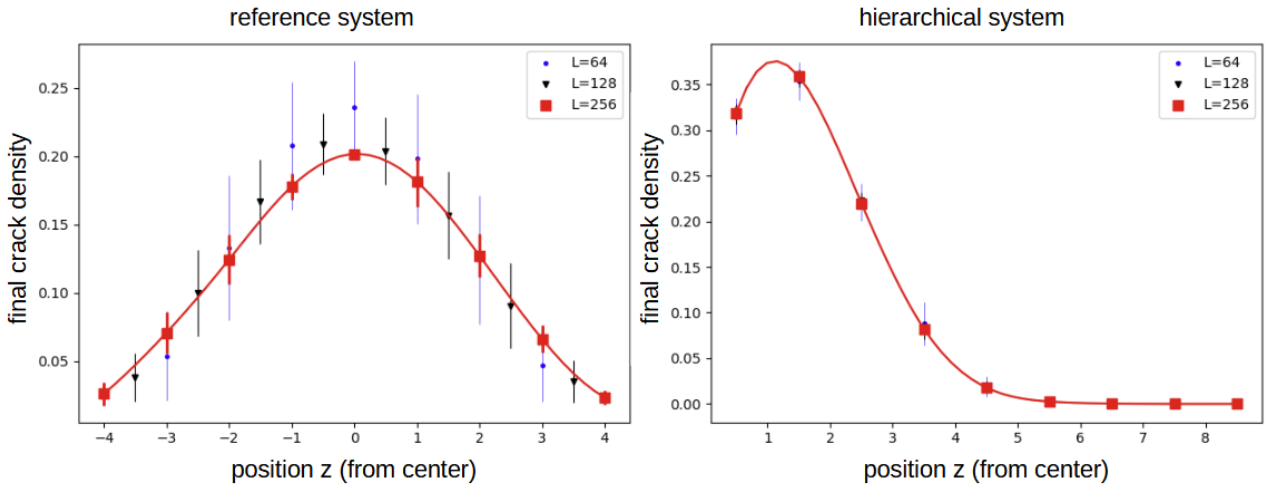

Figure 27: Position of the critical system-spanning crack in the thin film averaged over 80 random structures for system sizes L = 64 and 128 and 40 iterations for system size L = 256 for the case of the interface not being a weak layer (local strength equal to bulk).

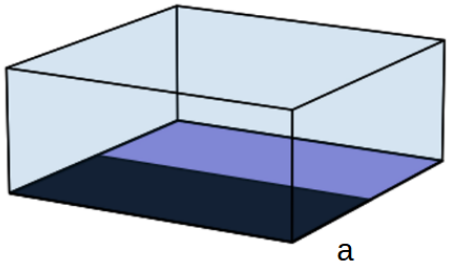

Figure 28: Schematic of the system with bulk of the film in blue, interface layer in violet and horizontal pre-crack of length a in black

a symmetric distribution over the film otherwise, as shown in Figure 27. Using this property to engineer a predetermined location of failure without adding a weak layer would be of interest, for which it must be determined whether applying hierarchical structuring does introduce weakness. Therefore, the performance of such systems with regards to work of fracture and peak stress was investigated in simulations of hierarchical and reference systems with horizontal pre-cracks of

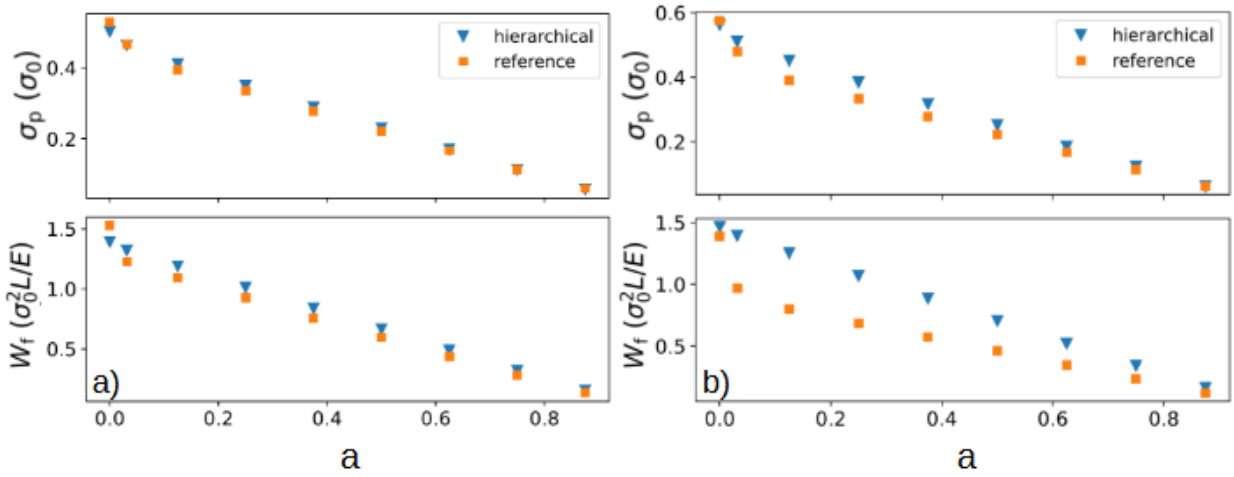

Figure 29: Peak stress σ_p and work of fracture W_f over initial horizontal crack size a for intermediate disorder of local strength with a) interface not being a weak layer and b) the interface as a weak layer.

length a in the interface, as shown schematically in Figure 28. A comparison of these measures between hierarchical and reference systems for intermediate disorder of local strength and the interface not being a weak layer can be seen in Figure 29a) and shows that the localization in the hierarchical systems is achieved at no performance cost. This is attributed to the mechanism of crack arrest active in hierarchical systems. While the reference systems show the typical behavior of quasi-brittle materials, namely growth of a horizontal critical crack through the system, the vertical gaps in the hierarchical systems suppress this. The network is therefore forced to fail by nucleating and coalescing individual cracks instead of growing a critical one, with additional work of fracture being expended for the nucleation processes. This mechanism can compensate for the

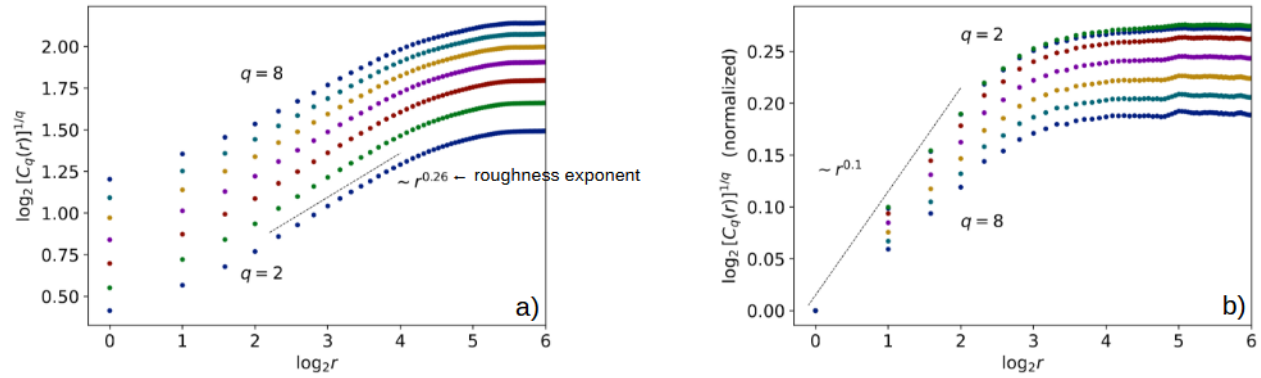

Figure 30: Structure factor Cq averaged over 40 a) reference and b) hierarchical systems (L = 256)

fact that the reference system can store damage throughout the whole system by crack roughening. If the interface is a weak layer, as in Figure 29b), the latter mechanism is not available anymore and the reference system consequently performs worse with the hierarchical one now outperforming it. The same holds true for a weak-layer interface and a high disorder in local strength. Only in the case of the interface not being weak and a high disorder of local strength does the localization induced by the hierarchical structuring come with a performance cost.

Scaling analysis of the fracture interfaces shows that the differences in mechanism between failure in the two types of systems lead to significantly different results. For this, structure factors C of differing orders q are calculated:

$$[C_q(r)]^{\frac{1}{q}} = [\langle |h(x+r) - h(x)|^q \rangle_x]^{\frac{1}{q}}$$

Plotting them over window size r shows curves where the slope of the curve is the roughness exponent. A non-zero slope indicates scaling and a constant line means a loss of correlations, which in these thin film systems occurs as a size effect for larger window sizes r. In Figure 30, the reference systems show curves with equal slopes for different orders q, therefore we observe (standard) scaling. In the hierarchical case, we instead find different slopes for different orders q, which points to multi-scaling behavior.

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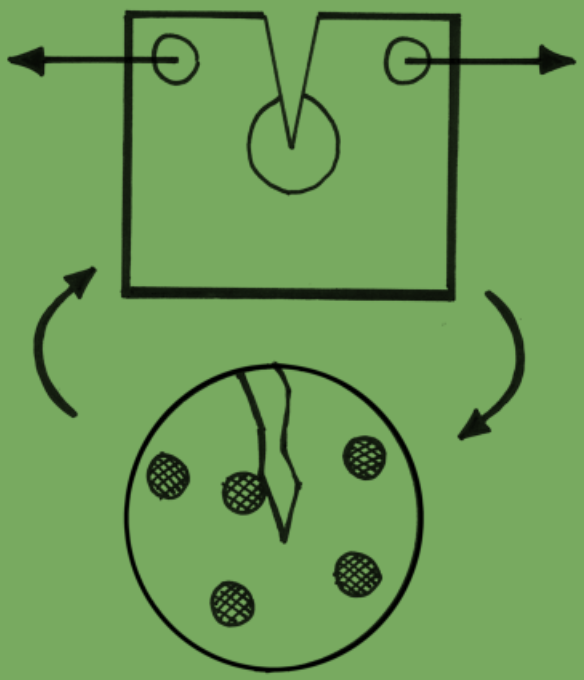

P8

FRACTURE IN POLYMER COMPOSITES: MESO TO MACRO

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P8: Influence of the irreversibility strategies in spatial adaptive phase-field fracture simulations

Maurice Rohracker, Julia Mergheim

The phase-field fracture method has received a lot of attention in the last decades due to its ability to simulate fracture in various materials. In this method, a discrete crack is captured by the smeared approximation (see Figure 31). For the simulation of fracture in brittle materials using the phase-field fracture method, problem (1) (see overview in [1]) must be solved. Find $\mathbf{u} \in \mathcal{B} \rightarrow \mathrm{R}^{\mathrm{dim}}, \mathrm{z} \in \mathcal{B} \rightarrow [0,\ 1]$, with $\mathrm{z} = 1 \Rightarrow$ intact and $\mathrm{z} = 0 \Rightarrow$ broken, s. t.

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

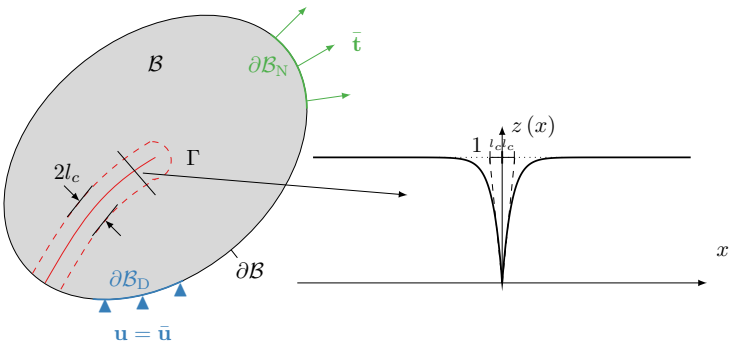

Figure 31: Smeared model of the phase-field fracture model.

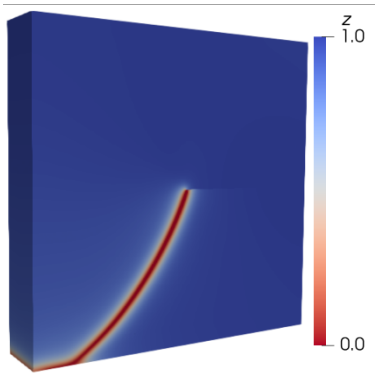

Figure 32: Phase-field contour of the 3D

For an accurate resolution of the phase-field function, suitable finite element meshes are required, which can lead to very computationally expensive simulations due to the large number of elements. In our recent publication [2] we introduced three different error indicators for adaptive spatial refinement (ASR) of the finite element mesh and compared them to each other. Special emphasis was put on the accuracy (error measure of the load-displacement curve) and efficiency (speedup) of the simulations. We have extended this comparative assessment to 3-dimensional numerical examples of crack growth in the single-edge notched shear (SENS) test (see Figure 32). For suitable parameters, they show very good accuracy and efficiency compared to the simulation on a pre-refined mesh. Another area of interest has been the crack irreversibility, or in other words, the method to prevent crack healing. In [3], a history function as the maximum of all tensile strain

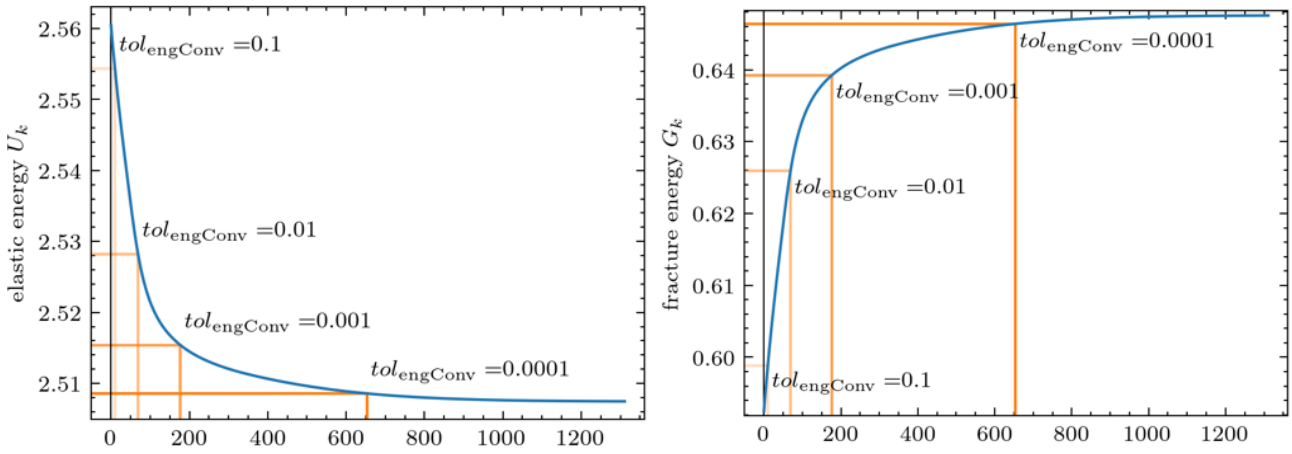

Figure 33: Elastic energy (left) and fracture energy (right) at $t = 10.2 \cdot 10^{-3}$ over the outer loops for the 2D shear test.

energies is introduced and used as the crack driving force. By defining this history function as a

function of the previous load step only, the residual equations in the staggered solution scheme are not coupled anymore, and hence convergence is achieved after a single staggered iteration. However, this strategy requires small time-step sizes to correctly capture the crack propagation. The counterexample to this strategy is the history current approach, where the history function depends on the current load-step, resulting in a two-way coupling of the residual equations. For

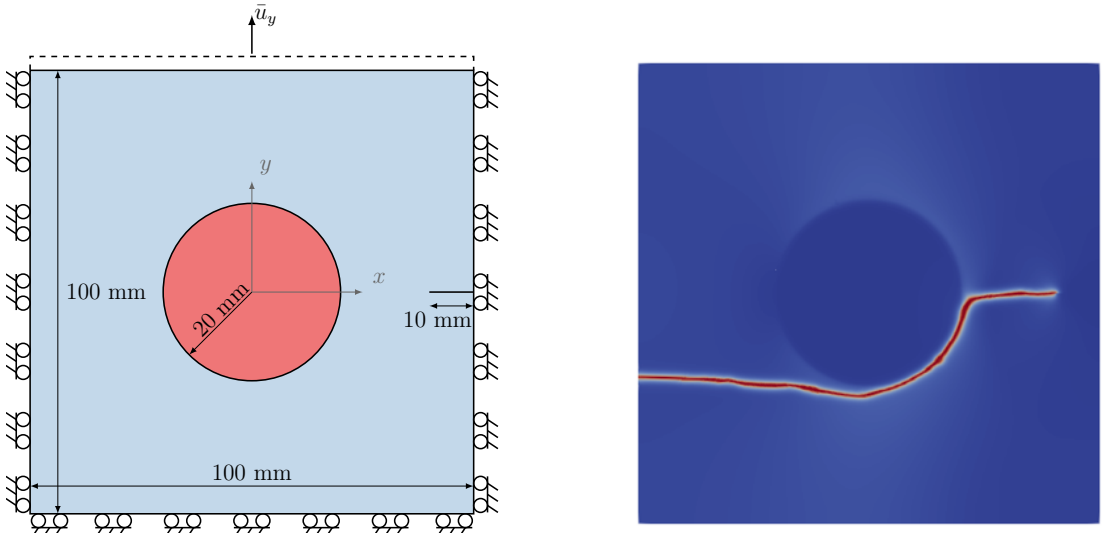

Figure 34: Geometry and loading configuration (left) and phase-field contour (right) of the single inclusion pre-crack tension test.

the simultaneous convergence of the two residual equations, multiple iterations (outer loops/ staggered iterations) are required, especially in the critical loading regime when the fracture occurs. Our goal here is to develop a new energy-based convergence criterion to reduce the number of outer loops while maintaining the accuracy of the fracture behavior. Based on the small

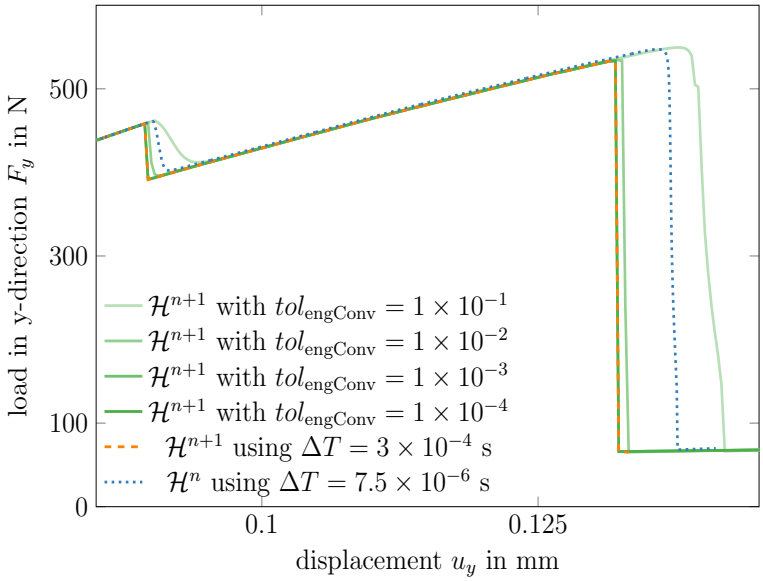

Figure 35: Load-displacement curves of the single inclusion pre-crack tension test.

changes in the elastic and fracture energies in the later outer loops, as seen in Figure 34, a relative energy difference-based criterion for the elastic energy $\left|\frac{\mathcal{E}^{el}_{k+1}-\mathcal{E}^{el}_{k}}{\mathcal{E}^{el}_{k+1}-\mathcal{E}^{el}_{1}}\right| < tol_{engConv}$ and for the fracture energy $\left|\frac{\mathcal{E}^{el}_{k+1}-\mathcal{E}^{el}_{k}}{\mathcal{E}^{el}_{k+1}-\mathcal{E}^{el}_{1}}\right| < tol_{engConv}$ is introduced for the convergence check. Here, a converged solution is obtained if either the residual-based criteria are satisfied simultaneously, or both the energy-based criteria are satisfied simultaneously. For different tolerance values tol_{engConv} the

convergence of the energy criterion is marked with different orange lines in Figure 34. To test this new convergence criterion, a tensile test on a pre-cracked single inclusion specimen was selected. The geometry setup with a stiff silica particle in an epoxy matrix is shown on the left side, and the resulting phase-field contour on the right side of Figure 35. For sufficient loading, the crack propagates until it reaches the particle (first peak in the load-displacement curve in Figure 35), arrests, and propagates further around the particle up to the second peak in the load-displacement curve. Furthermore, Figure 35 also shows the resulting curves for the different energy-based convergence tolerances tol_{engTol}, which converge with decreasing tolerance values. Correct results are observed with a tolerance of $1 \cdot 10^{-3}$ which results in a speedup of 1.4 compared to the residual-based converged solution (dashed orange line). The dotted blue line shows the corresponding solution when using the history previous approach with a time-step size of $\Delta T = 7.5 \cdot 10^{-6}\ s$ ($20{,}000$ load-steps), which does not correctly capture the brittle fracture behavior. Here, the crack propagation is slower compared to the history current approach. To incorporate ASR into the phase-field fracture simulations with the history current irreversibility approach, a repeating load-stepping scheme is necessary since ASR is a pure post-processing step, but crack propagation is observed within the load-steps. This further increased the speedup to 2.85 for similar accuracy, which reduced the simulation duration from $1395\ min$ to only $490\ min$. The combination of both strategies results in a speedup of 4.25 (simulation time: $328\ min$) for a phase-field refinement threshold of $th_{ref} = 0.8$, where elements are refined as soon as the phase field value falls below the given threshold, while still observing correct simulation results.

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aPJ: Mechanics of Generalized Interfaces and Grain Boundaries

Lucie Spannraft, Julia Mergheim, Fredrik Larsson, Kenneth Runesson & Paul Steinmann

Interfaces play an important role in numerous engineering applications, such as grain boundaries and adhesive layers. On the one hand, interfaces can increase the material's toughness, e.g. by acting as dislocation obstacles in polycrystalline metals. On the other hand, interfaces can be considered a weak link, predestined for decohesion and in-plane damage.

Our publications [1-3] present thermodynamically consistent interface laws for grain boundaries and generalized interfaces; and analyze their effects in FEM simulations.

Generalized interfaces allow for anisotropic decohesion and interface inelasticity. Interface inelasticity provides the interfaces with its own energetic and dissipative structures, i.e. membrane stresses causing resistance versus in-plane stretch. At finite strains, anisotropic decohesion introduces additional shear-like stresses for thermodynamical consistency. Our models account for a damage mode interaction, i.e. the damage modes normal cohesive, shear cohesive and in-plane (membrane) are coupled.

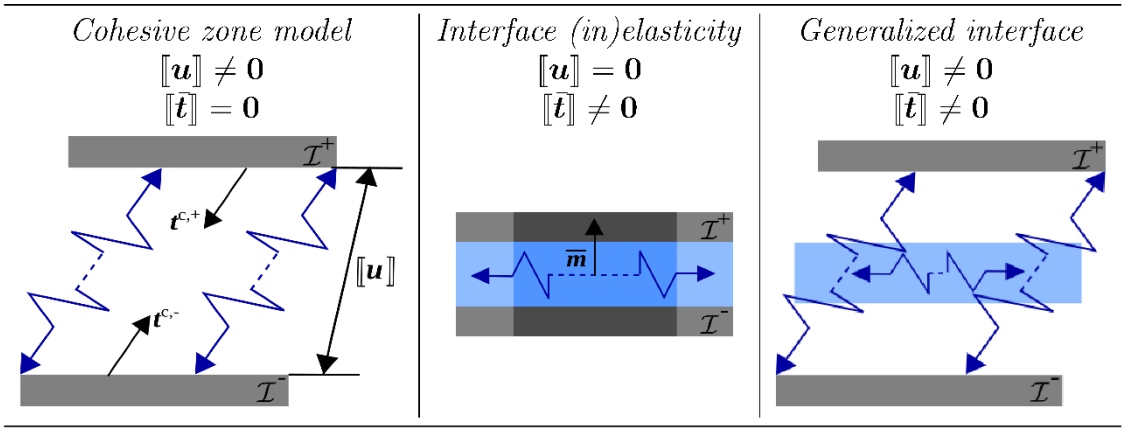

Figure 36: Categorization of interface models with regard to the displacement jump [[u]] and the traction jump $[[\bar{\boldsymbol{t}}]]:=\sigma\cdot\bar{\boldsymbol{m}}$, cf. [2].

Such generalized interface laws can be applied to a variety of materials undergoing different deformation modes, i.a. adhesive layers. The application of soft and brittle adhesives in industrial production has been steadily increasing for decades. For instance, adhesive layers are employed in lightweight construction, aircraft production, sealing applications and convenience products. Such adhesive layers are of small thickness and can be modeled by interphases with a finite thickness. Since interphases require high computational efforts, it is beneficial to approximate interphases by zero-thickness interfaces. Experiments in literature observe a damage mode interaction in adhesive layers. More precisely, in-plane damage increases cohesive degradation and normal and shear decohesion affect each other. Thus, we employ the models to capture the behavior of soft and brittle adhesives under deformations critical to their integrity, e.g. during manufacture or assembly.

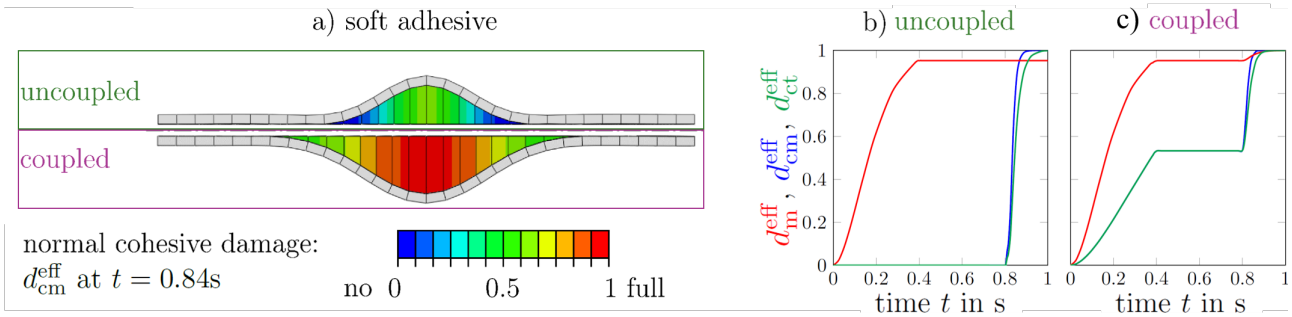

Figure 37: (a) The cohesive damage in a soft adhesive connecting two substrates during buckling. The damage variables d_{eff} for the (b) uncoupled and (c) coupled damage modes over time t, cf. [3].

Figure 37 depicts the results of a buckling simulation juxtaposing the case of not coupling the in-plane damage and the cohesive damage variables (uncoupled) and the coupled case. Two thin substrates are connected by a soft adhesive layer. Firstly, the body is stretched up to 300% strain (t=0.4s), unloaded (t=0.8s) and then compressed to 25% strain (t=1.0s). During the compression, buckling occurs, cf. Figure 37 (a). Accounting for a damage mode interaction (coupled) causes the structure to fail earlier, cf. Figure 37 (a), since the in-plane damage occurring through stretching impairs the cohesion. Compare Figure 37 (b) and (c) which oppose the damage variables for the cases of (b) uncoupled and (c) coupled damage modes. Accordingly, accounting for a complex model including a damage mode interaction is crucial for capturing the behavior of adhesives.

At grain boundaries, decohesion can also occur and be modeled by an anisotropic decohesion law. Furthermore, edge dislocations can be accumulated, submitted or transmitted at grain boundaries. In order to account for their behavior, a microtractions model considering a crystallographic mismatch is introduced within a gradient-extended crystal inelasticity framework. The microtractions along the grain boundary reduce for increasing decohesion, cf. [1]. Numerical results show that the crystallographic orientation of neighboring grains has a major impact on inter-granular fracture. Figure 38 opposes two cases of grain orientations visualized in (a) the set-up of a bicrystal under simple shear for (b,c) the edge dislocation densities and (d) the stress-strain curves. In Case 1 of no grain misorientation between both grains, the grain boundary is not felt by the edge dislocations. In contrast, the crystallographic misfit of Case 2 causes an accumulation of edge dislocations, i.e. an increase in the edge dislocation density, at the grain boundary. Furthermore, the distinct grain orientations change the material's toughness and consequently affect the stress-strain curves during decohesion, more specifically the damage initiation and the softening, compare Figure 38 (d).

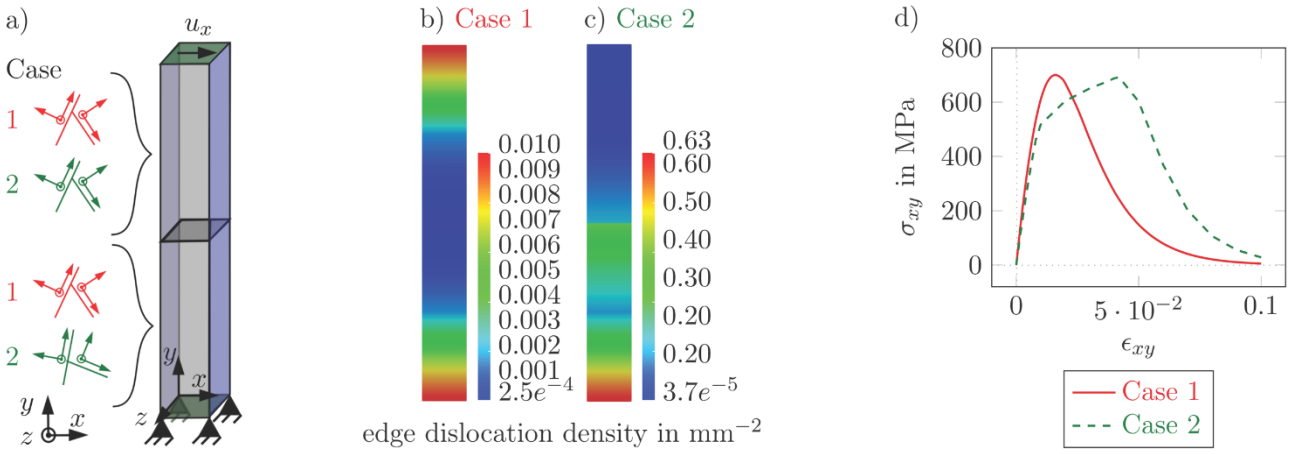

Figure 38: (a) Set-up of a bicrystal subjected to simple shear with two cases of grain orientations: Case 1 (red): no crystallographic misfit, Case 2 (green): crystallographic misfit. (b,c) Edge dislocation density and (d) stress-strain curves for cases 1 and 2, cf. [1].

These two examples indicate that an accurate modeling of interfaces is essential for capturing the behavior of the overall structure.

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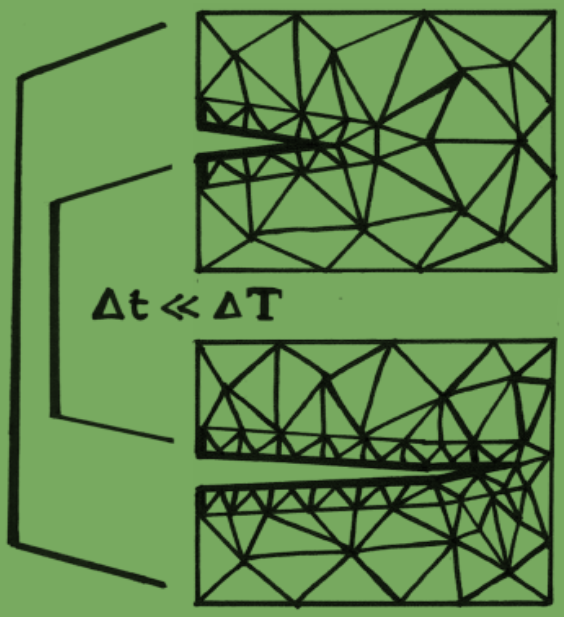

P9

ADAPTIVE DYNAMIC FRACTURE SIMULATION

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P9: Explicit asynchronous variational integrator for linear elastodynamics and numerical illustration of its convergence

Deepak Jadhav, Sigrid Leyendecker

In continuum mechanical simulations, it is a common practice to use different mesh sizes in various regions of interest. But, generally, the same time step (calculated by considering the smallest element size) is used for all the elements of the computational domain. This leads to very high computational costs while solving dynamic problems. To circumvent this problem, the idea of Asynchronous Variational Integrators (AVI) is employed [1]. These integrators are based on two primary concepts. Firstly, they employ spacetime discretizations, enabling different time steps for different elements within a finite element mesh. Secondly, they derive their time integration algorithms within the framework of discrete mechanics, utilizing a spacetime version of the Discrete Euler-Lagrange (DEL) equations derived from a discrete Hamilton's principle. These integrators exhibit symplecticity and good energy behavior. Furthermore, by using the variational derivation in the discrete time case, we can obtain a discrete time Noether's theorem implying the conservation of discrete momentum maps [1,2].

In this work, AVI for linear elastodynamic system is used. The discrete action sum for the same is formulated as

$$S_d = \sum_a \sum_{i=0}^{N_a-1} \frac{1}{2} m_a (t_a^{i+1} - t_a^i) \left[\frac{\boldsymbol{x}_a^{i+1} - \boldsymbol{x}_a^i}{t_a^{i+1} - t_a^i} \right]^2 - \sum_K \sum_{j=0}^{N_K-1} (t_K^{j+1} - t_K^j) V_K(\boldsymbol{x}_K^{j+1}, t_K^{j+1}) \tag{1}$$

where a is node number, $m_a$is nodal mass, $\boldsymbol{x}_a$ is nodal displacement, t_a is nodal time, K is element number, N_a is number of time steps for node a, N_K is number of time steps for element K, and V_K is potential energy of element K. Using discrete Hamilton's principle, DELs are formulated as

$$\delta S_d = 0 \implies D_a^i S_d = \mathbf{0} \tag{2}$$

$$\boldsymbol{p}_a^{i+\frac{1}{2}} - \boldsymbol{p}_a^{i-\frac{1}{2}} = -(t_K^j - t_K^{j-1}) D_a^i V_K(\boldsymbol{x}_K^j, t_K^j) \tag{3}$$

where, $\boldsymbol{p}_a$ is the momentum of node a, $\boldsymbol{p}_a^{i+\frac{1}{2}} = m_a \frac{\boldsymbol{x}_a^{i+1} - \boldsymbol{x}_a^i}{t_a^{i+1} - t_a^i}$, and D_a^i denotes the partial derivative with respect to $\boldsymbol{x}_a^i$. These DELs are then solved asynchronously by using a concept of priority queue to

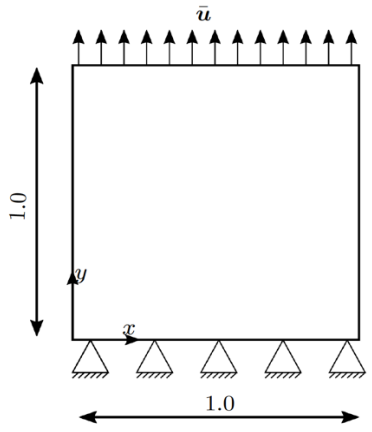

Figure 39: Geometry and boundary conditions of square plate

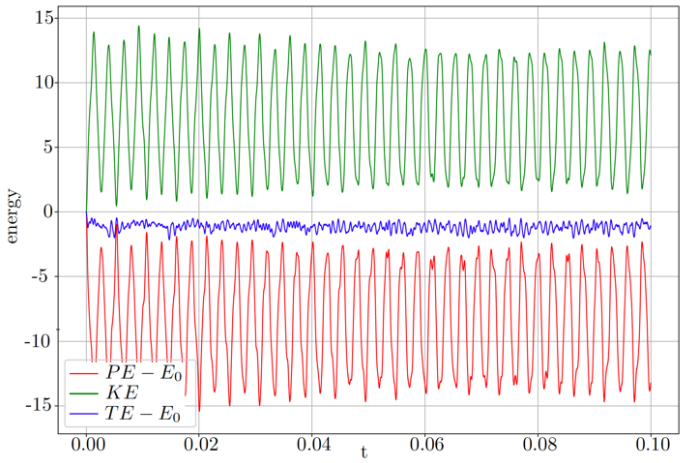

Figure 40: Good energy behavior of AVI

get the flow of the dynamic system. The priority queue holds the triangulated elements, ordered by their impending activation times. An element with the lowest activation time is the highest-

priority element in the queue, and thus the next one to be processed. Then, the current nodal velocities are employed to compute the new nodal displacements for this active element.

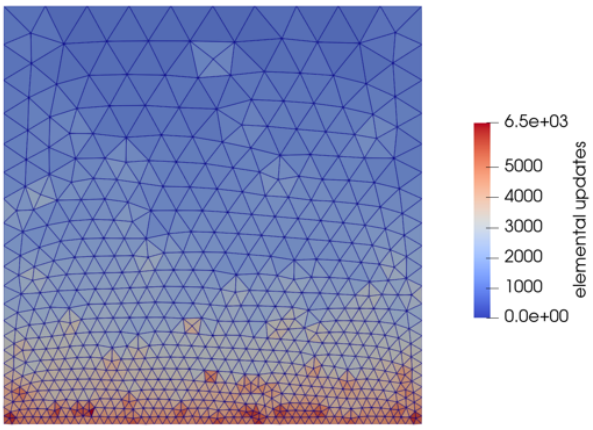

Figure 41: Distribution of elemental updates over mesh

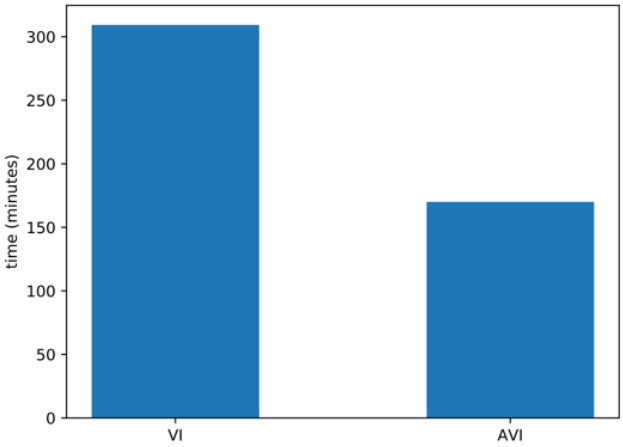

Figure 42: Computational time for VI and AVI

Subsequently, these velocities are adjusted by using the new element configuration. Finally, the next activation time for the element is calculated using the CFL condition, and the element is reinserted into the queue. If the activation time of an element is more than the end time of the simulation, an element is pushed out of the priority queue. This algorithm is iterated until the priority queue is empty [1].

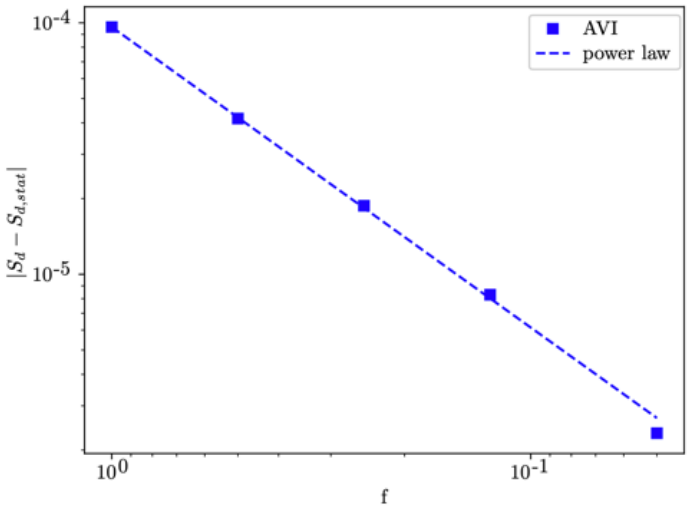

Figure 43: Convergence of discrete action sum

A benchmark case used to investigate the characteristics of AVI is shown in Figure 39. In this case, a 1 mm linear elastic square plate with elasticity modulus E = 1000 N/mm2, Poisson's ratio $\nu = 0.3$ and mass density $\rho = 2$ g/mm3 is fixed at one side and unrestricted on the other three sides. Initially, the plate is set in a stretched configuration under constant uniform strain and subsequently allowed to vibrate freely after being released from rest. As can be seen from Figure 40, AVI shows good energy behavior. Figure 41 shows the distribution of elemental updates over the mesh. Coarser elements get updated less frequently as compared to relatively finer elements in the mesh. This leads to significant computational savings. Figure 42 shows the nearly 50% reduced computational time of AVI as compared to its synchronous counterpart. A new numerical convergence framework for AVI is devised based on the convergence of discrete action sum [3].

As can be seen from Figure 43, explicit asynchronous variational integrator shows the linear convergence when temporal refinement is performed.

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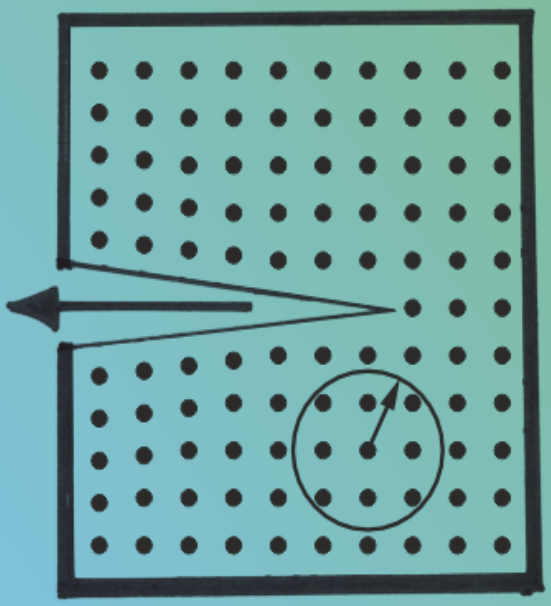

P10

CONFIGURATIONAL FRACTURE MECHANICS OF DISCRETE SYSTEMS

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P10 Modeling damage within continuum-kinematics-inspired peridynamics

Marie Laurien, Ali Javili and Paul Steinmann

Peridynamics (PD) is a nonlocal continuum formulation that was introduced by Silling in 2000 [1]. Nonlocality is introduced to the governing equations of PD through an integral term which computes the interactions of a continuum point and its neighboring points within a finite distance. The size of the considered neighborhood endows the model with a length-scale that allows to capture nonlocal effects that are of specific interest when modeling materials at small scales. In addition, a major advantage of PD is the straightforward modeling of damage by allowing for bond breakage, which is why it is widely used in fracture mechanics. The basic version of PD, i.e., bond-based PD, is restricted to a fixed Poisson ratio. We therefore employ an extension of PD, called continuum-kinematics-inspired peridynamics (CPD) [2]. There, in addition to pair-wise interactions, multi-neighbor interactions characterize the interplay of points via a kinematically exact description. In this manner, it is possible to capture changes not only in length, but also in area and volume.

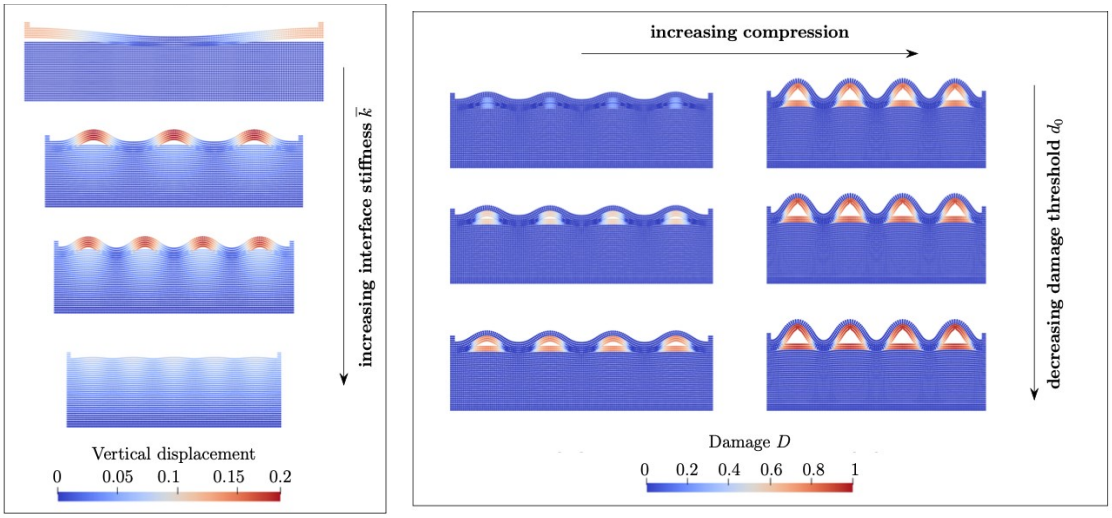

Figure 44: Wrinkling and delamination of a compressed bilayer: A decrease in wrinkling wavelength is observed with increasing interface stiffness (left). Damage is mitigated when larger interface damage thresholds are modeled (right).

In engineering structures, a material interface can be a weak spot, depending on the interfacial properties that result from the manufacturing process, e.g., the interface strength. As a consequence, the interface is an essential and at the same time a challenging component of an accurate material model. In [3], we developed a CPD model accounting for progressive damage within a finite-thickness interface, as opposed to the more common practice of abrupt bond breakage across a zero-thickness interface. The interactions across the interface are governed by an interface constitutive law similar to a traction-separation-law as employed in classical continuum mechanics. A thorough derivation of the theoretical framework employing a rate-variational principle demonstrates the compliance of the damage formulation with thermodynamics and balance laws. In order to ensure non-penetration at the interface, we present a simple approach to approximately track the interface during deformation using the neighboring points. This allows to penalize any penetration in the direction normal to the interface. The capabilities of the model are demonstrated in a series of numerical studies. Comparing the shape of the force-displacement curves resulting from a classical peeling test with different force-opening laws shows the ability to model a variety of interfacial behaviors. In a classical shear test, we investigate the effects of nonlocality that accompany a PD model and are of particular interest for small-scale applications.

It is found that increasing the size of the nonlocal interface leads to a stronger interfacial bonding and, hence, less damage. Furthermore, an increase in horizon size results in stiffer material behavior. In our example load case this provokes interfacial damage. The two aspects of nonlocality and progressive interfacial damage are linked for the first time to study the wrinkling and

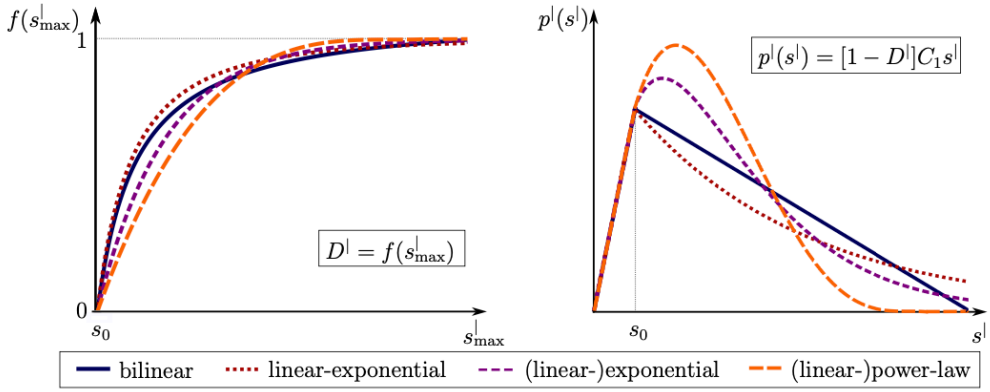

Figure 45: Damage laws (left) and resulting one-neighbour interaction forces (right).

delamination behavior of a stiff film bonded to a substrate, see Figure 44. Under compression the film becomes instable and buckles, leading to the well-known phenomenon of wrinkling instabilities.

The subject of current work is the modeling of damage in the bulk within the framework of CPD. For each type of interaction, i.e., one-neighbor, two-neighbor and three-neighbor interactions, we introduce a damage variable. The damage variables are obtained by evaluating a damage function at the current bond strain, area strain and volume strain, respectively. This allows to model not only abrupt damage but also progressive damage, which is illustrated by a selection of damage functions and the resulting interaction forces for one-neighbour interactions in Figure 45. In Figure 46, the damage propagation in a biaxially stretched square with a hole is compared for two different damage laws.

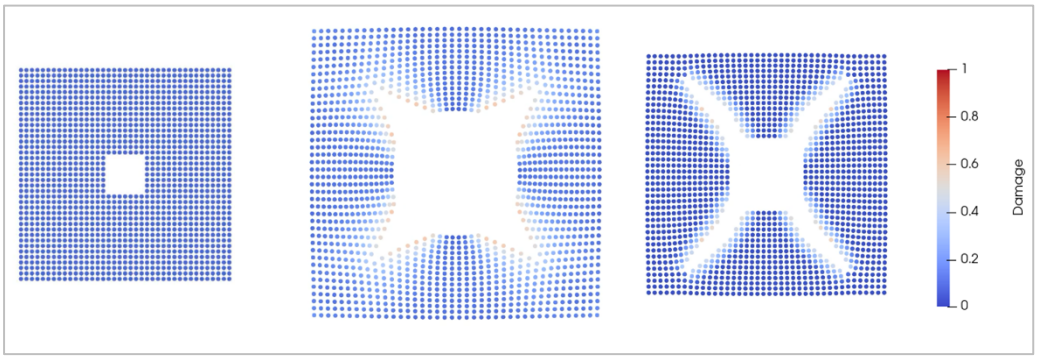

Figure 46: Expansion of a square with a hole. Left: Undeformed configuration. Center: Deformed configuration obtained using a progressive damage law. Right: Deformed configuration obtained using an abrupt damage function.

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aP10: A micromorphic approach captures non-local bone remodelling

A Titlbach, P. Steinmann, M. Stingl & A. Papastavrou, A.T. McBride

Our bones have the ability to adapt their internal microstructure to external mechanical stimulation. Overloading leads to bone formation, while underloading leads to bone resorption. In this process, it is mainly the inner, spongy part of the bone, the so-called cancellous bone, that changes. It consists of a microstructural network of rods, the trabeculae. Overload or underload

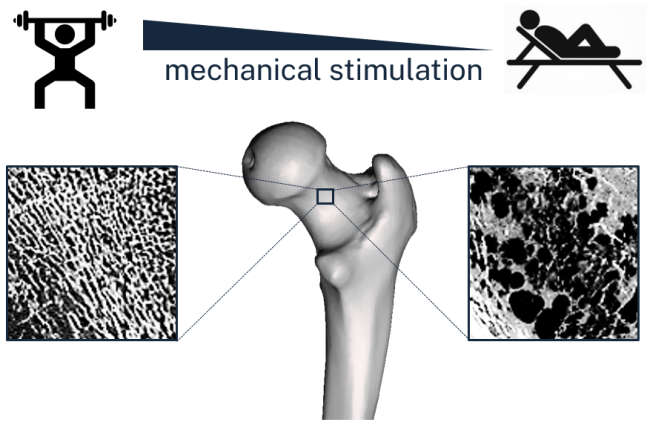

Figure 47: Mechanical stimulation of the bone strengthens or narrows the trabecular structure and thus influences the nominal bone density

causes the trabeculae to be strengthened or narrowed, leading to an increase or decrease in bone density, see Figure 47.

Microstructural effects are associated with bone heterogeneity, so two- or multi-scale approaches are often used to resolve trabecular structure at a subscale. However, this is algorithmically expensive to implement and increases computational costs. Therefore, we have developed a micromorphic approach, based on [1], in which we account for bone microstructure without

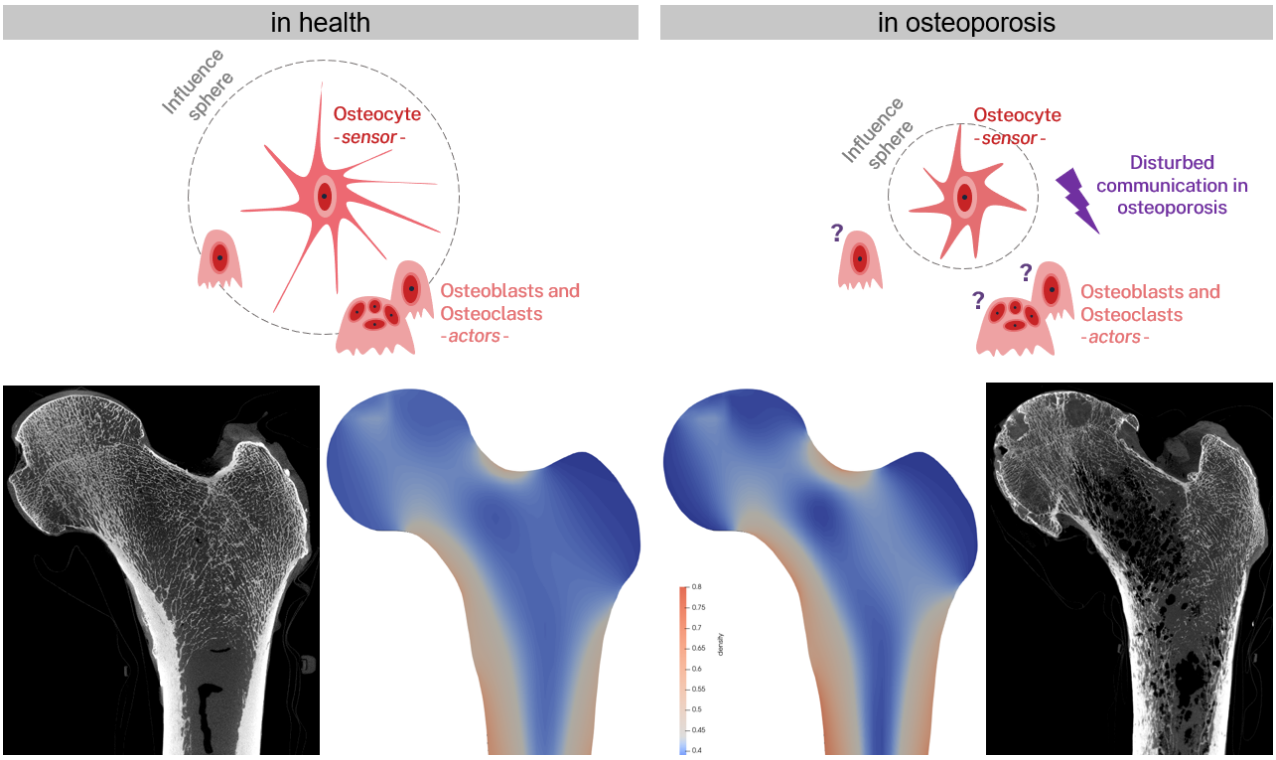

Figure 48: Disturbed osteocyte mechanosensing in the case of osteoporosis results in reduced non-local behaviour of the bone remodelling processes

explicitly resolving it, and which also allows us to capture the nonlocal behaviour of osteocyte mechanosensing, which is disrupted in the case of osteoporosis [2].

In the healthy case, the mechanical stimulation of the bone is detected by osteocytes, which act as mechanosensors. They are responsible for transmitting the information about overload or underload to the surrounding osteoblasts and osteoclasts, the executive cells for bone formation and degradation. This information signal acts in a certain area of influence and not only

Figure 49: Presentations at the international conferences CMBBE in May 2023 and ICCB in September

immediately locally. In the case of osteoporosis, this information signal is disrupted, i.e., the message about mechanical stimulation is not properly transmitted and the more distant osteoblasts and osteoclasts do not receive information about the mechanical stimuli in their environment. The disruption of the signaling pathways thus leads to a decrease in bone mass and strength, and the trabecular structure deteriorates, see Figure 48. This micromorphic approach was successfully published in the journal Computer Methods in Biomechanics and Biomedical Engineering in May 2023 [3]. The results were also presented in talks at the international conferences CMBBE in May 2023 in Paris, GACM and ICCB in September 2023 in Vienna, see Figure 49.

In the future, the micromorphic model will now be refined with regard to bone healing triggered by the flexoelectric effect, which has been demonstrated experimentally on bone material [4]. The validation for this has been successfully completed. The further procedure will be to apply the coupled flexoelectricity and micromorphic elasticity to bones, especially bones with microcracks. Bone models and meshes with cracks have already been prepared for this purpose.

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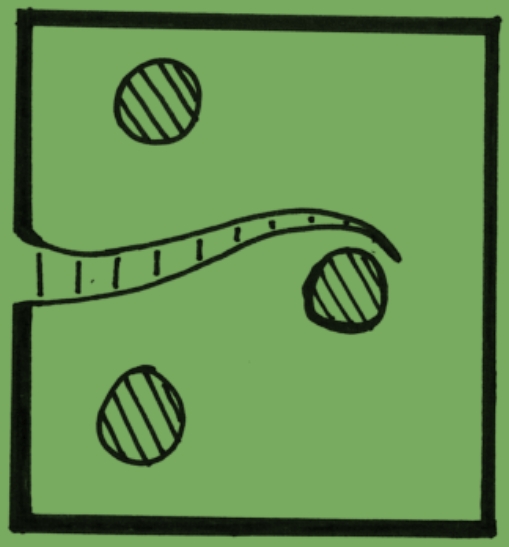

P11

FRACTURE CONTROL BY MATERIAL OPTIMIZATION

Lennart Igel

Prof. Dr. Michael Stingl
Applied Mathematics
(Continuous Optimization)
Department of Mathematics

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

Lennart Igel, Michael Stingl, Julia Mergheim & Lukas Pflug

Fracture optimization applications face a significant challenge: the discontinuity of objective functions in the design domain requires regularization, but the high computational cost of evaluating fracture simulations makes common regularization schemes impractical. Traditional approaches, such as transforming the problem into a robust optimization one by smoothing the objective with a mollifier, become unfeasible due to the superlinear increase in computational cost with growing design dimensions. However, in many cases, the resulting objective exhibits structural discontinuity along lower-dimensional submanifolds rather than across the entire design domain.

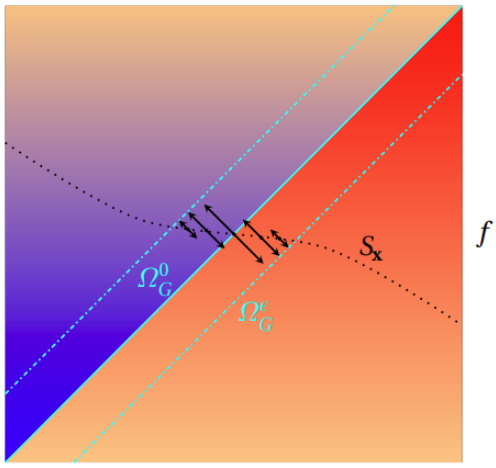

Figure 50: Visualization of each of the primary construction parts of the framework. The discontinuity set of the objective f is described by the zero set of the level set function G (Ω_G^0), a belt around the zero set (Ω_G^ε) denotes the set in which smoothing should be performed and scales the size 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.

Exploiting this localized discontinuity could be beneficial if it can be demonstrated that this assumption holds true. Motivated by this, we aimed to create an optimization algorithm capable of dynamically detecting nearby discontinuities and their positions relative to the current design point. The algorithm should selectively apply smoothing only where necessary, utilizing point evaluations of the objective to significantly reduce computational costs. Moreover, smoothing should exclusively target features requiring it; for example, there's no need to smooth in both x and y directions if the objective is only discontinuous along the y direction. This selective detection and smoothing of discontinuous features minimize the dimension of smoothing, detaching it from the design space dimension.

The key elements for creating our method as a mathematical framework are outlined in Figure 50. We introduce a new level set function to dynamically detect objective discontinuity, designed to have a zero set coinciding with the discontinuity set. The construction and assumptions on this level set function are explored in more detail in our upcoming publication. A crucial consideration involves the regularity of the zero set in the design domain. If these regularity assumptions hold, we can construct a dynamically oriented and scaled smoothing domain, utilizing the gradient of the level set function perpendicular to the zero set when close enough. Scaling is determined by the size of the level set function value, creating a smooth transition from point evaluation to line integral. This framework can be generalized to a larger number of level set functions.

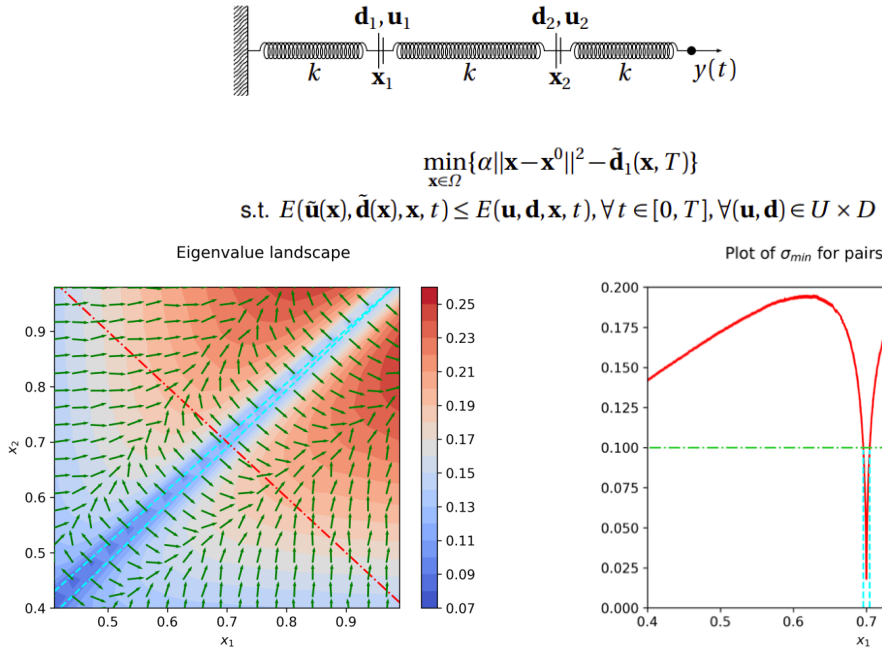

Figure 51: (Above) Simple design optimization problem with a spring model as subproblem. To evaluation the objective function, the subproblem has to be solved for the damage variable d_1 of the first interface, which has material strength x_1. The spring model has bifurcation points whenever x_1 = x_2, i.e. the diagonal line. (Below) The landscape for the minimal eigenvalue function and the associated set Ω^ε in light blue, as expected runs along the diagonal line over the design domain. On the right a cut across the counter diagonal red line of the minimal eigenvalue function is plotted as well, showing how close the eigenvalue comes to zero near the discontinuity.

Given the framework's reliance on the zero set of the level set function descriptor property of the discontinuity set, it is important to assess its practical applicability, especially in the context of fracture scenarios where no assurances of this property's general presence exist. To address these concerns, consider the spring system depicted in Figure 51. Nonuniqueness in objective functions, common in mechanical optimization problems, including fractures, arises from energy minimization subproblems. Nonuniqueness occurs only if multiple optimal solutions to the mechanical subproblem are allowed for a given design. This can be identified by tracking the minimal eigenvalue of the Hessian associated with the energy functional over the simulation time history and identifying where it becomes zero. By demonstrating that the defined eigenvalue function, under assumptions of analyticity on the energy and numerical solution operator, is itself analytic, we establish that both its zero set and the discontinuity set of the associated optimization problem form a submanifold in the design space. This result, obtained through our research over the past year, not only provides a level set function for problems meeting the given assumptions but also confirms our suspicions regarding the fracture setting. Our result justifies the application of our method, as it confirms that for such mechanical systems our assumptions hold. Furthermore, it allows us to employ the minimal eigenvalue function as a level set and thus yields a simple construction method for such general applications. In conclusion, we have constructed a novel approach for optimization of functions, which possess discontinuities along lower dimensional manifolds, with particular application to mechanical problems with a focus on fracture. The construction of the method allows for dynamic detection of the discontinuity during the optimization process and so greatly reduces the computational cost of smoothing by restricting it to dimensions and subdomains at which it is necessary.

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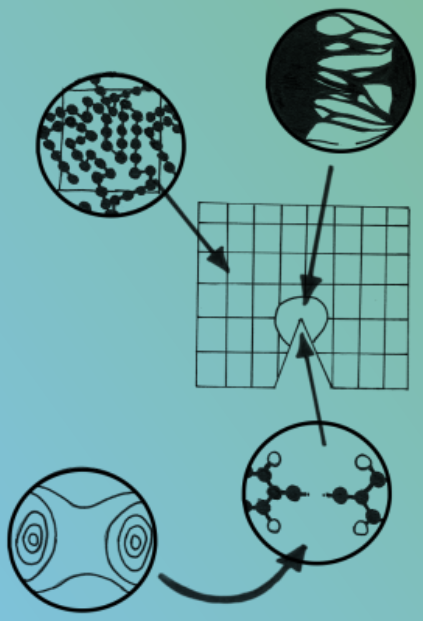

P12

QUANTUM-TO CONTINUUM MODEL OF THERMOSET FRACTURE

Dr. rer. nat. György Hantal

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Theoretical Physics
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P12: Coupling molecular dynamics with continuum mechanics for thermoset polymers

György Hantal, Sebastian Pfaller &Ana-Sunčana Smith

Introduction and motivation

Fracture in highly crosslinked thermosets, like epoxies, is inherently a multiscale phenomenon in which processes at all length- and timescales can contribute to the dissipation of energy and thus determine the fracture toughness. Fracture is ultimately caused by bond scission, which requires a quantum mechanical (QM) treatment. The reorganisation of the network occurs on the molecular scale, which is often captured by molecular mechanics. The macroscopic mechanical behaviour requires a continuum mechanics description. This project combines these three levels by integrating information from the QM level into the particle-based description and coupling it with a concurrently running continuum mechanical simulation. In practice, the system is split into a part that is propagated with molecular dynamics (MD) at atomic resolution, while a continuum description (finite element FE) is used in remaining regions of the sample to keep the computational cost to a minimum. FE and MD coupling is performed using stochastic boundary conditions as implemented in the Capriccio framework [1,2].

Work performed

PDR György Hantal has joined FRASCAL half way through the year and most of his work initially focused on familiarizing himself with the numerical tools and understanding the relation of P12 with the rest of the FRASCAL projects. Initial discussions soon led to realizing the importance of an aspect of the molecular-continuum coupling that was not considered before, namely the treatment of long-range electrostatic forces. His work was primary aimed at figuring out the necessary and technically feasible components and the shorter-term steps of achieving the coupling by considering the problematics of long-range interactions. Recently his work is directed towards the development of the computer model to be used in the project, as explained below.

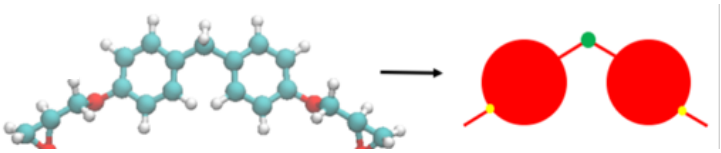

Figure 52: The planned coarse-graining of the DGEBA resin molecule to be represented by 3 interaction sites.

Since at the mesoscopic scale, particles or material elements are charge neutral with no further inner structure resolved, long-range electrostatic interactions do not arise and therefore, they are only relevant to the molecular scale. In fact, at the molecular scale, interaction sites carry partial charges in order to account for the charge distribution within the system, and the long-range nature of these electrostatic forces is appropriately accounted for by virtually extending the interaction calculation to an infinitely large medium. However, in our coupled molecular-continuum system the molecularly resolved part is effectively not in an infinitely large medium. Hence the question arises: How is the integrity of the molecular description maintained in this inherently non-periodic system and what happens to those long-range forces at the molecular-continuum boundary?

We propose to circumvent this problem by applying an intermediate, coarse-grained level between the molecular and the continuum resolution where the long-range forces can be eliminated in a physically consistent way. The coarse-grained model would retain the particle based description but at a coarser, simplified resolution where effective interaction sites account for entire molecules or molecular moieties. The coarse-grained interaction potential is obtained through a bottom-up

information transfer, which results in effective, short-ranged potentials that contain the effect of electrostatic interactions in an indirect, implicit way. Since the coarse-grained model will be still particle based, the machinery of molecular mechanics will be applied through the lammps simulation package [3]. To achieve this, both non-bonded and bonded coarse-grained potential parameters will be developed. As a first step of this development the degree of coarse-graining (the resolution of the coarsening) will need to be decided. As of now, we aim for the strongest reduction of the degrees of freedom that still reproduces the most basic molecular characteristics of the components in order to achieve the largest potential gain in length scale. Figure 52 illustrates the definition of the coarse-grained interaction sites proposed for the DGEBA epoxy resin

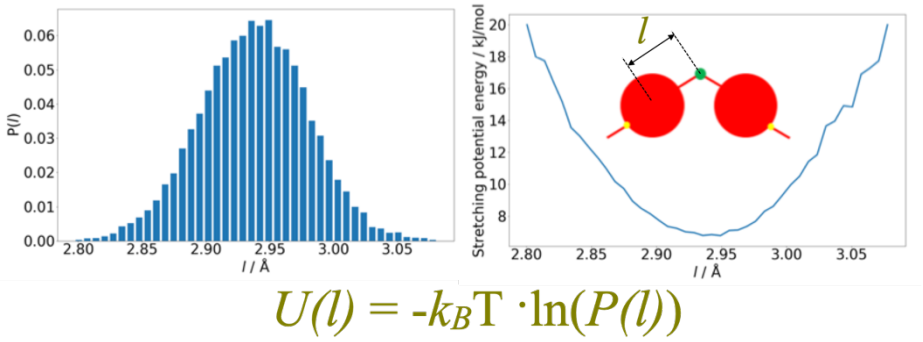

Figure 53: The development of the coarse-grained bond stretching interaction potential.

molecules. In the next step, conventional bonded and non-bonded interaction parameters will be developed between the a priory defined coarse-grained interaction sites. As of now, the application of the well-established "Iterative Boltzmann inversion" technique is planned, [4] whose primary goal is the development of a coarse-grained potential which is consistent with the average (equilibrium) structure determined at the highly resolved (atomic) level. The coarse-grained potentials arise as the "Boltzmann-inversed" structural functions (distribution and correlations) computed at the atomic scale between centres of moieties that are to be lumped together into the coarse-grained interactions sites. Figure 53 illustrates the development of a coarse-grained bond stretching interaction potential defined between the 3 coarse-grained interaction sites that represent the DGEBA molecule.

The last element of the model development is enabling the system to undergo fracture when bonds are highly stretched. Bond scission will be allowed only between coarse-grained interaction sites

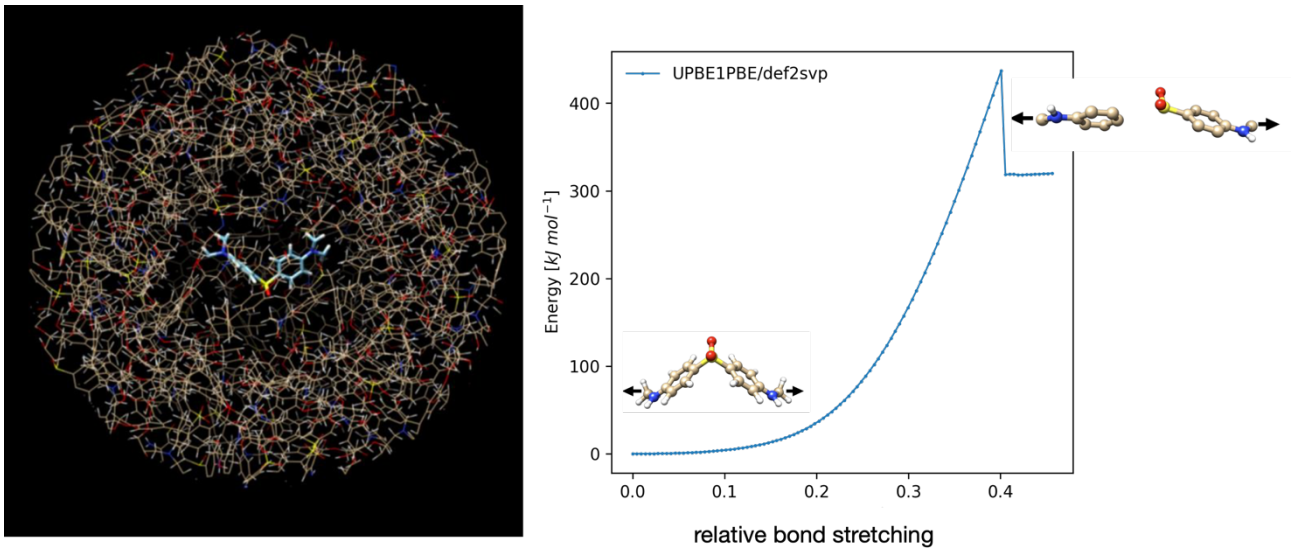

Figure 54: The development of the breakable coarse-grained bond potential.

(and not within them). The necessary effective breakable bond interactions will be studied using quantum chemistry based approaches. In practice, an automated protocol is being set up that identifies overly stretched bonds in an atomic simulation between groups that will be represented as single coarse-grained interaction sites. As it is already implemented in our in-house ChemBreak software, the stretched bond as well as the surrounding atoms are “scooped out” from the system and directly transferred to Gaussian software that sets up a QM/MM calculation. The energetics and the geometrical changes will be followed with Gaussian as the complex is further stretched until bond scission is observed. This procedure is illustrated in Figure 54.

Outlook

In the coming months the performance of different software will be compared that allow the development of coarse-grained interaction potentials based on the iterative Boltzmann inversion technique (see for example Ref 5). At the same time, ChemBreak will be adapted to identify the critical stretching of chemical bonds of interest for this project in order to develop the coarse grained breakable bond potential for the coarse-grained system.

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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 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 effects. ONIOM calculations were employed for this, analyzing a 30 Å radius around reaction sites as shown in Figure 55 to obtain accurate energy barriers. Using Quantum Mechanics/Molecular Mechanics (QM/MM) techniques we have included effects of local environment by allowing incorporation of factors like steric hindrance and hydrogen bonding. This approach enhances MD simulation accuracy for curing reactions, using parameters derived from QM/MM analysis. In the current stage, we have identified an optimal pre-curing strategy to obtain a densely packed liquid mixture comprising all possible DGEBA resin isomeric structures (Fig 56a). This ensures structural fidelity in the systems generated, which now exhibit densities closer to those reported experimentally[2]. Furthermore, based on QM studies we have applied a dihedral constraint (Fig 56b) over reaction mechanism in MD to facilitate least energetic reaction pathways. We are also performing a comprehensive QM/MM Transition state analysis to identify the different reaction sites from existing simulation and investigate the energetic barriers in presence of hydrogen bond.

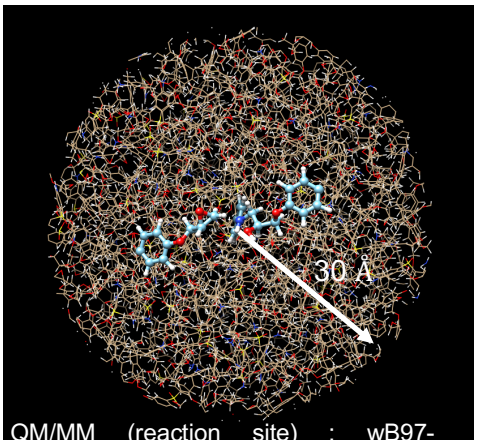

Figure 55: ONIOM system Stick model (QM) Wire model (MM).

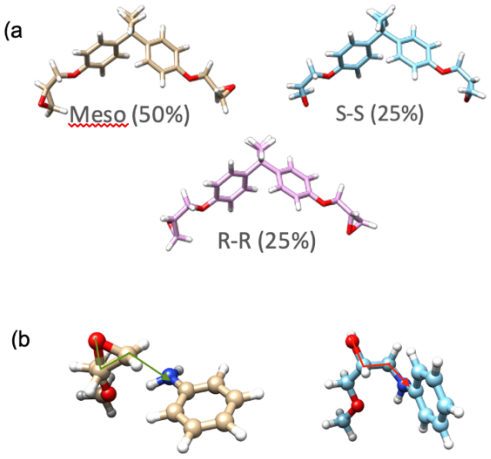

Figure 56: (a) Isomers of DGEBA resin in pre-cured liquid mixture (b) Dihedral constraint only allows back side reaction as observed in stepwise mechanism.

Conclusions, main achievements, and outlook

Adding on to the existing strategy to perform curing simulation by Block Chemistry approach[3], we have established an iterative annealing and stabilization cycle during curing this results in a lower energy state. These iterative cycles play a critical role in guiding system towards a stable configuration. Furthermore, using diffusion behaviour of un-crosslinked moieties and density correlation time of the system, we have minimized the time of curing simulation while preserving its full capabilities. This allowed us to successfully optimise the MD curing parameters. Using the

ONIOM systems around reaction sites, we have been able to fine tune the distance criterion used to search for the reactive ends in the MD simulation. Moreover, with inclusion of QMMM barriers in MD, we found energetic barriers for primary amine to be lower than secondary amine leading to deviation from previous behaviour as shown in Fig 57. Consequently, we have also found that variation in primary (k1) and secondary (k2) reaction kinetics alters polymer chain branching. When secondary reactions are faster or equal to primary ones, early branching occurs. Conversely, when primary reactions are leading, there is a linear growth initially, followed by crosslinking as shown in Fig 58. This branching behaviour is consistent with experimental literature [4]. In the next phase, we are developing an automated workflow to identify reaction sites and perform a posteriori QM/MM analysis, allowing higher accuracy in parametrizing MD curing simulation. Additionally, given the branching behaviour of polymer chains, graph theory will be employed to determine the shortest loop size, shedding light on the rigidity of the generated topology and characterizing the microstructure for further straining simulations.

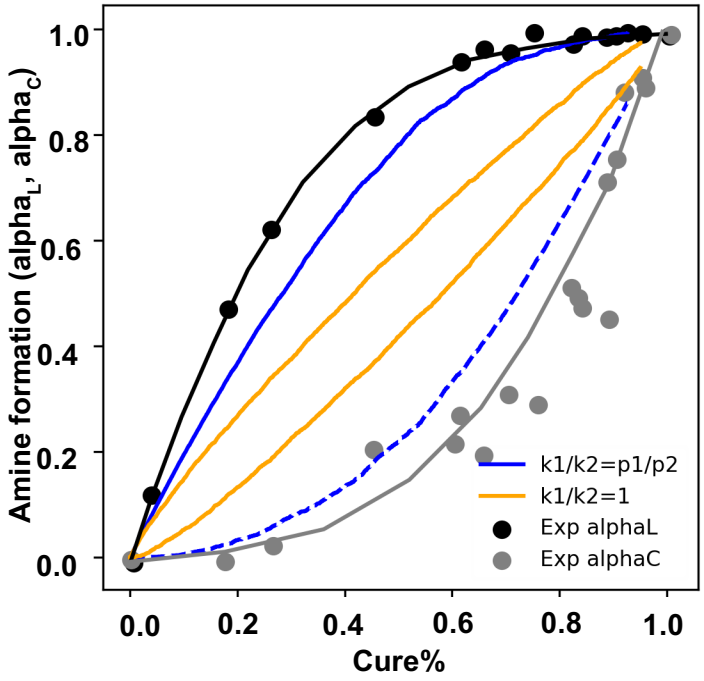

Figure 57: Percentage of amine formation over curing degrees (primary: alpha$_L$ and secondary: alpha$_C$).

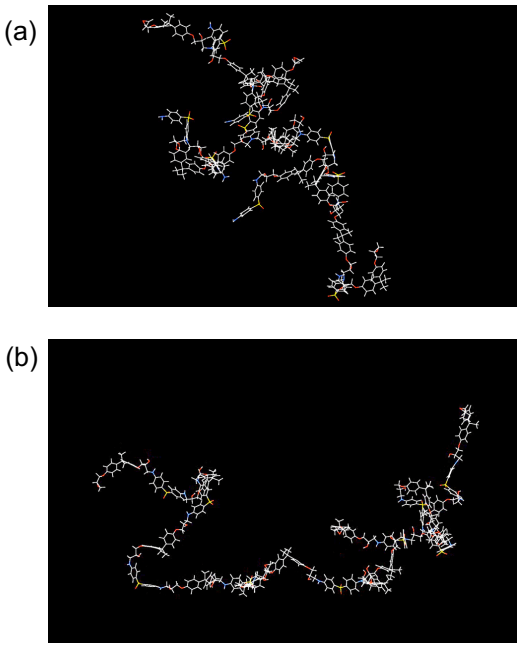

Figure 58: Chain growth (a) $k_1=k_2$ (b) $k_1 > k_2$.

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P13

FRACTURE IN ROCKS: FROM SINGLE GRAINS TO SEISMIC SCALE

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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

There is a general increasing trend across the globe towards alternative and renewable forms of energy as governments and corporations transition away from traditional sources such as oil and gas. Geothermal energy is becoming a popular renewable energy source in Germany (e.g., Weber et al., 2020). Currently major geothermal projects in Bavaria are primarily focussed in the south where high heat flows are present in both high and low permeable (K) reservoirs (Schulz et al., 2013). However, there is potential geothermal resources in Northern Bavaria where low permeable reservoirs have been identified in both the basement (granite) and overlying sedimentary basin (e.g., Kämmlein et al, 2019; Freitag et al., 2022). The primary mechanism for fluid flow in these types of reservoirs are fracture networks and therefore understanding the characteristics of these

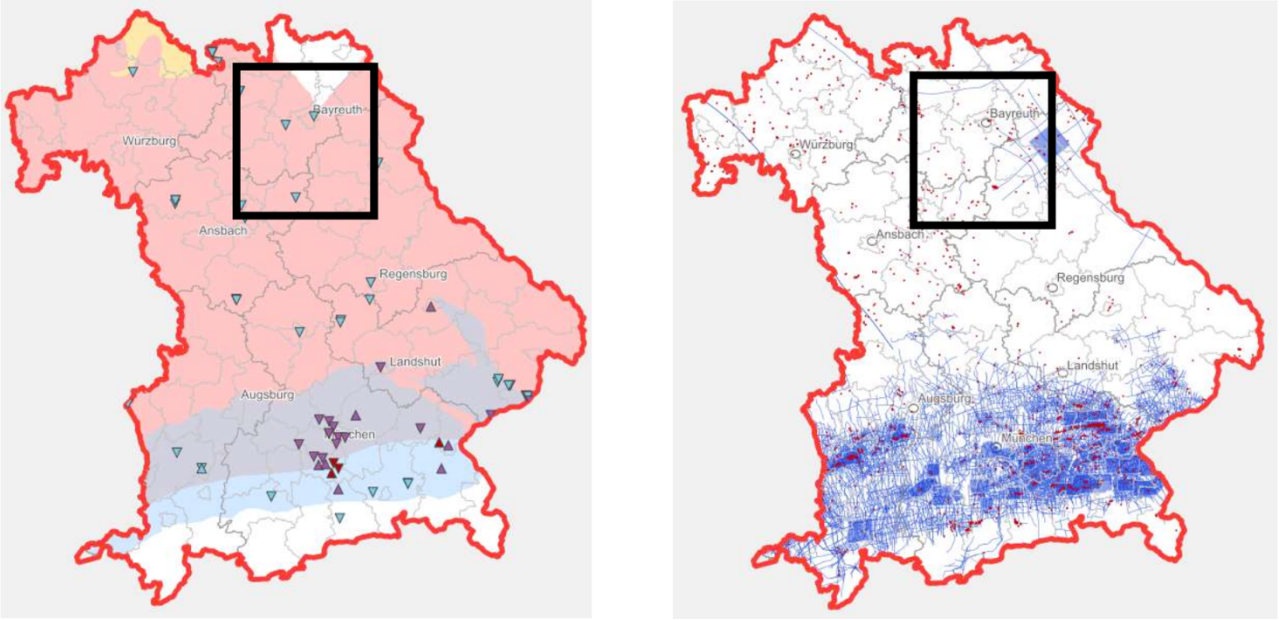

Figure 59: Left: Map showing the geothermal regions in Bavaria and current project installations (Schultz et al., 2013; GeotIS, 2014). Right: Map showing available subsurface data in Bavaria (Kühne et al., 2006; GeotIS, 2014). Black box shows the general research area.

features is vital for further exploration. There is limited research and few studies on the subsurface geology of Northern Bavaria and most fracture studies have been constrained to the south (Kühne et al., 2006). It is therefore useful to use the surface geology for interpretations and modelling of the subsurface. Outcrop analogues (such as quarries) can be used to measure and image fracture networks that are present in the geological formations at depth. This data can be integrated into subsurface models and simulations through upscaling workflows. The primary aims of this research is to understand and model the fractures present in Northern Bavaria and integrate data from both the surface and subsurface into large-scale fracture models of reservoirs and simulate geothermal fluid flow. Secondary aims of this research is to better understand the variability of fractures spatially and across scale and how network permeability is affected.

Methodology and Data Collection

Fracture data has been collected from several sites across Northern Bavaria primarily located along the Franconian Alb. Quarry sites include Kirchleus, Oberachtel and Gundelsheim. Data collection comprised of fracture measurements (azimuth and dip angle; aperture) and imaging fractured quarry sections (2D photogrammetry and 3D LiDAR and drone capture). 2D geometric analysis from the photogrammetry provide additional fracture network properties, such as fracture density/intensity, connectivity, and variations in fracture orientation. This process includes fingerprinting networks as spatial graphs. Fingerprints are a combination of block areas and shape factors used to uniquely define a fracture network. These are depicted as three bin area probability distributions plotted against shape factors that range from 0 to 1 approximating towards the circumscribing circular area. These 2D fracture networks can then be meshed (GMSH) for simulations. Using REDBACK (part of the MOOSE Framework), fluid flow simulations, can be undertaken to calculate the average fluid velocities within the 2D fracture network. These values can be used to determine the overall 2D permeability tensor of the network.

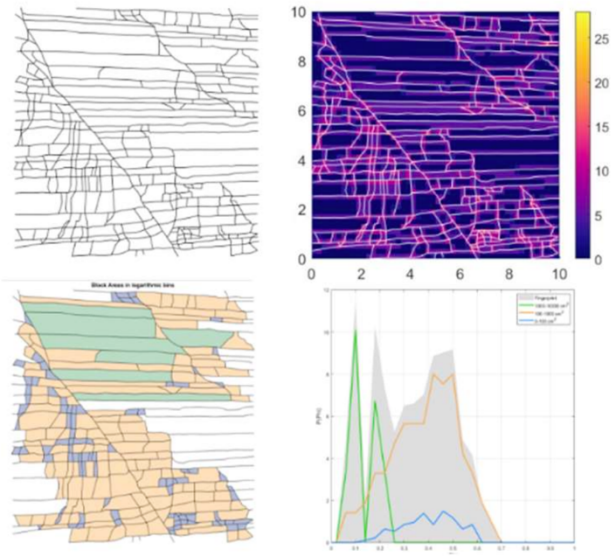

Figure 60: Clockwise from top left: Sampled fracture network from outcrop; P21 fracture intensity map of network; Fingerprint of fracture network; Distribution of shape sizes of the fingerprint.

Fractured Networks

The network fingerprints and geometrical analysis showed variation in the fracture networks across Northern Bavaria. Region 3 (Gundelsheim) showed higher shape factors in comparison with Regions 1 (Kirchleus) & 2 (Oberachtel). However, specific stress fields were identified affecting the different sites. Two compressional strike-slip regimes were observed in Regions 1 & 2 orientated ENE-WSW & WNW-ESE. Additionally, N-S & E-W orientated strike-slip regimes were observed in Region 3. The widespread distribution of these stress regimes throughout the regions aid in providing statistical data for driving large-scale fracture map network models.

Permeability Tensors

Using the outcrop sections, 2D permeability tensors can be obtained through numerical fluid flow simulations. 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. Investigation on the spatial and scalar influence of permeability tensors shows that larger sample sizes are less varied compared to smaller scales. This is important as we aim to find the scale at which the tensor

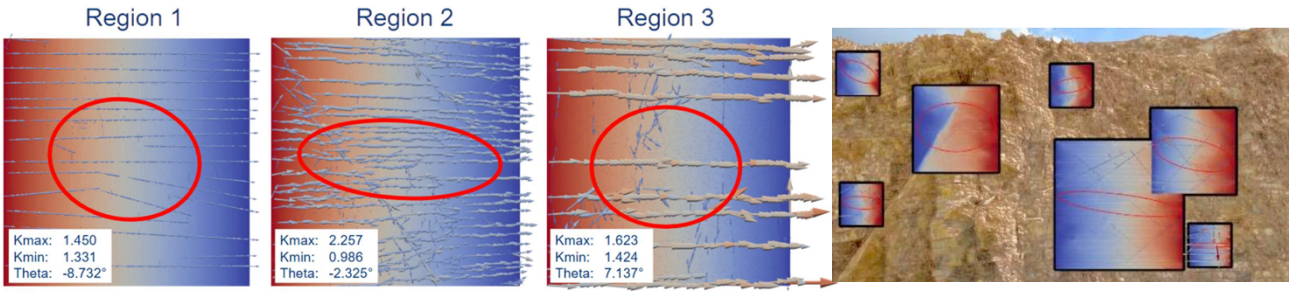

Figure 61: Left: 2D permeability tensor results from the different regions in Northern Bavaria. Reight: "D permeability tensor results from differing sample boxes. Scales vary from 2.5 m^2 to 7.5 m^2 and show increases variation in tensor orientiation and magnitude at lower scales.

becomes constant (i.e., little to zero variation) and as such the sample size that represents the network which is vital for generating upscaled fracture models.

Future Work and 3D Tensors

Planned work for 2024 includes extending the tensor simulation workflow to 3D through combining 2D tensors from three perpendicular sample sections. This will be tested through amphitheatre type quarry sections. Data from the different regions will also be integrated into a large-scale fracture model from which geothermal fluid flow simulations will be ran through. This will also be integrated with available subsurface data and compared with dynamic data from boreholes in the region to accurately test the simulations. Further collaborations are developing with FRASCAL projects P4 and aPC where fractures and natural fracturing mechanisms will be investigated using X-ray tomography and P2 on simulating small-scale mineralisation growth on fault planes observed in outcrop.

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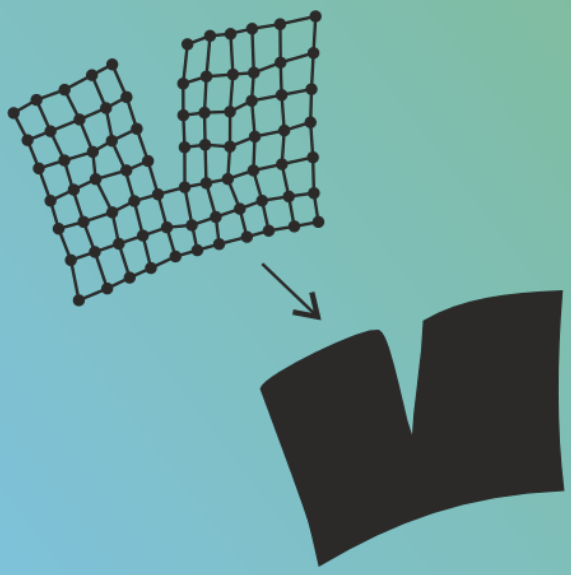

P13

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

Joscha Seutter

Prof. Dr. Manuel Friedrich

Applied Analysis

Department of Mathematics

P14: Atomistic-to-Continuum Convergence for quasi-static crack growth in brittle materials

Joscha Seutter, Prof. Dr. Manuel Friedrich

Ever since the work of Francfort and Marigo [5], a natural mathematical framework for theoretical studies of fracture behavior is given by so-called free discontinuity problems, where displacements and crack paths are determined from an energy minimization principle. 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 limit energy [3]. However, for the investigation of crack evolution in time, an understanding of the connection between atomistic and continuum systems is completely missing. The goal of our project is to fill this gap and provide a rigorous analysis of the relation between atomistic and continuum models in the setting of quasi-static evolution.

Our investigations this year build upon the previous work [6], which was published last year. There, we introduced an atomistic model for quasi-static crack growth that includes an irreversibility condition. More precisely, we considered systems of interacting particles arranged in an atomic lattice occupying the bounded reference domain of the material. The interactions were modelled by classical potentials from Molecular Mechanics, e.g., Lennard-Jones-type potentials. Here, our evolution is solely driven by time-dependent boundary condition, and we followed the principle of global energy minimization. The irreversibility constraint was implemented by a rather simplistic approach: If the distance between two atoms exceeds a certain threshold, the interaction is considered to be 'damaged' and the system should be affected at all future times. This was modelled by a 'maximum-memory-variable' that tracks the deformation history of each 'spring' in our system by taking the supremum over all past time steps. Such an approach resembles the use of a maximal-opening memory variables in cohesive continuum models for crack evolution (see e.g. in [4]). In [6], we were able to prove the existence of a continuous-in-time evolution that solves a delay differential equation, taking the complete history of the deformation into account.

While in [6], we kept the modelling framework rather general, we decided to make some additional assumptions for the atomistic-to-continuum analysis. More precisely, we adopt the setting from [3], which means we consider only nearest-neighbour energy contributions and restrict ourselves to a triangular atomistic grid. Moreover, we consider the case of only anti-plane strain, i.e., the material can only deform in vertical direction. A further underlying assumption of our approach is, that the boundary loading varies slowly in time compared to the elastic wave speed of the material. This means we neglect inertial effects and treat fracture as a rate-independent process.

At the beginning of the year, we were hoping to make use of the results from [7], where the authors address the issue of global stability for a unilateral minimality condition in a very general setting. However, we realized that our attempt to adapt and apply their techniques to our problem was not doable. Instead, we focused on setting up a suitable incremental minimization scheme as the starting point of our analysis. In contrast to the previous research, now not only the time step size δ, but also the inter-atomic distance ε varies. We hence needed to consider a simultaneous limit of the resulting sequence of minimizers as both of these parameters vanish. Following an idea from [3], 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. However, this turned out to be more involved than initially assumed. This is partly due to the fact, that changing from a bond-wise viewpoint to a triangle-wise perspective leads to uncertainties that need to be controlled in the limit. The major issue, however, is that there might be interaction-pairs that are considered 'broken' on the atomistic level but don't necessarily lead to a crack in the continuum limit. Therefore, one must distinguish these interactions also in the triangle-reformulation and to prove that these contributions actually don't play a role in the limit. To tackle this problem, we introduced a new notion of set-convergence which accounts for jump-sets with vanishing jump height separately and proved the necessary compactness and lower-semi continuity results. However, just recently we realized that his adjustment of sigma-p-convergence (see [2]) can be avoided by resorting to the original notion, only with integrability $p<4$.

A further difficulty was to figure out the correct scaling for the displacement field and the energy, that would lead to finite energy and meaningful limiting evolution. This means, we had to find the correct scaling regime, in which energy contributions that include a crack and the energy contribution of a purely elastic displacement, are of the same order. With this being accomplished, we were able to adjust the compactness proofs from [3] and show that there exists a limiting evolution. Our ultimate goal was then to prove that this limiting evolution satisfies 3 conditions: (1) A global stability at all times, (2) an irreversibility condition and (3) an energy balance law. For the global stability, we must prove that $t \to (u(t), K(t))$ is a minimum energy configuration at all times t. For this, we had to come up with a suitable adaptation of a jump-transfer argument from [1] to the atomistic setting, which turned out to be the most delicate part of the proof. While the irreversibility condition (2) is a direct consequence of the irreversibility incorporated in the discrete model, the proof of the energy balance demanded some extra work. For this, we followed the general strategy from [2], i.e., we made use of the global stability result, the lower semi-continuity of the energy and the regularity of the boundary conditions. Moreover, we also realized that for the limiting evolution $t \to (u(t), K(t))$, the notion of sigma-convergence from [7] indeed coincides with sigma-p-convergence.

Finally, despite some temporary setbacks, we were able to complete a full proof for the desired result, namely an atomistic-to-continuum convergence for quasi-static fracture evolution. From a mathematical point of view, the novelty of our approach is the investigation of irreversibility in an atomistic model and the application of a jump transfer argument to this setting. From a mechanical perspective we establish a rigorous link between particle-based fracture models and the realm of continuum mechanics, where we account for the irreversibility of crack growth. However, a valid understanding of the exact interplay between the modelling parameters on the atomistic scale, in particular the breakage threshold R, and the parameters of the resulting continuum model, is not provided by our analysis.

The paper is currently being finalised and planned to be submitted at the beginning of January 2024. One possible idea for subsequent research includes a non-local to local convergence study for a model from peridynamics that contains a memory variable and thus accounts for irreversibility.

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

All FRASCAL publications for 2023 are listed below with the corresponding abstract. They are assigned 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 **17 publications** in 2023. Datasets can be published on the zenodo platform - with or without an associated text-based publication. A total of **9 datasets** were published here in 2023.

P3 | Fracture in polymer composites: nano to meso

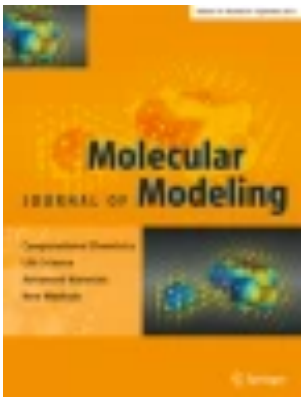
Konrad J. (PDR), Zahn D. (PA):

Interfaces in reinforced epoxy resins: from molecular scale understanding towards mechanical properties

In: Journal of Molecular Modeling (2023), Art-Nr.: 243

ISSN: 0948-5023

DOI: 10.1007/s00894-023-05654-w



“Context

We report on atomic level of detail analyses of polymer composite models featuring epoxy resin interfaces to silica, iron oxide, and cellulose layers. Using “reactive” molecular dynamics simulations to explore epoxy network formation, resin hardening is investigated in an unprejudiced manner. This allows the detailed characterization of salt-bridges and hydrogen bonds at the interfaces. Moreover, our sandwich-type composite systems are subjected to tensile testing along the interface normal. To elucidate the role of relaxation processes, we contrast (i) direct dissociation of the epoxy-metal oxide/cellulose contact layer, (ii) constant strain-rate molecular dynamics studies featuring (visco-)elastic deformation and bond rupture of the epoxy resin, and (iii) extrapolated relaxation dynamics mimicking quasi-static conditions. While the fracture mechanism is clearly identified as interface dissociation of the composite constituents, we still find damaging of the nearby polymer phase. The observed plastic deformation and local cavitation are rationalized from the comparably large stress required for the dissociation of salt-bridges, hydrogen bonds, and van der Waals contacts. Indeed, the delamination of the contact layers of epoxy resins with slabs of silica, magnetite, and cellulose call for a maximum stress of 33, 26, and 21 MPa, respectively, as compared to 84 MPa required for bulk epoxy yielding.

Methods

Molecular dynamics simulations using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code were augmented by a Monte Carlo–type procedure to probe epoxy bond formation (Macromolecules 53(22): 9698–9705). The underlying interaction models are split into conventional Generalized Amber Force Fields (GAFF) for non-reacting moieties and a recently developed reactive molecular mechanics potential enabling epoxy bond formation and cleavage (ACS Polymers Au 1(3): 165–174)”

P4 | Fragmentation in large scale DEM simulations

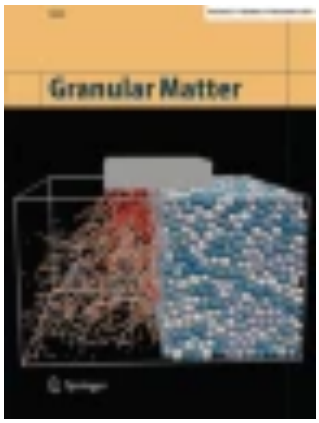
Santarossa A. (aPhD), D`Angelo O., Sack A., Pöschel T. (PA):

Effect of particle size on the suction mechanism in granular grippers

In: Granular Matter (2023), Art.-Nr.: 16

ISSN:

DOI: 10.1007/s10035-022-01306-7



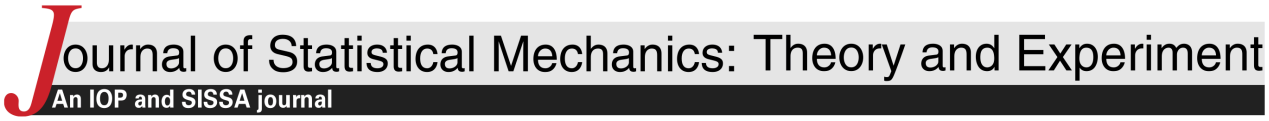
“Granular grippers are highly adaptable end-effectors that exploit the reversible jamming transition of granular materials to hold and manipulate objects. Their holding force comes from the combination of three mechanisms: frictional forces, geometrical constraints, and suction effects. In this work, we experimentally study the effect of particle size on the suction mechanism. Through X-ray computed tomography, we show that small particles (average diameter μ) achieve higher conformation around the object than larger particles (), thus allowing the formation of air-tight seals. When the gripper is pulled off, mimicking lifting of an object, vacuum pressure is generated in the sealed cavity at the interface gripper–object. If the particles used as filling material are too large, the gripper does not conform closely around the object, leaving gaps between the gripper’s membrane and the object. These gaps prevent the formation of sealed vacuum cavities between the object and the gripper and in turn hinder the suction mechanism from operating.”

P5 | Compressive failure in porous material

Ritter J. (PDR), Shegufta S. (PhD), Zaiser M. (PA):

Effects of disorder on deformation and failure of brittle porous materials

In: Journal of Statistical Mechanics-Theory and Experiment 2023 (2023), Art.Nr.: 053301
ISSN: 1742-5468
DOI: 10.1088/1742-5468/acccdf



“The mechanical behavior of porous materials depends strongly on porosity and pore geometry, but also on morphological parameters characterizing the spatial arrangement of pores. Here we use bond-based peridynamics to study effects of disorder on the deformation and failure behavior of brittle porous solids both in the quasi-static limit and in case of dynamic loading scenarios. We show that structural disorder, which has a strong influence on stiffness, strength and toughness in the quasi-static limit, becomes less relevant under dynamic loading conditions.”

P6 | Fracture in thermoplastics: discrete-to-continuum

Weber F. (PhD), Ries M. (PDR), Bauer C. (PhD), Wick C. (PA), Pfaller S. (PA):

On equilibrating non-periodic molecular dynamics samples for coupled particle-continuum simulations of amorphous polymers

In: Forces in Mechanics 10 (2023), Art.Nr.: 100159

ISSN: 2666-3597

DOI: 10.1016/j.finmec.2022.100159

URL: https://nbn-resolving.org/urn:nbn:de:bvb:29-opus4-200639

“In the context of fracture simulations of polymers, the molecular mechanisms in the vicinity of the crack tip are of particular interest. Nevertheless, to keep the computational cost to a minimum, a coarser resolution must be used in the remaining regions of the numerical sample. For the specific case of amorphous polymers, the Capriccio method bridges the gap between the length and time scales involved at the different levels of resolution by concurrently coupling molecular dynamics (MD) with the finite element method (FEM). Within the scope of the Capriccio approach, the coupling to the molecular MD region introduces non-periodic, so-called stochastic boundary conditions (SBC). In similarity to typical simulations under periodic boundary conditions (PBC), the SBC MD simulations must reach an equilibrium state before mechanical loads are exerted on the coupled systems. In this contribution, we hence extensively study the equilibration properties of non-periodic MD samples using the Capriccio method. From a thorough parameter study, which in general reveals only minor effects of the considered quantities on the equilibrium state, a best set of parameters follows. The behavior of an exemplary system equilibrated with this parameter set is further studied under uniaxial tension and we observe some peculiarities in view of creep and relaxation phenomena. This raises important questions to be addressed in the further development of the Capriccio method.”

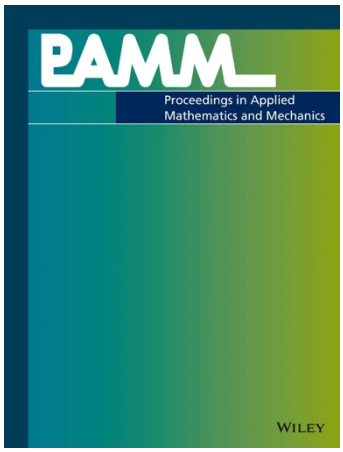
Torres Huamani D., Zhao W. (PDR), Pfaller S. (PA):

A particle-continuum coupling method for amorphous polymers with multiple particle-based domains

In: Proceedings in Applied Mathematics and Mechanics 22 (2023)

ISSN: 1617-7061

DOI: 10.1002/pamm.202200245



“This contribution presents a partitioned-domain particle-continuum coupling method for amorphous polymers with multiple particle-based domains. The coupling method treats the particle-based domains with molecular dynamics (MD) simulations and the continuum domain discretized by the Finite Element (FE) method. In the continuum domain, a viscoelastic-viscoplastic (VE-VP) constitutive model derived from MD simulation results of the polymer at molecular resolution is employed. The effects of the minimum distances between the domains, the distribution and the number of the MD domains as well as the strain rates are studied under uniaxial tension. This method is a precursor for multiscale simulations of polymer-based nanocomposites (PNC).”

Ries M. (PDR), Reber S., Steinmann, P. (PA) Pfaller S. (PA):

Extending a generic and fast coarse-grained molecular dynamics model to examine the mechanical behavior of grafted polymer nanocomposites

In: Forces in Mechanics 12 (2023)

ISSN: 2666-3597

DOI: 10.1016/j.finmec.2023.100207

URL: https://doi.org/10.1016/j.finmec.2023.100207

“Polymer nanocomposites are an important class of materials for engineering applications due to their high versatility and good mechanical properties combined with low density. By directly attaching the polymer chains to the nanofillers, the so-called grafting, a better load transfer between matrix and filler is achieved, and, in addition, a better dispersion of the fillers is obtained. Both result in enhanced mechanical properties. Since experimental investigations on the nanoscale are extremely challenging, complementary numerical studies are needed to unravel the mechanical behavior of polymer nanocomposites. To this end, molecular dynamics is ideally suited since it captures the microstructure, but is also numerically expensive. Therefore, this contribution presents a fast coarse-grained molecular dynamics model for the investigation of the mechanical behavior of grafted polymer nanocomposites. For this purpose, we extend an existing model by grafting bonds, which allows us to compare the effect of untreated and grafted fillers directly. In particular, we investigate the influence of filler content, grafting degree, and filler size on the stiffness and strength of the polymer (grafted) nanocomposites. We conclude that the grafting bonds have little effect on the stiffness, while the strength is significantly improved compared to the untreated fillers, which is in agreement with the literature. The presented molecular dynamics model for polymer grafted nanocomposites provides the basis for further investigations, particularly of the crucial matrix-filler interphase. In addition, this contribution translates molecular dynamics insights into mechanical properties, which bridges the gap to the engineering scale and thus represents a step towards exploiting the full potential of polymer (grafted) nanocomposites.”

Ries M. (PDR), Bauer C. (PhD), Weber F. (PhD), Steinmann, P. (PA) Pfaller S. (PA):

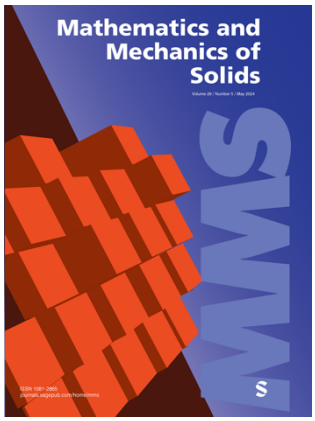
Characterization of the material behavior and identification of effective elastic moduli based on molecular dynamics simulations of coarse-grained silica

In: Mathematics and Mechanics of Solids (2023), Volume 28, Issue 5

ISSN: 1081-2865

DOI: 10.1177/10812865221108099

URL: https://doi.org/10.1177/10812865221108099



“The addition of fillers can significantly improve the mechanical behavior of polymers. The responsible mechanisms at the molecular level can be well assessed by particle-based simulation techniques, such as molecular dynamics. However, the high computational cost of these simulations prevents the study of macroscopic samples. Continuum-based approaches, particularly micromechanics, offer a more efficient alternative but require precise constitutive models for all constituents, which are usually unavailable at these small length scales. In this contribution, we derive a molecular-dynamics-informed constitutive law by employing a characterization strategy introduced in a previous publication. We choose silicon dioxide (silica) as an exemplary filler material used in polymer composites and perform uniaxial and shear deformation tests with molecular dynamics. The material exhibits elastoplastic behavior with a pronounced anisotropy. Based on the pseudo-experimental data, we calibrate an anisotropic elastic constitutive law and reproduce the material response for small strains accurately. The study validates the characterization strategy that facilitates the calibration of constitutive laws from molecular dynamics simulations. Furthermore, the obtained material model for coarse-grained silica forms the basis for future continuum-based investigations of polymer nanocomposites. In general, the presented transition from a fine-scale particle model to a coarse and computationally efficient continuum description adds to the body of knowledge of molecular science as well as the engineering community.”

Dötschel V., Pfaller S. (PA), Ries M. (PDR):

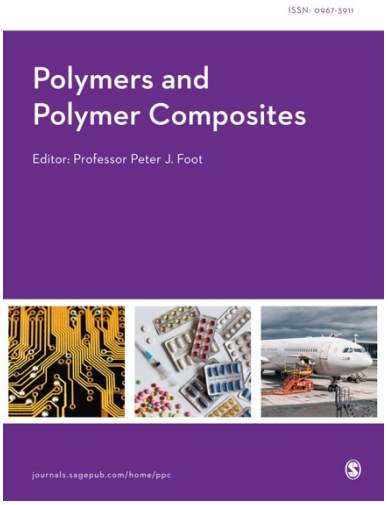
Studying the mechanical behavior of a generic thermoplastic by means of a fast coarse-grained molecular dynamics model

In: Polymers and Polymer Composites (2023)

ISSN: 0967-3911

DOI: 10.1177/09673911231208590

URL: https://doi.org/10.1177/09673911231208590



“Polymers play an emerging role in modern engineering applications due to their comparatively low cost, low density, and versatile manufacturing. The addition of nano-sized fillers further enhances the polymer’s properties but also induces a strong dependence on the resulting microstructure, particularly the matrix-filler interphase. Since an experimental characterization of this nano-sized interphase is extremely difficult, molecular dynamics (MD) simulations are used to study the effects at such small scales. However, MD’s high computational costs usually limit the scope of a mechanical characterization. Therefore, this study presents the methodology and tools to generate and analyze samples of an efficient generic thermoplastic model. In this first contribution, we focus on the neat polymer and introduce a versatile and numerically stable self-avoiding random walker with adjustable linearity of chain growth. Moreover, we verify our equilibration procedure by preparing samples in liquid and solid state which behave physically sound. Finally, we perform uniaxial tensile tests with a maximum strain of 10 % to evaluate the mechanical properties. In the liquid case, the polymer chains are sufficiently mobile, such that the tensile stresses fluctuate only around zero, while the solid exhibits an almost linear elastic regime followed by a nonlinear part. This contribution forms the basis for a thorough mechanical characterization of polymer nanocomposites which we will address in future studies. The methodology and tools introduced are not limited to our generic polymer, but applicable to many coarse-grained models.”

Seibert J., Pfaller S. (PA), Ries M. (PDR):

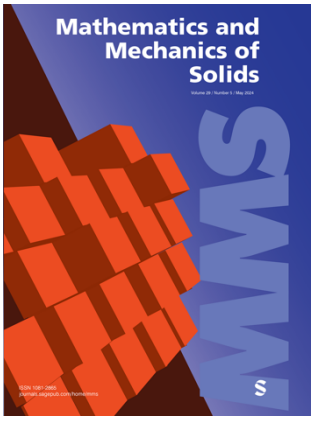
Investigation of the influence of nano-sized particles on the entanglement distribution if a generic polymer nanocomposite using molecular dynamics

In: Mathematics and Mechanics od Solids (2023), Volume 29, Issue 3

ISSN: 1081-2865

DOI: 10.1177/10812865231206547

URL: https://doi.org/10.1177/10812865231206547



“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.”

P8 | Fracture in polymer composites: meso to macro

Rohracker M. (PhD), Kumar P. (PDR), Mergheim J. (PA):

A comparative assessment of different adaptive spatial refinement strategies in phase-field fracture models for brittle fracture

In: Forces in Mechanics 10 (2023), S. 100157

ISSN: 2666-3597

DOI: 10.1016/j.finmec.2022.100157

URL: https://www.sciencedirect.com/science/article/pii/S2666359722000853

“For the smeared approximation of a discrete crack, phase-field fracture simulations of brittle materials require suitable finite element meshes in regions where crack propagation is expected to get an accurate resolution of the phase-field function. The straightforward option is to pre-refine the mesh in regions of the expected crack paths. However, this could lead to very computationally intensive simulations due to the high number of elements. Alternatively, adaptive spatial refinement of the finite element mesh is utilized based on appropriate error indicators to obtain the required accuracy in the areas of crack propagation. Different error indicators can be used: the most common one for phase-field fracture simulations is the threshold-based approach, in which elements are refined depending on the value of the phase-field function. Alternatively, the Kelly error indicator can be used as a criterion for spatial adaptivity. It considers the jumps in the gradients of the phase-field function between the elements. We additionally introduce here an error indicator based on configurational forces, that depend on the Eshelby stress tensor. For mode I loading in linear elastic fracture mechanics, the configurational forces have a close connection to the -Integral and the critical fracture energy, respectively. Therefore, a suitable norm of the configurational forces is introduced as an error indicator here. These three error indicators are introduced and compared to each other in terms of accuracy and efficiency by means of numerical examples for crack growth in the single edge notched shear test.”

Spannkraft L. (aPhD), Steinmann P. (PA), Mergheim J. (PA):

A generalized anisotropic damage interface model for finite strains

In: Journal of the Mechanics and Physics of Solids (2023), Art.-Nr.: 105255
DOI: 10.1016/j.jmps.2023.105255

“This contribution presents a generalized mechanical interface model for nonlinear kinematics. The interface’s response is non-coherent, i.e. allows for a jump in the deformations and for cohesive failure, and also includes interfacial (in)elasticity, which means that an additional membrane stiffness is introduced in the interface. This can result in a jump in the tractions across the interface and induces membrane stresses for in-plane stretches. An anisotropic cohesive law, i.e. dependent on the spatial interface normal, is formulated which induces for nonlinear kinematics additional shear-like stresses within the interface to satisfy the balance of angular momentum. The cohesive and membrane degradations are coupled via damage variables of the different deformation modes to account for an interaction. It is shown that the model is thermodynamically consistent, fulfills the balance equations and material frame indifference. An interface element with the generalized interface model is implemented as a user element in Abaqus. Numerical examples illustrate the influence of damage coupling on the mechanical response of adhesive layers.”

Kumar P. (PDR), Mergheim J. (PA):

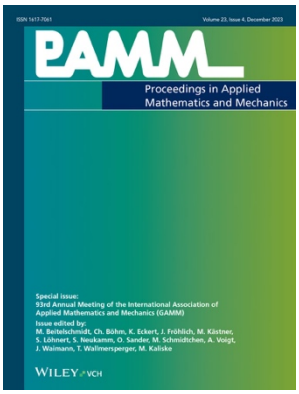
Computational modeling of fracture in polymer nanocomposites undergoing large deformations via the graded-interphase-enhanced phase-field fracture approach

In: Proceedings in Applied Mathematics and Mechanics (2023), Volume 23, Issue 4

ISSN: 1617-7061

DOI: 10.1002/pamm.202300247

URL: https://doi.org/10.1002/pamm.202300247



“The phenomenon of fracture in polymer composites, polymer nano-composites in particular, entails a multitude of intricate mechanisms including branching and merging of several cracks along with particle debonding and subsequent plastic void growth. This work involves an extension of the standard phase-field fracture approach by means of the graded interphase concept in order to facilitate the modeling of a wide-spectrum of fracture responses, which can be observed in experimental studies concerning the fracture behavior of polymer nano-composites. Herein, motivated by the microstructure morphology of polymer nano-composites, a continuous grading of the elastic and fracture properties is considered within a finite thickness interphase region around the filler particles. Appropriate tuning of the graded-interphase model parameters enables to capture a variety of fracture responses, including cohesive failure between the filler particle and the matrix, as demonstrated via the presented numerical examples, which focus on polymer nano-composites undergoing large deformations prior to fracture.”

P9 | Adaptive dynamic fracture simulation

Phansalkar D (PDR)., Jadhav D. (PhD), Weinberg K., Ortiz M. (MF), Leyendecker S. (PA):

Extension of the spatially adaptive phase-field model to various forms of fracture

In: Forces in Mechanics 10 (2023), Art.Nr.: 100161

ISSN: 2666-3597

DOI: 10.1016/j.finmec.2022.100161

“The phase field approach has proved to be efficient and has received ample attention amongst the available techniques to model fracture. However, high computational cost still imposes substantial difficulties in the phase-field simulation of fractures. This contribution is based on a recently proposed variational approach for spatial adaptivity in a phase-field model of fracture. The main idea is to consider the regularisation length as a space-dependent variable in the argument of the energy functional. We extend this now by implementing a strain energy split to ensure that only the tensile energy drives the crack propagation. The displacement, phase field, and optimal regularisation length are then determined locally by minimisation of the modified energy functional. Subsequently, the computed optimal regularisation length is used to refine the mesh size locally. The resultant solution procedure is implemented in the finite element library FEniCS. Numerical investigations on selected examples of different fracture modes demonstrate that the spatially adaptive phase field model has a comparable convergence rate, but a subjacent energy convergence curve resulting in significant computational savings. Moreover, it also computes the peak force more accurately illustrating its potential for usage in practical applications.”

P10 | Configurational Fracture | Surface Mechanics

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

Peridynamic modeling of nonlocal degrading interfaces in composites

In: Forces in Mechanics 10 (2023)
ISSN: 2666-3597
DOI: 10.1016/j.finmec.2022.100124

“When modeling composite materials at small scales, the consideration of nonlocal effects is fundamental. In addition, the overall response of matrix-inclusion composites is strongly affected by the behavior of the interface between inclusion and matrix. This can be attributed to a possible detachment of the constituents as well as the high interface-to-volume ratio especially for nano-sized inclusions. Peridynamics is a nonlocal theory that is suitable to introduce a length-scale into a continuum description and take into account nonlocal interactions. Complex interface models within a peridynamic framework are, however, rarely studied. The objective of this work is to present a modeling approach to nonlocal interfaces accounting for opening and degradation within the framework of continuum-kinematics-inspired peridynamics (CPD). The proposed method is employed to study nonlocal effects in matrix-inclusion composites with focus on the effect of nonlocal interfaces. In our approach, the nonlocal interface is modeled as a finite thickness interface, i.e. a region where the subdomains overlap. Within this region, the constituents are pair-wise connected through interface bonding forces that follow a characteristic force-opening law. In computational experiments, our model captures the influence of the strength and size of the interface as well as the inclusion volume fraction on the overall response. In particular, nonlocality manifests itself through a “smaller–stiffer” material behavior and an increased influence of the interface, which highlights the importance of an appropriate nonlocal interface model.”

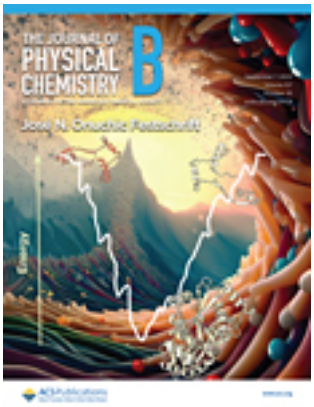
P12 | Quantum-to-continuum model of thermoset

Livraghi M., Pahi S. (aPhD), Piotr Nowakowski, Smith D., Wick C. R. (PA), Smith A.-S. (PA):

Block Chemistry for Accurate Modeling of Epoxy Resins

The Journal of Physical Chemistry B 2023, Art.Nr: 127

DOI: 10.1021/acs.jpcb.3c04724



“Accurate molecular modeling of the physical and chemical behavior of highly cross-linked epoxy resins at the atomistic scale is important for the design of new property-optimized materials. However, a systematic approach to parametrizing and characterizing these systems in molecular dynamics is missing. We therefore present a unified scheme to derive atomic charges for amine-based epoxy resins, in agreement with the AMBER force field, based on defining reactive fragments—blocks—building the network. The approach is applicable to all stages of curing from pure liquid to gelation to fully cured glass. We utilize this approach to study DGEBA/DDS epoxy systems, incorporating dynamic topology changes into atomistic molecular dynamics simulations of the curing reaction with 127,000 atoms. We study size effects in our simulations and predict the gel point utilizing a rigorous percolation theory to recover accurately the experimental data. Furthermore, we observe excellent agreement between the estimated and the experimentally determined glass transition temperatures as a function of curing rate. Finally, we demonstrate the quality of our model by the prediction of the elastic modulus based on uniaxial tensile tests. The presented scheme paves the way for a broadly consistent approach for modeling and characterizing all amine-based epoxy resins.”

P13 | Modelling of the development of deformation bands in porous rocks and their influence on the permeability evolution of reservoirs

Mathur B. (PhD), Prabhakaran R., Köhn D. (PA):

Evolving geometries, topologies, and apertures in fracture networks: Quantitative insights from lattice modeling

In: Forces in Mechanics 12 (2023), Art.Nr.: 100197

ISSN: 2666-3597

DOI: 10.1016/j.finmec.2023.100197

“Fracture networks are crucial in controlling rock mass permeability. Some of the important features of the fracture networks like the density, interconnectivity, spatial distribution, and fracture apertures determine the success of the subsurface operations. Fracture networks can be studied with analogue studies, physical experiments, and numerical modeling. In this study, we analyse the evolution of a two-dimensional fracture network under gravitational and shear loads using the lattice modeling capabilities of the microstructural modeling environment “Elle”. The simulation cases include varying gravitational loads and Young’s moduli of the formations. The topological progression of the modeled fracture network from isolated to interconnected nodes depicts a realistic network evolution process. The study shows that the rock stiffness exhibits a direct correlation with the number of fractures influencing the average aperture size of the network. A higher gravity load resulted in the development of a sparse fracture network. Stiffer rock models also showed an early onset of fracturing.”

Hutka GA., Cacace M., Hofmann H., Mathur B. (PhD), Zang A.:

Investigating seismicity rates with Coulomb failure stress models caused by pore pressure and thermal stress from operating a well doublet in a generic geothermal reservoir in the Netherlands

In: Netherlands Journal of Geosciences-Geologie En Mijnbouw 102 (2023), Art.Nr.: e8
ISSN: 0016-7746
DOI: 10.1017/njg.2023.7

“The utilisation of geothermal energy in the Netherlands is primarily focused on deep sedimentary aquifers, which are often intersected by major faults. Geothermal operations (i.e. fluid production and injection) may alter the effective stress state along these faults and trigger induced seismic events. Pore pressure perturbations have been generally considered the main driver of injection-induced seismicity. However, thermal stresses caused by temperature gradients between the re-injected cold fluid and the reservoir rock may also contribute to the triggering of earthquakes in geothermal reservoirs. While existing geothermal power plants operating in sandstone reservoirs did not produce any major induced seismicity, it is a matter of debate whether a reduction in the temperature of the re-injected fluid could increase the seismic hazard potential. In this study, we applied modified Gutenberg–Richter statistics based on frictional Coulomb stress variations implemented in a coupled thermo-hydro-mechanical model to estimate the seismic hazard caused by the operation of a geothermal doublet. We conducted a systematic parametric study to assess and rank the impact of different intrinsic (geological) and extrinsic (operational) parameters on the induced seismic hazard potential. We identified a competing mechanism between induced variations in pore pressure and thermal stress within the reservoir in controlling induced seismicity. We found that stress changes induced by pore pressure variations are the main cause of seismic hazard, although thermally induced stresses also contribute significantly. The results indicate that by optimising the operational parameters it is possible to increase production efficiency while maintaining a long-term control over the fluid injection-induced seismicity.”

3.1 Dataset publications on Zenodo

January 25

Esfandiary N.(PDR), Zaiser M. (PA) & Moretti P. (PA):

Statistical aspects of interface adhesion and detachment of hierarchically patterned structures

Journal of Statistical Mechanics: Theory and Experiment 023301

https://doi.org/10.1088/1742-5468/ac52a4

"We introduce a three dimensional model for interface failure of hierarchical materials adhering to heterogeneous substrates. We find that the hierarchical structure induces scale invariant detachment patterns, which in the limit of low interface disorder prevent interface failure by crack propagation ('detachment fronts'). In the opposite limit of high interface disorder, hierarchical patterns ensure enhanced work of failure as compared to reference non-hierarchical structures. While the study of hierarchical adhesion is motivated by examples of fibrous materials of biological interest, our results indicate that hierarchical patterns can be useful in engineering scenarios in view of tuning and optimizing adhesion properties."

March 10

Ritter J. (PDR), Shegufta, S. (PhD) & Zaiser, M. (PA):

Effects of disorder on deformation and failure of brittle porous materials

"The mechanical behavior of porous materials depends strongly on porosity and pore geometry, but also on morphological parameters characterizing the spatial arrangement of pores. Here we use bond-based peridynamics to study effects of disorder on the deformation and failure behavior of brittle porous solids both in the quasi-static limit and in case of dynamic loading scenarios. We show that structural disorder, which has a strong influence on stiffness, strength and toughness in the quasi-static limit, becomes less relevant under dynamic loading conditions."

March 23

Titelbach A. (aPhD), Papastavrou A., McBride A. & Steinmann P. (PA):

A novel micromorphic approach captures non-locality in continuum bone remodelling

"In continuum bone remodelling, bone is considered as continuous matter on the macroscale. Motivated by i) the underlying trabecular microstructure of bone resulting in size-dependence and ii) the non-local characteristics of osteocyte mechanosensing, a novel phenomenological approach based on a micromorphic formulation is proposed. Via illustrative benchmark examples, i.e. elementary unit cube, rod-shaped bone samples, and a 3D-femur sample, the novel approach is compared to the established local formulation, and the influence of the characteristic size of the microcontinuum and the coupling between macro- and microscale deformation is analysed. Taken together, the interaction between continuum points at the macroscale and their neighbourhood is effectively captured by the micromorphic formulation thus influencing the resulting distribution of nominal bone density at the macroscale."

May 11

Laubert L. (aPhD):

Establishing a framework for conducting comparative one- and multidimensional studies on the coupling of the finite element method with particle-based techniques

"This thesis presents a framework for conducting comparative one- and multidimensional studies on the coupling of the finite element (FE) method with particle-based techniques. The framework includes both a mathematical-mechanical description as well as a code-based implementation for its execution: A one-dimensional (1D) setup imitates the staggered scheme underlying coupled three-dimensional (3D) simulations, which are based on the Capriccio method, and allows for a fast detection of parameter influences on the system behavior. However, it lacks some features of typical 3D coupled systems, such as nonlinear material behavior and particle interactions beyond the next neighbors. The 1D model and its domains are set with equal dimensions corresponding to a reference 3D system along the studied dimension. Significant quantities such as the number of anchor points in the bridging domain and the stiffnesses of all domains are transformed by various mathematical approaches for achieving interdimensional comparability. The framework further includes a method for projecting mean displacements of molecular dynamics (MD) particles, anchor points, and FE nodes of the 3D reference system along the investigated spatial dimension to the corresponding coordinate axis of the 1D model. This technique proves to be highly suitable for comparing the displacement behavior of all domains of the 1D and 3D systems during deformation tests. To further demonstrate the capabilities of the developed framework, the convergence behavior, measuring how fast the coupled domains across the dimensions align, as well as the force responses in the FE domain of the 1D model are compared to those of the 3D reference model. The results show that the methods used for realizing interdimensional comparability result in a rather similar convergence behavior as well as force responses of the 1D and 3D model. Discrepancies observed between the 1D and 3D systems might be due to the limitations of the 1D system imitating the 3D model, including the present inelastic behavior of the 3D MD domain, and due to slight deliberately incorporated deviations in the domain stiffnesses inside the coupling region of the 1D and 3D models. Overall, the present work provides promising tools for conducting comparative studies on the coupling of FEM with particle-based techniques, although further research is required to assess how to eliminate or reduce the deviations."

Laubert L. (aPhD)

One dimensional framework imitating the Capriccio method for coupling the finite element method with particle-based techniques

"This readme contains explanations on the application of the source code for conducting 1D experiments as applied in the associated project thesis [1], published on the following dataset: https://doi.org/10.5281/zenodo.7924367"

Laubert L. (aPhD)

Framework for projecting displacements of particles and nodes resulting from Capriccio method coupled deformation simulations to a one dimensional representation

"This readme contains explanations on the application of the source code for projecting displacements of any particle or node described through Cartesian coordinates in a 3D space to one of the three axis as applied in the associated project thesis [1], published on the following dataset: https://doi.org/10.5281/zenodo.7924367"

Laubert L. (aPhD)

Deformation simulation results of Capriccio method coupled systems for conducting comparative one- and multidimensional studies on the coupling of the finite element method with particle-based techniques

"This readme explains the content and path structure of the results obtained from a deformation test conducted on slightly different MD-FE coupled systems performing the Capriccio method in a three-dimensional space within the associated project thesis [1], published on the following dataset: https://doi.org/10.5281/zenodo.7924367Furthermore, input files and parameters as well as potential tables required to reproduce the obtained data are provided as well. The molecular dynamics (MD) part is executed in LAMMPS and the finite element (FE) method part by a MATLAB script as described in Section 4.1 of [1]. The whole setup of the 3D models is elaborated in Section 4.2 of [1]. A discussion of some results is given in Chapter 6 of [1] in the context of assessing their comparability with the corresponding 1D model."

August 1

Mathur B. (PhD), Köhn D. (PA) & Prabhakaran R.:

Evolving geometries, topologies, and apertures in fracture networks: Quantitative insights from lattice modelling

"Fracture networks are crucial in controlling rock mass permeability. Some of the important features of the fracture networks like the density, interconnectivity, spatial distribution, and fracture apertures determine the success of the subsurface operations. Fracture networks can be studied with analogue studies, physical experiments, and numerical modeling. In this study, we analyse the evolution of a two-dimensional fracture network under gravitational and shear loads using the lattice modeling capabilities of the microstructural modeling environment "Elle". The simulation cases include varying gravitational loads and Young's moduli of the formations. The topological progression of the modeled fracture network from isolated to interconnected nodes depicts a realistic network evolution process. The study shows that the rock stiffness exhibits a direct correlation with the number of fractures influencing the average aperture size of the network. A higher gravity load resulted in the development of a sparse fracture network. Stiffer rock models also showed an early onset of fracturing."

September 8

Ries M., Reber S., Steinmann P. & Pfaller S.:

Extending a generic and fast-coarse-grained molecular dynamics model to examine the mechanical behavior of grafted polymer nanocomposites: data set

“Polymer nanocomposites are an important class of materials for engineering applications due to their high versatility and good mechanical properties combined with low density. By directly attaching the polymer chains to the nanofillers, the so-called grafting, a better load transfer between matrix and filler is achieved, and, in addition, a better dispersion of the fillers is obtained. Both result in enhanced mechanical properties. Since experimental investigations on the nanoscale are extremely challenging, complementary numerical studies are needed to unravel the mechanical behavior of polymer nanocomposites. To this end, molecular dynamics is ideally suited since it captures the microstructure, but is also numerically expensive. Therefore, this contribution presents a fast coarse-grained molecular dynamics model for the investigation of the mechanical behavior of grafted polymer nanocomposites. For this purpose, we extend an existing model by grafting bonds, which allows us to compare the effect of untreated and grafted fillers directly. In particular, we investigate the influence of filler content, grafting degree, and filler size on the stiffness and strength of the polymer (grafted) nanocomposites. We conclude that the grafting bonds have little effect on the stiffness, while the strength is significantly improved compared to the untreated fillers, which is in agreement with the literature. The presented molecular dynamics model for polymer grafted nanocomposites provides the basis for further investigations, particularly of the crucial matrix-filler interphase. In addition, this contribution translates molecular dynamics insights into mechanical properties, which bridges the gap to the engineering scale and thus represents a step towards exploiting the full potential of polymer (grafted) nanocom”

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

The following is a tabular list of academic activities that took place in 2023 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
13.03.2023 15.03.2023	MGMS 2023	Erlangen	**Talk:** Accelerating plane-wave based ab initio molecular dynamics by optimization of Fast-Fourier transforms for modern HPC architectures
26.03.2023 31.03.2023	DPG 2023	Dresden	**Poster:** Accelerating plane-wave-based ab initio molecular dynamics by optimization of Fast-Fourier Transforms for modern HPC architectures
08.08.2023 10.08.2023	SFB 953 Symposium	Erlangen	**Poster:** Characterization of Novel Carbon-Rich Architectures by First-Principles Calculations

P3 | Pascal Franck

Name	Supported researcher	Course | field of study	Tasks relating to FRASCAL
Bakhmetau, Sviataslau	Pascal Frank, P3	Molecular Science	MD simulation of polymer composite using coarse-grained models

P4 | Utku Canbolat

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
03.02.2023	CBI Symposium	Erlangen	**Poster:** Plastic deformation, wear and heat transfer in fracture of complex-shaped particles
17.09.2023 21.09.2023	DEM9	Erlangen	**Talk:** Image-informed fracture model for complex-shaped particles in discrete element simulations

P4 | Angel Santarossa

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
17.09.2023 21.09.2923	DEM9	Erlangen	**Poster:** Tomographic imaging-based finite element analysis of 3D mixed-mode cracks

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
23.10.2023 26.10.2023	CFRAC	Prague	Participation and organisation of a MS titled "Connecting scales and disciplines to model fracture"

from | to	Name of school	Location
23.10.2023 26.10.2023	Peridynamic models for material degradation: from fracture/fragmentation to corrosion; from models to computer codes	Udine, Italy

P6 | Felix Weber

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
30.05.2023 02.06.2023	93rd GAMM Annual Meeting	Dresden	**Talk:** Fracture simulations of polymers: coupling molecular & continuum models
19.06.2023 21.06.2023	7th ECCOMAS YIC	Porto	**Talk:** Fracture in polymers: discrete-to-continuum coupling

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

Supervised Bachelor Student	Topic	Supervisor | Date
Adams, Annina	Advancing the Capriccio method: parameter study with respect to load application	Felix Weber 14 Jul 23

P6 | Wuyang Zhao

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
30.05.2023 02.06.2023	93rd GAMM Annual Meeting	Dresden	**Talk:** Multiscale modelling of fracture behavior of glassy polymers across molecular and continuum scales
05.09.2023 07.09.2023	COMPLAS	Barcelona	**Talk:** Fracture of glassy thermoplastics based on multiscale simulations across molecular and continuum scales

Collaborating Institution	Research topic	Researchers involved
Theoretical Physical Chemistry Group at TU Darmstadt	Coupled MD-FE fracture simulations of amorphous polymers	Yash Jain, M.Sc Prof. Dr. Florian Müller-Plathe

Supervised Master Student	Topic	Supervisor | Date

Torres Huamani, David	Gekoppelte MD-FE Simulation für polymerbasierte Nanokomposite mit mehreren MD-Gebieten	Wuyang Zhao 29 Mar 23

Submitted publications

W. Zhao, R. Xiao, P. Steinmann, and S. Pfaller. "Time-temperature correlations of amorphous thermoplastics at large strains based on molecular dynamics simulations," submitted to Mechanics of Materials, 2023.

P6 | Maximilian Ries

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
19.06.2023 21.06.2023	YIC 2023	Porto	**Talk:** A coarse-grained molecular dynamics model to analyze fracture in polymer nanocomposites
10.10.2023 13.10.2023	CMCS	Eindhoven	**Poster:** Studying the mechanical performance of polymer nanocomposites with molecular dynamics-informed continuum models
16.11.2023 17.11.2023	MOANSI Annual Meeting	Stuttgart	Participation only

Submitted publications

M. Ries, L. Laubert, P. Steinmann and S. Pfaller, "Impact of the molar mass distribution on the mechanical behavior of polymer nanocomposites: A generic, coarse-grained molecular dynamics study," 2023.

P6 | Lukas Laubert

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
29.05.2023 02.06.2023	93rd GAMM Annual Meeting	Dresden	Participation only

Collaborating Institution	Research topic	Researchers involved
Institut de Chimie et des Matèriaux Paris-Est (ICMPE) at the Université Paris-Est Créteil Val de Marne (UPEC)	BIO ART	Agustín Ríos De Anda Stephanie Chedid
Laboratoire Modélisation et Simulation Multi-Échelle (MSME) at the Univerité Gustave Eiffel (UGE)	BIO ART	Fabrice Detrez Moussa Lamamra
Department of Polymer Engineering (PE) at the Universität Bayreuth	BIO ART	Martin Demleitner Denise Schweser

Submitted publications

Ries M., Laubert L., Steinmann P., Pfaller S., "Impact of the Molar Mass Distribution on the Mechanical behavior of Polymer Nanocomposites: a Generic, Coarse-grained Molecular Dynamics Study", submitted to European Journal of Mechanics / A Solids.

Research stay from | to	Institute visited	Local supervisor	Research activities performed and skills acquired during stay
19.07.2023 22.07.2023	BIO ART Kick-off Meeting		BIO ART: project planning

P7 | Christian Greff

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
20.06.2023 23.06.2023	CFRAC	Prague	**Talk:** Hierarchical microstructure controls interface failure patterns

P8 | Paras Kumar

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
30.05.2023 02.06.2023	GAMM 2023	Dresden	**Talk:** Phase-field modelling of fracture on polymer nano-composites via graded interphases
11.06.2023 16.06.2023	ICF 15	Atlanta	**Talk:** A versatile phase-field fracture model for polymer composites: capturing their multi-faceted fracture behavior via graded interphases

from | to	Name of school	Location
17.07.2023 21.07.2023	CISM Advanced Course on variational methods for complex materials and processes	Udine, Italy
31.07.2023 04.08.2023	8th FAMM Juniors summer school on scientific machine learning	Hannover, Germany

Supervised Student	Topic	Supervisor | Date
Rodschei, Maxim	Computational modeling of viscoelastic polymer nano-composites	Paras Kumar 03 Mar 23
Mut, Ece (CE-TSE)	Development of a spline function based finite element solver for plates	Paras Kumar 18 Sep 23

Student assistant	Course/ field fo study	Funded Member of FRASCAL (from | to)	Tasks relating to FRASCAL
Prateek, Prateek	Computational Engineering	15.08.22 15.02.23	Support on conducting enhanced computational homogenization-based simulations involving large sized systems in 3D and generation of RVEs with elliptical particles.

P8 | Maurice Rohracker

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
06.02.2023 07.02.2023	8th GAMM Workshop on phase-field modeling	Zurich	**Talk:** Comparison of adaptive spatial refinement in phase-field fracture simulations of brittle materials
18.04.2023	DGM Meeting, Expert Comitee materials modelling, simulation and data	Aachen	**Talk:** Comparative assessment of adaptive spatial refinement in 3D phase-field fracture simulations
21.07.2023 23.07.2023	7th CFRAC	Prague	**Talk:** Comparison of irreversibility strategies in phase-field fracture simulations

Supervised Master Student	Topic	Supervisor | Date
Maxim Rodschei	Phase-field modelling of fracture in rate dependent materials	Julia Mergheim Maurice Rohracker Dez 2023

P8 | Lucie Spannraft

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
10.10.2023 13.10.2023	CMCS 2023	Eindhoven	**Poster:** Mechanics of generalized interfaces and grain boundaries

Collaborating Institution	Research topic	Researchers involved
Chalmers University of Technology, Gothenburg, Sweden	Grain boundary mechanics	Prof. Kenneth Runesson Prof. Frederik Larsson

P9 | Deepak Jadhav

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
06.02.2023 07.02.2023	8th GAMM Workshop on phase-field modeling	Zurich	**Talk:** Investigation of dofferent forms of fracture using a spatially adaptive phase-field model

P10 | Marie Laurien

from | to	Name of school	Location
23.10.2023 26.10.2023	Peridynamic models for material degradation: from fracture/fragmentation to corrosion; from models to computer codes	Udine, Italy
Submitted publications		
M. Laurien, A. Javili und P. Steinmann, „Nonlocal interfaces accounting for progressive damage within continuum-kinematics-inspired peridynamics," submitted to International Journal of Solids and Structures, 2023		

P10 | Anna Titlbach

from | to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
03.05.2023 05.05.2023	CMBBE Conference	Paris	**Talk:** Considering nonlocality in continuum bone remodelling – a micromorphic approach
10.09.2023 13.09.2023	GACM Colloquium	Vienna	**Invited Talk:** A novel micromorph approach capturing non-local cone remodelling: analysis of bone specimens and loading scenarios
20.09.2023 22.09.2023	ICCB Conference	Vienna	**Invited Talk:** Exploring bone remodelling via a novel micromorphic approach
from | to	**Name of school**		**Location**
23.10.2023 26.10.2023	Peridynamic models for material degradation: from fracture/fragmentation to corrosion; from models to computer codes		Udine, Italy

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 FRASCAL schools, soft skills trainings, and seminars. Furthermore, all presentations of student theses supervised by FRASCAL doctoral researchers take place within the framework of the so-called student seminar series of FRASCAL (S^3 FRASCAL). Social events accompanying qualification days encourage close exchange between the doctoral researchers and the mentoring teams.

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.

Mini Lectures 2023

	Date	Title	Lecturer
01	10 February 2023	Introduction to geometric time evolution integration (IGETI)	S. Leyendecker
02	17 February 2023	Introduction to material modelling	J. Mergheim
03	05 May 2023	Introduction to mathematical optimization	M. Stingl
04	14 July 2023	Introduction to numerics	G. Capobianco R. T. Sato de Almargo
05	21 July 2023	Introduction to density functional theory	B. Meyer
06	10 November 2023	ML-Introduction: phase-field fracture modelling & FE simulation	T. Wick
07	24 November 2023	Introduction to peridynamics	A. J. Javili

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

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.

5 special seminars were held in 2023. The scientists Dr. Ignatios Athanasiadis (School of Engineering, University of Glasgow), PD Dr. Sebastian Pfaller & Dr. Maximilian Ries (FAU), Prof. Dr. Lasse Laurson (Tampere University of applied Sciences, Finland) and Dr. Maxime Vassaux (Institute of Physics, Rennes, France) could be engaged for the special seminar days.

Special seminars 2023

	Date	Title	Lecturer
01	12 May 2023	Computational framework for crack propagation	Dr. Ignatios Athanasiadis (School of Engineering, University of Glasgow)
02	26 May 2023	Generating scientific diagrams with pgfplots	PD Dr.-Ing. Habil Sebastian Pfaller & Dr. Maximilian Ries (FAU)
03	13 June 2023	Modelling planar crack front propagation	Prof. Dr. Lasse Laurson (Tampere University of applied Sciences, Finland)
04	15 September 2023	Mini-Tutorial high performance computing (HPC)	Erlangen National High Performance Computing Centre
05	06 October 2023	Probing mechanical properties	Dr. Maxime Vassaux (Institute of Physics, Rennes, France)

FRASCAL Soft Skills Trainings

In 2023 one soft skills seminar was held. Dr. Iris Wangermann focussed on the topic “unconscious bias”. This concerned questions such as “how do unconscious biases arise (focus on gender equality)” and shed light on the neuroscientific/psychological backround.

Further presented aspects were:

- Understand the impact of biases on decisions
- Reflecting on one`s own blind spots in everyday work – as a person affected and a person causing them
- Developing a more responsible approach
- Awareness instead of guilt and shame
- Practising self- reflection
- Accept that imperfection ist poart of reality
- Practising empathic listening with genuine interest

Text & pictures: Ann-Sophie Herzner

How many unconscious biases prevail in academia? Too many, according to the inclusive leadership expert, Dr. Iris Wangermann. Female-authored papers tend to be cited less frequently than male-authored papers. Further, the ease with which one's family name is pronounced can have an impact on whether one is promoted or not.

It is an integral part of the FRASCAL curriculum to create awareness of decision-making processes regarding gender, equality and diversity. In this context, PhD students annually invite an expert on this topic to gain further knowledge in this area. On April 14th, the PhD students welcomed Dr. Iris Wangermann, who visited the Graduate College to hold a workshop on our unconscious biases. Dr. Iris Wangermann is an expert in inclusive leadership, intercultural teambuilding, and consciousness. During the workshop „Unconscious bias: how our brain tricks us" participants studied the neuroscientific and psychological basics of unconscious biases. Through personal examples and experiences, participants discovered their blind spots.

Dr. Wangermann encouraged participants to accept that imperfection is part of our reality and that we need to practice empathic listening, showing genuine interest, in order to have so called „aha" experiences. The workshop included many practical exercises, such as self-reflection and mindfulness practices, storytelling and listening, as well as judging a picture of a woman at different phases of her life.

Through the experiences gained during the workshop, it became quite apparent to the participating students that unconscious biases are deeply ingrained in our psyche. However, by understanding how these biases arise and affect our behaviour, we can work towards mitigating their impact. Overall, the workshop provided a valuable learning experience for participants and an opportunity to make new connections with colleagues.

Feedback from participants was positive, with many describing the workshop as enriching and intense. There were numerous lively debates amongst the future inclusive leaders.

FRASCAL Seminars

In each lecture period (except those with a FRASCAL retreat), 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.

On Friday, 28 April 2023 the FRASCAL seminar took place at the LTM, where the doctoral researchers and associated doctoral researchers of the second cohort had the opportunity to present the research results.

PROGRAMME

9:00 – 9:10 WELCOME and INTRODUCTION
Paul Steinmann

9:10 – 9:40 Utku Canbolat (P4)
Fragmentation in Large Scale Discrete Element Simulations for Complex-Shaped Particles

9:40 – 10:10 Pascal Frank (P3)
MD-Simulation of Polysiloxanes

10:10 – 10:40 Deepak Jadhav (P9)
Numerical Illustration of Γ-Convergence for Variational Integrators

10:40 – 11:00 COFFEE BREAK

11:00 – 11:30 Maurice Rohracker (P8)
Comparative Assessment of Adaptive Spatial Refinement Strategies in 3D Phase-Field Fracture Simulations

11:30 – 12:00 Shucheta Shegufta (P5)
Effect of Disorder on Failure of Porous Materials

12:00 – 12:30 Felix Weber (P6)
Coarse-Grained Molecular Dynamics Simulations of Polystyrene: Considering Bond Scission

12:30 – 13:40 LUNCH BREAK

13:40 – 14:10 Sampanna Pahi (aPO)
Modelling Mechanochemical Bond Scission of Epoxy Resins under Stress

14:10 – 14:40 Lucie Spannraft (aPJ)
Generalized Interfaces to Model Structural and Soft Adhesives and their Failure

14:40 – 15:10 Julian Konrad (P3/start up)
Multi-Scale Modelling of Epoxy Resin and Composites: from Curing to Fracture

15:10 – 15:40 PERIPATETIC CLOSING DISCUSSION

FRASCAL Retreat

The 3rd RTG Retreat took place from 17th to 18th of November 2023 at Kloster Banz. Each doctoral researcher must participate, focusing on the internal evaluation of FRASCAL's scientific progress. For this purpose, the doctoral researchers and associated doctoral researchers report on their scientific activities to all members of FRASCAL, which enables further assessment of the scientific progress of the doctoral projects. The scientific dialogue was rounded off by workshops, reports on career paths and social activities for informal get-togethers.

Text: Ann-Sophie Herzner | Pictures: Nicole Güthlein

In a brief welcome speech the two spokespersons, Prof. Dr. Steinmann and Prof. Dr. Stingl, set the tone for the upcoming two days. Shortly after, each doctoral researcher presented research findings and updates. Late in the afternoon, members of the FRASCAL External Advisory Board offered practical advice to our doctoral researchers, sharing valuable insights into their own CVs. However, even scientists need

after so many stimulating thoughts a break. Upon returning from a „Scientific Hiking Tour" to the monastery, dinner and a team-building activities awaited the participants.

Day two had as plenty to offer as day 1, beginning with the remaining presentations of doctoral researchers and ending by various special activities. For instance, Lukas Laubert shared his experiences from the French-German Collaboration BIO ART. The afternoon session featured a workshop on ‚Research Data Management (RDM), by PD Dr. Sebastian Pfaller and concluded with a so called „Poster Blitz." In other words, each researcher had precisely one minute to present their poster, providing a visual overview of their dissertation in an entertaining manner.

After all, the third FRASCAL Retreat at Kloster Banz proved again as a milestone of each cohort. Interactions among researchers from diverse backgrounds not only encouraged collaboration but also incubated new research ideas.

PROGRAMME

Friday, November 17

09:00 - 09:20 CHECK-IN & COFFEE

09:20 - 09:30 Welcome & Introduction
Paul Steinmann and Michael Stingl

09:30 - 09:50 Christian Ritterhoff (P1)
Fracture of polar perovskite oxides

09:50 - 10:10 Pascal Frank (P3)
MD-Simulation of Polysiloxanes

10:10 - 10:30 Utku Canbolat (P4)
Image-Informed Fracture Model for Complex-Shaped Particles in Discrete Element Simulations

10:30 - 11:00 COFFEE BREAK

11:00 - 11:20 Shucheta Shegufta (P5)
Failure of Highly Porous Material

11:20 - 11:40 Felix Weber (P6)
Multiscale Fracture Simulations of Silica Glass

11:40 - 12:00 Christian Greff (P7)
Fracture Surface Geometry in 3D Hierarchical Material Adhesion

12:00 - 13:00 LUNCH BREAK

13:00 - 15:30 Walk & Talk
Scientific Hiking Tour

15:30 - 16:00 COFFEE BREAK

15:30 - 16:00 COFFEE BREAK

16:00 - 16:20 Maurice Rohracker (P8)
Influence of the Irreversibility Strategy in Phase-Field Fracture Simulations

16:20 - 16:40 Deepak Jadhav (P9)
Asynchronous Variational Integrators for Elastodynamics and for a Phase Field Model of Dynamic Fracture

16:40 - 17:30 CVs and experiences of FRASCAL External Advisory Board Member

17:30 - 18:30 DINNER

19:00 Team Building Activities

Saturday, November 18

07:30 - 09:00 BREAKFAST

09:00 - 09:20 Marie Laurien (P10)
Peridynamic Fracture Mechanics

09:20 - 09:40 Lennart Igel (P11)
Stochastic Optimization with High Dimensional Uncertainties with Application to Fracture Control

09:40 - 10:00 Lukas Laubert (P6)
French-German Collaboration BIO ART

10:00 - 10:30 COFFEE BREAK

10:30 - 10:50 György Hantal (P12)
Coupling molecular dynamics with continuum mechanics for thermoset polymers

10:50 - 11:10 Joscha Seutter (P14)
Variational Models for Brittle Fracture and Crack Growth

11:10 - 12:00 Sebastian Pfaller
Research Data Management (RDM)

12:00 - 13:00 LUNCH BREAK

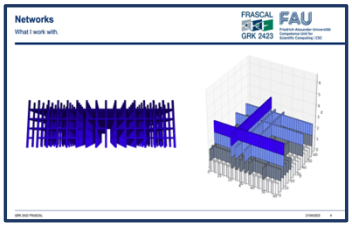
13:00 - 13:20 Miguel Ángel Moreno-Mateos
Soft Fracture: Electro-Magnetical Modulation & Configurational Mechanics

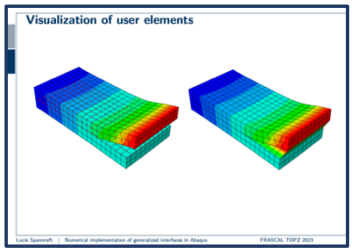
13:20 - 13:40 Poster Blitz
Associated projects and Start-Ups

13:40 - 15:00 Poster Session with Coffee

15:00 - 15:10 CLOSING

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.

Language Coaching in Scientific English

Paul Gahman and Paul Hobbs-Koch from the "FAU Language Centre", professional English language coaches were also in 2023 available for the FRASCAL participants to train oral presentations, to proofread English publications, and to give English classes in each lecture period. Attendance of English classes is optional. The individual learning units were structured as following:

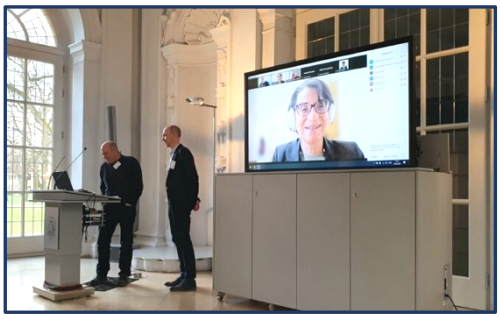
Language Coaching 2023

	Date	Title
01	27 April 2023	Expository Work with Subject-Specific Terminology
02	4 May 2023	Online Writing and Research Tools
03	11 May 2023	Linking and Assimilating
04	25 May 2023	Shadowing
05	15 June 2023	Ensuring Structural Development with Thematic Progression
06	29 June 2023	Discourse Critique for Language and Content Accuracy
07	13 July 2023	Spontaneous Speech trough Concept Explanation
08	23 October 2023	Spoken Mediation
09	06 November 2023	Mediation across Registers

2nd FRASCAL Symposium

Text & pictures: Ann-Sophie Herzner

On 15 March 2023. The 2nd FRASCAL Symposium was held at the venerable Orangerie of Erlangen. The symposium aimed to provide a platform for the FRASCAL principal advisors and prospective Mercator Fellows to share their insights on the fracture problem from a higher-level perspective. As expected, the event was well-attended by colleagues and young researchers from various institutions who had an interest in the fracture problem.



Throughout the day, seven guest speakers delivered talks that provided valuable insights into the fracture problem. Laura De Lorenzis from ETH Zurich opened the stage with her talk on „The role of multi-physics and multi-scale approaches in fracture mechanics“. Manuel Friedrich from FAU followed with a talk on „Modelling of the fracture process using cohesive zone models“. Paolo Moretti from FAU reported thereupon on „Fracture of thin films and interfaces“. Christian Wick, also from FAU, shared his insights on „Microstructure and fracture of advanced materials“, while Erik Bitzek from MPIE Düsseldorf presented „Atomistic simulations of fracture: From continuum to discrete models“. Daniel Koehn from FAU dived into „Machine learning approaches for fracture prediction“, and Anna Pandolfi from Politecnico di Milano wrapped up the symposium with a talk on „Fracture of biological and soft materials“. Each talk was followed by a stimulating discussion among the attendees, which helped to deepen their understanding of the fracture problem. The symposium concluded at 4:15 p.m., with closing remarks from the organizers. In summary, the 2nd FRASCAL Symposium provided a valuable opportunity for principal advisors, doctoral researchers and prospective Mercator fellows to share their insights on the fracture problem. Overall, it was a successful event that contributed to the advancement of knowledge in the field of fracture mechanics.

At the end of the event, the doctoral researchers honored Andrea Dakkouri-Baldauf. Recently, we had learned with regret that our FRASCAL coordinator would soon be leaving the team. To express our appreciation for her leadership and support, our team prepared a small gift for her. We wish Andrea all the best as she moves forward in her career!

4.2 Visiting researcher programme

Scientists from a wide range of countries travelled to FAU for seminars on various key topics. They were also in dialogue with various scientists from FAU beyond the days of the seminars.

Visiting researchers 2023

Date	Guest	Topic
12 May 2023	Dr. Ignatios Athanasiadis | School of Engineering, University of Glasgow	**Special Seminar:** Computational framework for crack propagation
13 June 2023	Prof. Lasse Laurson | Tampere University of Applied Sciences, Finland	**Special Seminar:** Modelling planar crack front propagation
06 October 2023	Dr. Maxime Vassaux | Institute of Physics, Rennes, France	**Special Seminar:** Probing mechanical properties with chemical specificity using molecular and multiscale simulations

Text & picture: Sebastian Pfaller

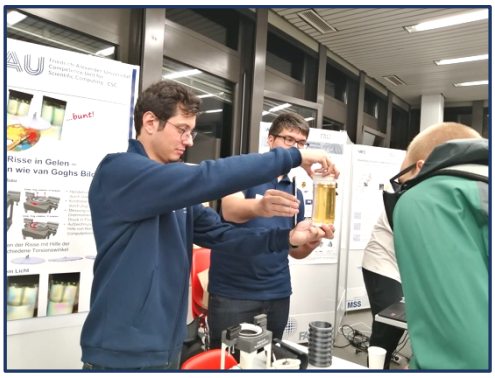
From October 2 to 7, Dr. Maxime Vassaux from France visited the Capriccio group. Maxime is a CNRS Researcher at the Institute of Physics in Rennes and is planning to use the Capriccio method for multiscale FE-MD simulations of silica glass. During the week of his visit, we were able to take the first steps in this direction and have already obtained some very promising results.

On October 6, Maxime gave a special seminar in the research training group FRASCAL (https://www.frascal.research.fau.eu/) on "Probing mechanical properties with chemical specificity using molecular and multiscale simulation". Not only after the seminar, but also during the whole week, many exciting discussions with colleagues from FRASCAL and from the Institute of Applied Mechanics took place. Apart from the scientific program, we still found some time for joint activities: For example, on October 3, which is a public holiday in Germany, Felix and Maxime biked to Nuremberg and met up with Sebastian, who gave a guided tour of the premises of the Fränkische Museums-Eisenbahn e.V. Nürnberg and after this of the city centre of Nuremberg. Another highlight was a joint lunch with the PULS group (https://puls.physik.fau.de/) on October 5. In conclusion, the week was a complete success and we are very much looking forward to the upcoming joint activities with Maxime.

5. Selected Highlights

5.1 Long night of Sciences

Text & picture: Ann-Sophie Herzner



During the "Lange Nacht der Wissenschaft" an October 23, 2023 numerous FAU institutes in Erlangen, Fuerth, and Nuremberg welcomed all kind of science lovers from 6 pm to 12 pm, among them the Research Training Group GRK 2423 FRASCAL. The Long Night of Science (Lange Nacht der Wissenschaft, LNdW) is one of the largest science events in the Nuremberg Metropolitan Region and a great opportunity for our young scientists to transfer their knowledge to the general public. Our Graduate College showcased its involvement through several interactive stations and small experiments. Why and under which circumstances do cracks occur? And how can this knowledge help humanity to prevent for example accidents? On a daily basis, the researchers at FRASCAL contemplate these questions. People of all ages – among them the youngest – thought this would be interesting and were attracted by fractures in all its diversity. During the whole night they discovered fractures in their everyday surrounding as in food packaging. The researchers also took the experiments to the molecular scale and to the visualization of the cracks under polarized light. Some visitors might already crave for more demonstration material as candy wrappers and most importantly – for more science!

5.2 FRASCAL Mini-Symposium at CFRAC 2023 in Prague

Text & pictures: Maurice Rohracker & Shucheta Shegufta

The 7th International Conference on Computational Modeling of Fracture and Failure of Materials and Structures (CFRAC) took place from 21. to 23. June 2023 in the beautiful city of Prague. FRASCAL organized a mini-symposium „Connecting scales and disciplines to model fracture" at CFRAC comprising three sessions with four presentations each. We were very pleased to welcome Prof. Marc Geers from the Eindhoven University of Technology as the keynote speaker at our symposium. Christian Greff and Maurice Rohracker also presented their current work in one of the sessions. Furthermore, Stefan Hiemer gave a talk on his research covered in his recently achieved doctoral degree. A special thanks go to Maurice Rohracker and Shucheta Shegufta for co-organizing the mini-symposium. Besides the very interesting scientific discussions at the conference, the organizers also convinced with a very fitting social program. In addition to the conference dinner at Letenský zámeček, in the heart of Letná Park next to the popular beer garden, there was also an invitation to the classical concert by the soloists Marie Fajtová and Roman Patočka accompanied by the Bohemia Chamber Orchestra in the Bethlehem Chapel – presenting a further highlight at CFRAC 2023.

Many thanks to the organizers of CFRAC 2023.

5.3 8th GAMM workshop on phase-field modelling at ETH Zürich

Text & pictures: Maurice Rohracker & Deepak Jadhav

At the eight edition of the GAMM workshop on phase-field modelling at the ETH Zürich Deepak Jadhav and Maurice Rohracker participated and gave a talk about their research within FRASCAL. In this two-day workshop, different researchers from several disciplines met together in the Alumni Pavilion at ETH to talk about their recent insights of their research with a focus on theoretical and application-related aspects of the phase-field approach to study physical phenomena such as fracture. Further, also other physical phenomena, such as diffusion, thermal conduction, ferro- and piezo-electric effects, phase transformation and separation processes, biomechanics, fluid mechanics, as well as coupled problems involving multiple processes, have been presented. On top of everything, also, the development of novel, efficient numerical algorithms has been discussed along with innovative approaches based on data-driven and/or machine-learning methods. Deepak Jadhav showed his investigations of different forms of fracture using a spatially adaptive phase-field model, and Maurice Rohracker presented a comparison of different adaptive spatial refinement strategies in phase-field fracture simulations of brittle materials. One highlight of the event was the dinner in the Dozentenfoyer on top of the main building of ETH Zürich with a very nice view over the city. A special thanks to the organizers of this event and FRASCAL for the assumption of all travel costs.

5.4 Doctoral degree

We are pleased to announce two successfully completed FRASCAL dissertation projects in 2023:

Dr. Wuyang Zhao

Text & picture: Sebastian Pfaller

We are delighted to announce that Wuyang Zhao successfully defended his dissertation entitled "Multiscale modeling of the fracture behavior of glassy polymers across the atomistic and continuum scale" on August 29, 2023. In his thesis, he revisits the basics of continuum mechanics, atomistic simulations, and their coupling and thoroughly investigates the material behaviour of amorphous polymers at large strains based on molecular dynamics simulations with particular focus on the numerical sample preparation and the effect of simulation parameters as well as physical phenomena like degree of polymerisation, cooling rate, and aging time. Based on this, he demonstrates the capability of the molecular model to render plausible time-temperature superposition at small and large strains. After this, he discusses constitutive modelling approaches and introduces

his novel viscoelastic-viscoplastic model to capture the material behaviour based on molecular dynamics simulations. The last section concentrates on Wuyang's extension of the Capriccio method to inelastic material behaviour and large strains and gives an outlook to coupled fracture simulations with the vicinity of the crack tip resolved at the molecular level. We wish Wuyang a successful continuation of his research activities and all the best for his future!

His thesis is openly available via https://opus4.kobv.de/opus4-fau/frontdoor/index/index/docId/23843

Dr. Maximilian Ries

Text & picture: Sebastian Pfaller

We are delighted to announce the graduation of Dr.-Ing. Maximilian Ries.

In his thesis "Characterization and modeling of polymer nanocomposites across the scales," Maximilian introduces a methodology to derive continuum mechanical models for polymer nanocomposites (PNCs) based on molecular dynamics. He thus combines the advantages of particle-based and continuum approaches. Furthermore, the obtained constitutive descriptions for matrix, filler, and interphase form the prerequisite for analyzing representative volume elements (RVEs). Using these RVEs, he evaluates the influence of filler content and distribution on the polymer nanocomposite's overall stiffness. Consequently, his interdisciplinary work contributes significantly to understanding polymer nanocomposites, especially the crucial matrix-filler interphase, and thus complements experimental insights. Moreover, the transfer of molecular-scale insights into continuum mechanical models forms an essential link between the chemistry and engineering communities for the numerical modeling of polymer nanocomposites.

Maximilian will continue his academic career as a postdoctoral researcher in the Capriccio group, where he will switch his research focus to polymer fracture and the mechanical behavior of adhesives.

His thesis is openly available via doi.org/10.25593/opus4-fau-23638

5.5 FRASCAL moves on to the next round

FRASCAL celebrates the entry into the second DFG-funded research phase – the DFG approves the funding of the Research Training Group for a further 4.5 years!

Text & pictures: Heidi Zinser

The FRASCAL project focuses on what holds matter together at its core. Material fractures in planes, ships or trains can lead to catastrophes and cost lives – for example, the ICE train accident in Eschede 25 years ago was triggered by the fracture of a wheel tyre. In 13 projects, the Research Training Group FRASCAL is developing computer-based simulation methods that can capture the character of fracture processes on different length scales.

The aim is to study the fracture processes of materials from the crack visible to the naked eye down to the atomic level in the nanometre range. The focus will be on materials such as plastics, which

are becoming increasingly important in helping to make aircraft, for example, lighter and more energy efficient. Unlike metals – for example, tyres – the fracture behavior of plastics has not yet been researched as intensively and interdisciplinary as in the FRASCAL Research Training Group.

The DFG will now fund the Research Training Group for another 4.5 years with around 5.6 million euros.

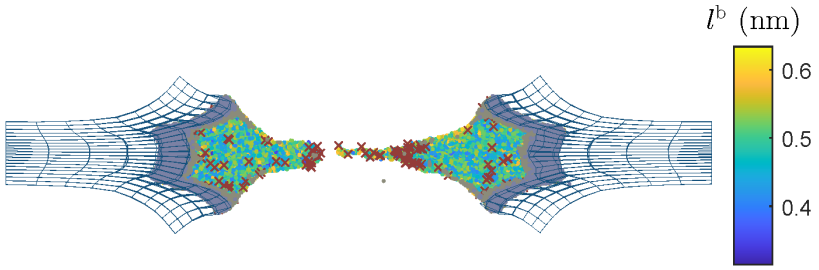
We are all looking forward to continuing this exciting collaborative work until the end of 2027. A hearty thanks goes to all those involved for their great efforts!

5.7 Startup funding

In 2023, the young researchers Paras Kumar, Ina Schmidt, Julian Konrad and Wuyang Zhao were supported with the FRASCAL startup foundation. Wuyang Zhao and Paras Kumar kindly made the effort to explain what research contribution was made as part of this funding.

Wuyang Zhao

With FRASCAL Start-Up funding 2023, Wuyang Zhao continued his research on the fracture of glassy polymers following the completion of his dissertation. Building on the multiscale simulation method for glassy polymers developed during his doctoral work, he studied the fracture behavior of glassy polymers under non-uniform deformation, addressing the limitations of uniform deformation in pure molecular dynamics simulations with periodic boundary conditions. The figure below illustrates the distribution of bond length l^{b} and the location of broken bonds in a thermoplastic model after fracture under uniaxial tensile loading. Beyond this ongoing work, which investigates the effects of geometric loading conditions and bond breakage criteria on fracture behavior, he has also explored time-temperature correlations at large strains [1] and proposed a constitutive model for steady-state strain hardening behavior [2] of glassy polymers. These contributions are essential for further studies on the fracture of glassy polymers at different strain rates and temperatures. They form a significant part of the preliminary work for a DFG project proposal on investigating the physical origin of brittle-to-ductile transition in glassy polymers, which was submitted at the end of March 2024.



References

[1] W. Zhao, R. Xiao, P. Steinmann, S. Pfaller. Time--temperature correlations of amorphous thermoplastics at large strains based on molecular dynamics simulations. Mechanics of Materials, 2024, 190, 104926

[2] W. Zhao, P. Steinmann, S. Pfaller. Modeling steady state rate- and temperature-dependent strain hardening behavior of glassy polymers. 2024, Under Review.

Paras Kumar

The FRASCAL startup funding grant supported Paras Kumar in his endeavor to envisage a post-doctoral research project aiming at development of efficient schemes for multiscale modeling of heterogeneous materials undergoing large deformations and exhibiting nonlinear-inelastic constitutive response. The central idea here is to reduce the formidable computational cost of the microscale calculations involved in a usual two-scale concurrent (FE2 like) scheme by means of efficient surrogate models which are to be trained in the off-line phase using the data generated from microscale calculations conducted on the expected input parameter space. A combination of conventional physics-based and machine-learning-based approaches is being explored for the development of efficient multiscale simulation procedures to enable accurate modeling of the above-mentioned class of materials.