FAU

Friedrich-Alexander-Universität
Erlangen-Nürnberg

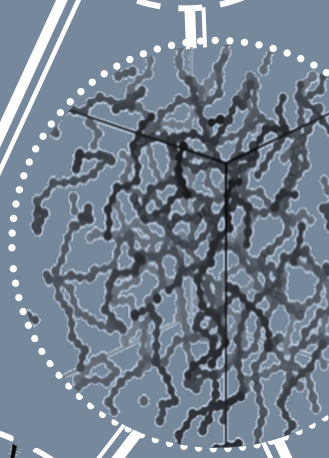
# FRACTURE ACROSS SCALES

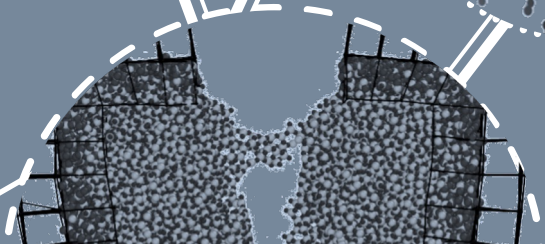
Integrating Mechanics, Materials Science, Mathematics, Chemistry and Physics

ANNUAL REPORT 2025

FRASCAL

GRK 2423





**Annual Report**
of the Research Training Group GRK 2423

# FRASCAL

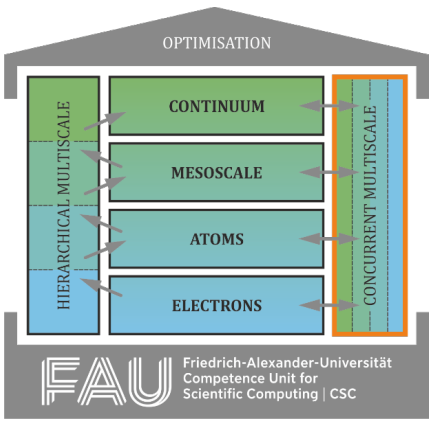
## Fracture across Scales

### 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)

# 2025




www.frascal.fau.de

## IMPRESSUM

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# Preface

In 2025, we welcomed the third cohort to FRASCAL. This enriched FRASCAL with a wide variety of new characters. The initial phase was particularly exciting as we got to know each other, new research topics developed, and over the course of the year we grew together into a harmonious group. The overlap between the cohorts allowed the “newbies” to learn from the “oldies,” and the „oldies‘“ benefitted from fresh input by the „newbies".
Within their first year, the third cohort experienced and achieved a great number of milestones and was able to take full advantage of the qualification program. These included research stays and initial publications as part of their doctoral thesis research.
There were also many opportunities for social interaction: numerous events—both internal FRASCAL events such as the retreat and university-wide events such as the Long Night of Science.
After this successful first year, we are very much looking forward to the upcoming two years and are confident that they will be fantastic!

Erlangen, January 2026

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:**

Ba Duc Duong

**Doctoral researchers' gender representative:**

Leon Pyka

### Participating supervisors

| Principal Advisors (PAs) | Chair, Department, Work Address | Contact Data | Research Area |
|---|---|---|---|
| **Friedrich**, Manuel, Prof. Dr. rer. nat. | Modeling and Numerics, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen | +49 9131 85-67 214 / - 67 225, manuel.friedrich@fau.de, www.mso.math.fau.de | **Applied Analysis, Calculus of Variations** |
| **Koehn,** Daniel, Prof. Dr. rer. nat. | Tectonics, Dep. of Geography and Geosciences, Schlossgarten 5, 91054 Erlangen | +49 9131 85-22626 daniel.koehn@fau.de, www.gzn.nat.fau.eu | **Structural Geology and Tectonics** |
| **Leyendecker** Sigrid, Prof. Dr.-Ing. | Applied Dynamics, Dep. of Mechanical Engineering, Immerwahrstraße 1, 91058 Erlangen | +49 9131 85-61 001, sigrid.leyendecker@fau.de, www.ltd.tf.uni-erlangen.de | **Computational Dynamics** |
| **Mergheim**, Julia, Prof. Dr.-Ing. | Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen | +49 9131 85-28 505 / -503, julia.mergheim@fau.de, www.ltm.tf.fau.eu | **Computational Mechanics** |
| **Meyer**, Bernd, Prof. Dr. rer. nat. | Computational Chemistry, Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen | +49 9131 85-20 403 / -404, bernd.meyer@fau.de, www.chemistry.nat.fau.eu/ccc/groups | **Surface Science** |
| **Moretti**, Paolo, PD Dr. | Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth | +49 911 65078-65 071 / -066, paolo.moretti@fau.de, www.matsim.techfak.uni-erlangen.de | **Complex Microstructures** |

| | | | |
|---|---|---|---|
| **Pfaller**, Sebastian, PD Dr.-Ing. habil. | Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen | +49 9131 85-28 507/ -503, sebastian.pfaller@fau.de, www.ltm.tf.fau.eu | **Scale Coupling Methods** |
| **Pflug**, Lukas Dr. rer. nat. | FAU Competence Center Scientific Computing, Cauerstr. 11, 91058 Erlangen | +49 9131 85-67139 lukas.pflug@fau.de www.zisc.fau.de/zisc/staff | **Optimisation** |
| **Pöschel**, Thorsten, Prof. Dr. rer. nat. | Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraße 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, Cauerstraße 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, Cauerstraße 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** |
| **Ries,** Maximilian Dr. rer. nat. | Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen | +49 9131 85-67 619/ -503, maximilian.ries@fau.de, www.ltm.tf.fau.eu | **Multiscale Simulation of Amorphous Polymers** |

| Doctoral Researchers | Chair, Department, Work Address | Contact Data | Research Area |
|---|---|---|---|
| **Canbolat**, Utku | Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraße 3, 91058 Erlangen | +49 9131 85-70 490 / -518, utku.canbolat@fau.de, www.mss.cbi.fau.de | **Large Scale Simulations for Fragmentation of Granular Materials** |

| Doctoral Researchers | Chair, Department, Work Address | Contact Data | Research Area |
|---|---|---|---|
| **Duong**, Ba Duc | Modeling and Numerics, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen | ba.duc.duong@fau.de www.mso.math.fau.de | **Discrete-to-Continuum Passage for Variational Fracture Models** |
| **Greff**, Christian | Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth | +49 911 65078-65 063 / -066, christian.greff@fau.de, www.matsim.techfak.uni-erlangen.de | **Tuning Adhesion Properties of Hierarchical Materials** |
| **Igel**, Lennart | Mathematical Optimisation, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen | +49 9131 85-67 083 / -20785, lennart.g.igel@fau.de, www.mso.math.fau.de | **Fracture Control by Material Optimisation** |
| **Jadhav**, Deepak Balasaheb | Applied Dynamics, Dep. of Mechanical Engineering, Immerwahrstraße 1, 91058 Erlangen | +49 9131 85-61 002 / -011, deepak.jadhav@fau.de, www.ltd.tf.uni-erlangen.de | **Adaptive Dynamic Fracture Simulation** |
| **Karimi**, Javad | Tectonics, Dep. of Geography and Geosciences, Schlossgarten 5, 91054 Erlangen | javad.karimi@fau.de www.gzn.nat.fau.eu | **Fragmentation and Fracture in Geological Rocks** |
| **Kirsan,** Azad | Computational Chemistry, Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen | +49 9131 85-20421, azad.kirsan@fau.de, https://www.chemistry.nat.fau.eu | **Chemistry at the Crack Tip** |
| **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** |
| **Luo,** Yuxin | Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth | yuxin.luo@fau.de, www.matsim.techfak.uni-erlangen.de | **Compressive Failure in Porous Materials** |
| **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** |
| **Prateek** | Applied Dynamics, Dep. of Mechanical Engineering, Immerwahrstraße 1, 91058 Erlangen | 2404.prateek@fau.de, www.ltd.tf.fau.de | **Adaptive Dynamic Fracture Simulation** |
| **Puhlmann**, Pascal | Theoretical Chemistry, Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen | +49 9131 85-20422 pascal.puhlmann@fau.de www.chemistry.nat.fau.eu/ccc/groups/zahn-group/ | **Fracture in Polymer Composites: Nano to Meso** |
| **Pyka,** Leon | Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth | leon.pyka@fau.de, www.matsim.tf.fau.de | **Tuning Adhesion Properties of Hierarchical Materials** |

| Doctoral Researchers | Chair, Department, Work Address | Contact Data | Research Area |
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| **Richter,** Eva | Applied Mechanics, Dep. of Mechanical Engineering, Paul-Gordan-Straße 3, 91052 Erlangen | +49 9131 85-64400, eva.richter@fau.de, https://www.ltm.tf.fau.de/ | **Multiscale Fracture of Thermoplastic Polymers** |
| **Ritterhoff**, Christian | Computational Chemistry, Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen | +49 9131 85-20 421 / -404, christian.ritterhoff@fau.de, www.chemistry.nat.fau.eu/ccc/groups | **Chemistry at the Crack Tip** |
| **Rohracker**, Maurice | Applied Mechanics, Dep. of Mechanical Engineering, Paul-Gordan-Str. 3, 91052 Erlangen | +49 9131 85-64 410 / -413, mau.rohracker@fau.de, www.ltm.tf.fau.eu | **Fracture in Polymer Composites: Meso to Macro** |
| **Seutter**, Joscha | Modeling and Numerics, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen | +49 9131 85-67 215 / - 67 225, joscha.seutter@fau.de, www.mso.math.fau.de | **Discrete-to-Continuum Passage for Variational Fracture Models** |
| **Sharma**, Aditi | Applied Mechanics, Dep. of Mechanical Engineering, Paul-Gordan-Straße 3-5, 91052 Erlangen | adt.sharma@fau.de, https://www.ltm.tf.fau.de/ | **Continuum-kinematics-inspired peridynamic modelling of fracture** |
| **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 | **Compressive Failure in Porous Materials** |
| **Weber**, Felix | Applied Mechanics, Dep. of Mechanical Engineering, Paul-Gordan-Str. 3, 91052 Erlangen | +49 9131 85-64 410 / -413, felix.w.weber@fau.de, www.ltm.tf.fau.eu | **Multiscale Fracture of Thermoplastic Polymers** |
| **Zetzmann,** Max | Mathematical Optimisation, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen | max.zetzmann@fau.de, www.mso.math.fau.de | **Fracture Control by Material Optimisation** |

## Associated doctoral researchers

| Associated Doctoral Researchers | Chair, Department, Work Address | Contact Data | Research Area |
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| **Arican,** Bariscan | Theoretische Physik I, Dep. of Physics, Cauerstr. 3., 91058 Erlangen | +49 9131 85-70561, bariscan.arican@fau.de | **Quantum-to-Continuum Model of Thermoset** |
| **Laubert,** Lukas | Applied Mechanics, Dep. of Mechanical Engineering, Paul-Gordan-Str. 3, 91052 Erlangen | +49 9131 85-644/ -10, lukas.laubert@fau.de, www.ltm.tf.fau.eu | **Multiscale Fracture of Thermoplastic Polymers** |
| **Santarossa**, Angel | Multiscale Simulation, Dep. of Chem. & Biol. Engineering, | +49 9131 85-70 482, angel.santarossa@fau.de, | **Crack Front Segmentation** |

| | | | |
|---|---|---|---|
| | Cauerstraße 3, 91058 Erlangen | www.mss.cbi.fau.de | **in I+III Mixed Mode Loading** |
| **Smith**, Ruaridh | Tectonics,<br>Dep. of Geography and Geosciences, Schlossgarten 5<br>91054 Erlangen | +49 9131 85 25915<br>ruaridh.smith@fau.de,<br>www.gzn.nat.fau.eu | **Modelling Geothermal Systems through Fractured Media** |
| **Titlbach,** Anna | Faculty of Mechanical Engineering<br>Kesslerplatz 12,<br>90489 Nürnberg | +49 157 59611854<br>anna.titlbach@th-nuernberg.de | **Computational Bone Remodelling** |

## Mercator Fellows

| Mercator Fellows | Affiliation | Expertise |
|---|---|---|
| **Bitzek**, Erik<br>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,<br>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,<br>Dr. | Politecnico di Milano, Italy | Computational mechanics, development of advanced fracture techniques (cohesive elements, eigenerosion), particle methods for the discretization of failure of solids and diffusion of fluids, and multiscale material models for porous brittle materials (brittle damage) to simulate fracking |

### External Advisory Board

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

## 1.3 Coordination and administration

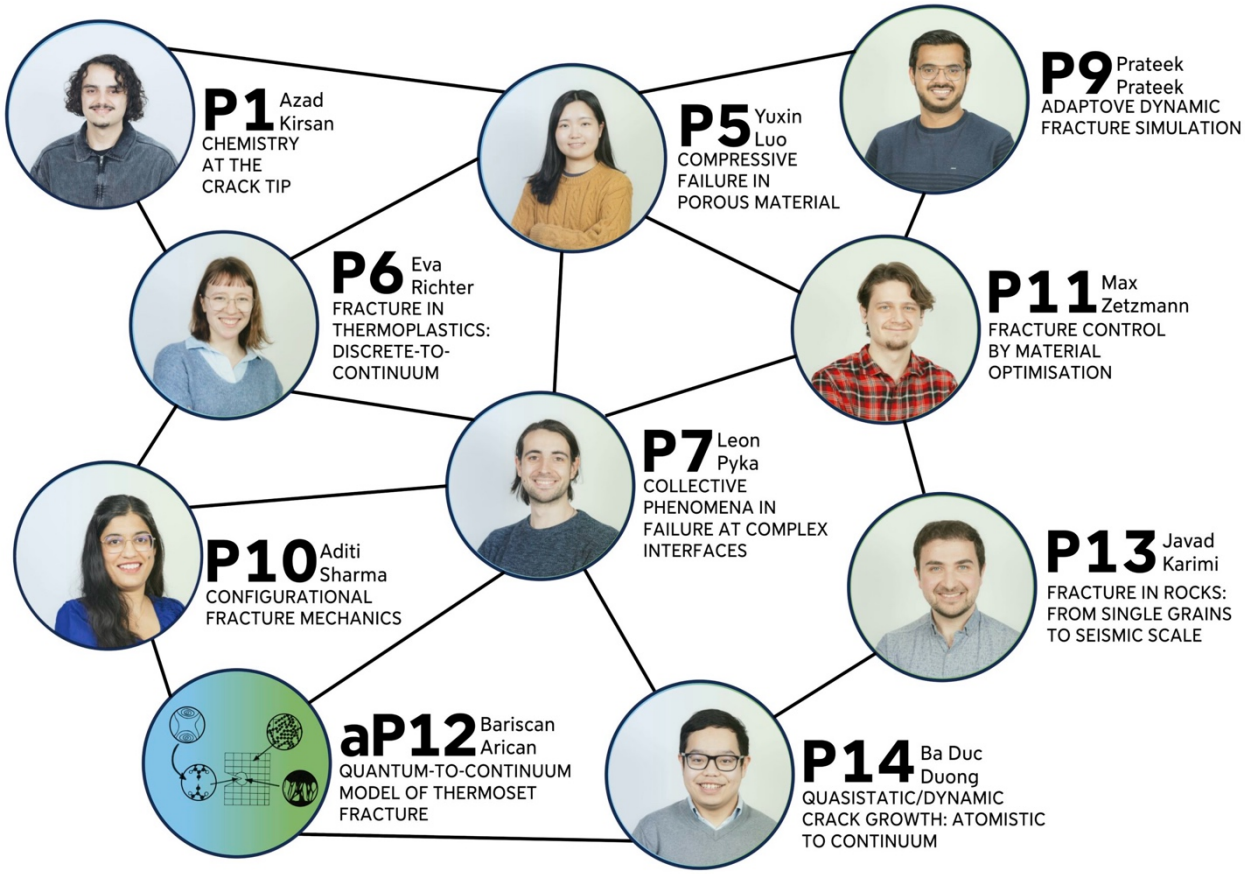
### Coordination and administration of GRK 2423 FRASCAL

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

## 1.4 Reporting period

01 January 2025 to 31 December 2025

# 2 Research Programme



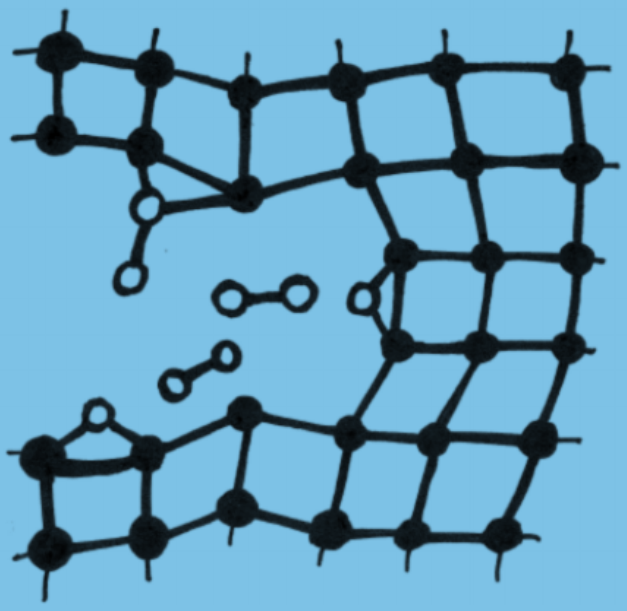

## 2.1 Research projects

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 realize a concurrent multiscale modelling approach for fracture, ranging from quantum to continuum treatment. The effect of heterogeneities on fracture behavior is a common scientific question underlying all projects. Heterogeneities can exist on an atomic scale in the form of locally changed bonding or density (P1, P12, P14), or on larger scales, where heterogeneities include second phases as in composites (P3, P6, P8, P11), porous and geological structures (P5, P13), as well as interfaces, surfaces and/or (micro) cracks (P4, P7, P9, P10).

## FRASCAL's projects:

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

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



# P 1

## CHEMISTRY AT THE CRACK TIP


**Azad Kirsan**

**Christian Ritterhoff**

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

# P1: Simulations of crack propagation in Li2O with a machine-learned potential

Azad Kirsan and Bernd Meyer

Lithium metal batteries (LMBs) are a leading candidate for next-generation energy storage systems due to the usage of a highly reactive Li metal anode, offering a significantly higher energy density than the commonly used lithium ion batteries (LIBs), which rely on intercalation-type electrodes. However, the practical use of LMBs is hindered by problems occurring due to inhomogeneous Li plating. During the charging process, the Li ions depositing back onto the Li electrode prefer to adsorb at defect or non-uniform sites of the surface. This leads to a plethora of problems, including a phenomenon called "dead lithium", where Li clusters split-off of the electrode surface and are surrounded by a passivating layer, which renders them unable to take part in any electrochemical reactions, thus reducing the efficiency of the battery. Another, more serious issue related to inhomogeneous Li deposition is the formation of dendritic structures. These so-called dendrites are long tree-branch like structures that grow on the Li metal electrode and pose a severe safety risk, since they can get so large that they reach the membrane separating the two half-cells of the battery and pierce it, leading to a short-circuit.[1,2]

The solid electrolyte interphase (SEI) is a heterogeneous, passivating layer forming on the Li electrode that mediates ionic transport. The SEI is formed due to the electrolyte molecules decomposing upon contact with the reactive Li metal and its properties fundamentally determine the batteries efficiency, long-term stability, and ion deposition and thus reduce or even inhibit the formation of dead Li and dendrites. Close to the electrode, the SEI consists mostly of Li2O. As Li ions move through the battery, the stresses occurring can lead to mechanical fracture of the SEI, which is a critical aspect of its degradation, as cracks can expose fresh Li metal to the electrolyte, leading to more unwanted reactions and promoting the growth of dendrites. Understanding the mechanisms of SEI fracture, its initiation and propagation is therefore of utmost importance for the establishment of better and more robust LMBs.[1,2]

Due to their high computational cost, ab initio calculations are restricted to small systems sizes and are thus not suited for the simulation of larger bulk structures necessary for the modeling of cracks. On the other hand, molecular mechanics simulations employing empirical force fields don't have the required chemical accuracy and cannot confidently predict chemical reactions. This is why in this project we developed a machine-learned interatomic potential (MLIP) for Li2O, which makes up the largest part of the SEI, to perform more reliable and reactive fracture simulations. Employing the atomic cluster expansion (ACE[3]) potential training method, we used 8964 structures and performed density functional theory (DFT) calculations at the PBE+D3 level of accuracy to train our potential. The dataset consisted of Li2O (6391), Li metal (1674), and Li2O2 (899) structures, encompassing a wide variety of atomic environments. In order to validate the trained potential, some material properties were benchmarked. Firstly, the lattice constant of the Li2O crystal structure was determined as 4.6048 Å with the MLIP, matching the DFT reference of 4.6088 Å. Secondly, Li migration barriers in Li2O were determined by creating a Li vacancy and then calculating the energy difference of the transition state (as seen in Fig. 1b) from the initial structure (Fig. 1a). The predicted energy barrier of 0.22 eV again matches our reference DFT value of 0.20 eV very well. With the last two benchmarks we verified that the MLIP predicts surface energies and elastic constants correctly, see Tables 1 and 2, since they are fundamental for accurate fracture

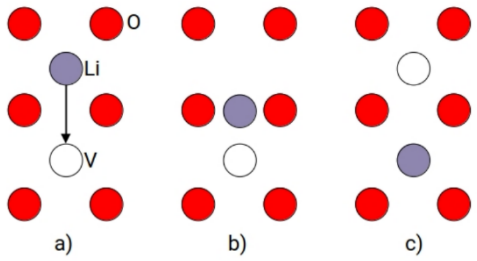



**Fig. 1:** Migration of a Li atom into a neighboring vacancy.

simulations. The MLIP predicted the trends of the Li2O surface energies successfully, determining the (111)-surface as the lowest-energy surface and (100) as the highest, however the absolute surface energies were overestimated. The elastic constants, other than the Poisson ratio, were also slightly overestimated by about 12-13% in each case. For both, the surface energies as well as the elastic constants, the deviations lie within the expected range of errors for MLIPs reported in the literature, which is why we were satisfied with these results and went on to perform crack simulations for Li2O. The setup for the fracture simulations is shown in Fig. 2. The structure with a

| Surface | PBE+D3 | MLIP |
|---|---|---|
| 100 | 83.4 | 91.2 |
| 110 | 66.0 | 74.5 |
| 111 | 40.9 | 51.1 |

**Table 1:** Reference and MLIP surface energies of $Li_2O$ in meV $Å^{-2}$.

| Constant | PBE+D3 | MLIP |
|---|---|---|
| Bulk modulus / GPa | 78.6 | 88.3 |
| Shear modulus / GPa | 70.4 | 79.6 |
| Elastic modulus / GPa | 162.6 | 183.6 |
| Poisson ratio | 0.155 | 0.153 |

**Table 2:** Reference and MLIP predicted elastic constants of Li2O.

(111) cleavage plane consists of 3456 atoms. The molecular dynamics simulations were performed at 300 K for 15 ps each, using different initial structures at varying given stress intensity factors KI (mode I fracture). The atoms at the border of the structure were fixed and periodic boundary conditions were applied along the crack front. Three Li-Li distances across the crack tip were analyzed in order to determine the critical stress intensity factors at which the crack starts either to heal or to propagate. The three Li pairs are shown in Fig. 2, where the distance marked in green corresponds to a Li pair at the crack tip, the purple one to a pair in front of the tip, and the blue one to a Li pair behind the tip. Fig. 3 shows the average Li-Li distance divided by the equilibrium Li-Li distance in a Li2O crystal plotted against the stress intensity factor of the initial structure. The graph colors correspond to the color of the marked distances in Fig. 2. A bond was considered broken at an elongation of 25%. Based on this criterion it was found that the crack closes for stress intensity factors below ~55 GPa Å1/2. As expected, the healing happened along the crack plane, meaning that the underlying crystal structure was reformed. The critical loading for crack opening was found to be ~70 GPa Å1/2, after which the crack started propagating. The MLIP predicted that the crystal sustains brittle cleavage, which is also the expected behavior for the (111) plane in a Li2O crystal, since it is the most stable surface. Any stress intensity factor between the two boundaries results in metastable states, where the crack is stationary.

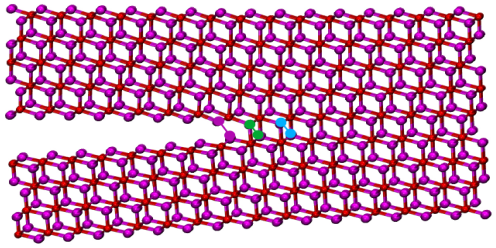


**Fig. 2:** General setup for the crack simulations of a $Li_2O$ crystal with a (111) cleavage plane.

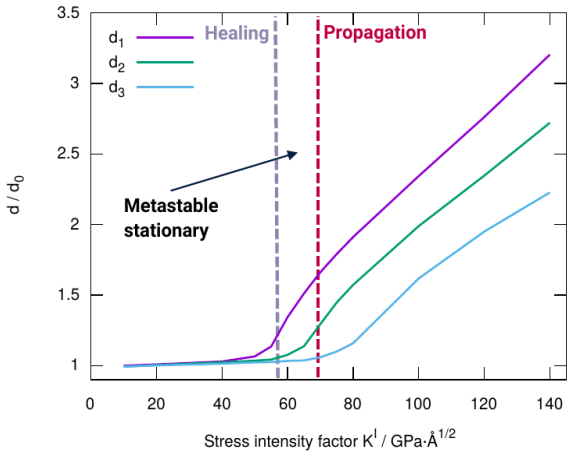



**Fig. 3:** Li-Li distances across the crack tip depending on the applied stress intensity factor. Graph colors correspond to the Li pairs marked in Fig. 2.

In summary, we benchmarked our Li-O MLIP trained with the ACE method on various properties and used it to perform first fracture simulations on a Li2O crystal, which showed promising results.

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## P1: Chemistry at the Crack Tip

Christian L. Ritterhoff and Bernd Meyer

In my FRASCAL PhD project, I investigated the polarization emerging when cleaving certain perovskite oxides. Using first-principles calculations, I elucidated the influence of the ferroelectric and antiferrodistortive effect on the resulting structure and composition of the crack surfaces and thus could provide an explanation of experimental findings. An originally planned switch from a quantum mechanical approach to using machine learned interatomic potentials (MLIPs) was thwarted by the complexity of the problem, as reaching chemical accuracy with the latter is difficult for polarized configurations. My quantum-mechanical investigation was therefore confined to a supercell of the size of a few crystal unit cells.

However, this brief step into the field of MLIPs sparked my interest and thus, as part of my future postdoc project, I made contact with researcher from the Ruhr University of Bochum of the group of Ralf Drautz. They are the developers of the pacemaker[1] and gracemaker[2] program suites, which enable scientists around the world to generate their own interatomic potentials based on DFT reference datasets. With their expertise and support, I started an investigation of the pre-train → fine-tune → distill (PFD) workflow, a recent development towards cheaper and systematically improvable interatomic potentials.

The first step implies the pre-training of a so-called foundation model. Using reference datasets of enormous size (100M+ structures), spanning nearly the complete periodic table, a single potential is fitted, with the goal to subsequently serve as the foundation of future potentials. The idea is that most basic interactions of most elements are already included in this parametrization. Its accuracy suffices for many applications in material science. However, chemistry often requires an accuracy beyond that of most foundation models, as they are not trained on e.g. reaction pathways or rare events. At the same time, they are multiple magnitudes slower than previous lightweight MLIPs as consequence of their large number of parameters and increased complexity.

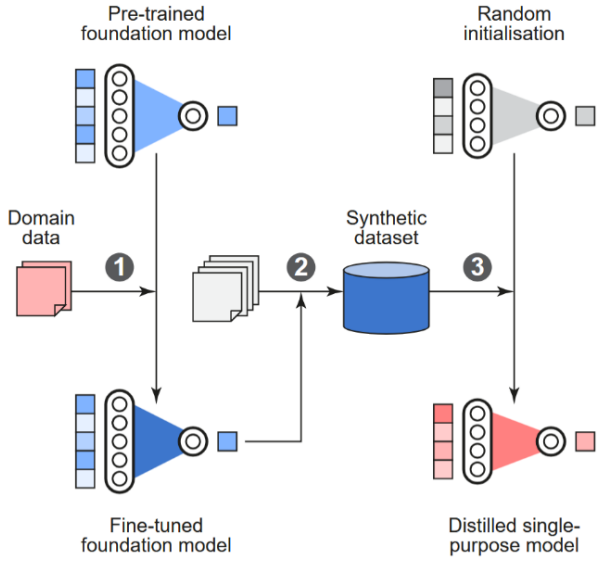


**Fig. 1:** Illustration of the foundation model → fine-tuning → distillation workflow; taken from Ref. [3].

Thus, the second and third step in the PFD workflow are fine-tuning and distillation. Figure 1 summarizes these two steps. The foundation model is fine-tuned on a task-specific dataset to boost the accuracy for the system of interest consisting of a small subset of elements. The resulting high-fidelity "teacher" model then serves to distill its knowledge into a compact surrogate “student” model via supervised training on predictions from the “teacher” (synthetic dataset from the fine-tuned foundation model, not DFT!). Following this procedure yields a lightweight potential suitable for large-scale simulations while preserving near-DFT accuracy. Notably, this procedure reduces the required DFT reference data since the basic interactions of the system of interest are already included in the foundation model and only specifics have to be taught in the fine-tuning step.

We chose to test this paradigm using a large set of carbon-only configuration, since carbon's diverse hybridization (sp/sp2/sp3), competing isomers, and multi-scale bonding motifs perfectly

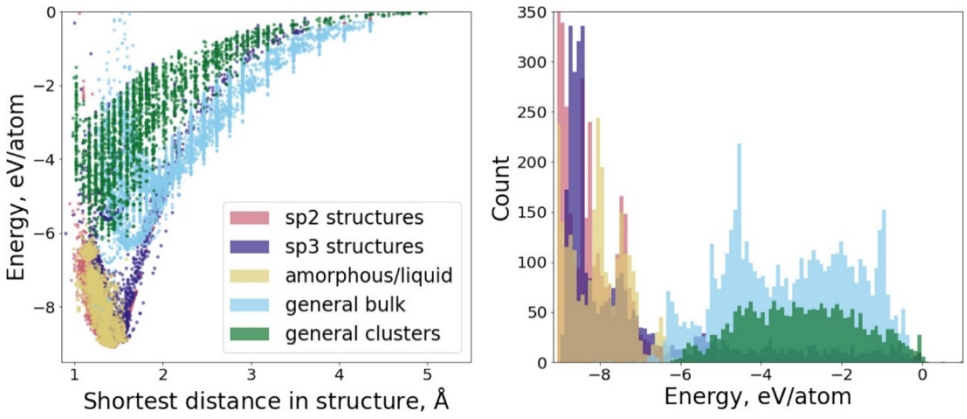


**Fig. 2:** Structure of the carbon dataset from Ref. [3]. Left: Structural distribution. Right: Energy distribution.

challenge MLIP expressivity. Rather than generating new DFT data, we re-used a dataset by Minaam et al. [3] of 17,293 VASP calculations of diverse carbon structures (Figure 2).

A major advantage of fine-tuning a potential from a foundation model is the reduction of required DFT reference data. Our first goal was to test this paradigm. For this purpose, we first need a reference evaluation set which quantifies the quality of our potentials. We chose a small dataset of 1912 structures published by Bochkarev et al.,[2] which shows a similar distribution as the training dataset. We then evaluated all structures with the GRACE-1L-OMAT foundation model to receive a baseline reference. Following this, we fine-tuned the foundation model on a subset of the complete dataset comprising randomly chosen structures and re-evaluated the evaluation set. Repeating this procedure for subsets of increasing sizes yields potentials of increasing quality.

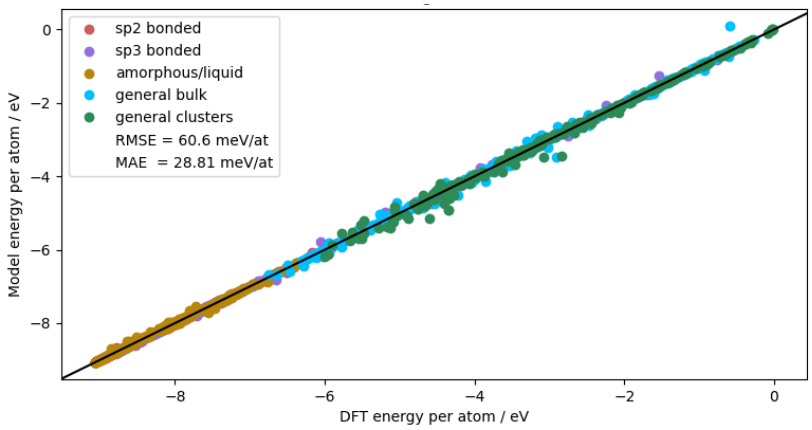


**Fig. 3:** Model energy prediction vs. DFT reference data. 2800 carbon structures have been used for fine-tuning.

Figure 3 shows that a fraction of the complete dataset is enough to obtain a highly accurate potential: 2800 randomly chosen structures suffice to reduce the MAE to 28 meV per atom. The next step is then to compare these potentials to others which had the same training data but were trained from scratch rather than having the foundation model as a starting point. For these experiments, we expect a quantifiable advantage of the latter, especially in the low-data regime.

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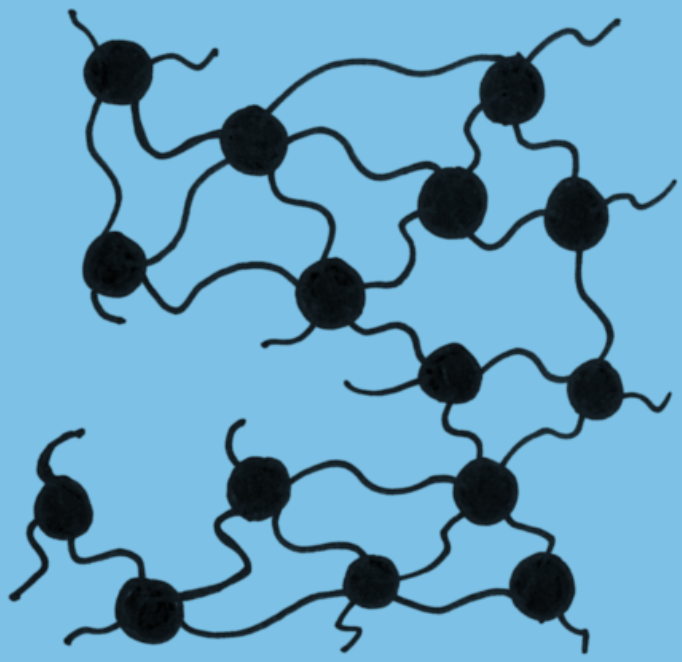

# P3

## FRACTURE IN POLYMER COMPOSITES: NANO TO MESO

**Pascal Puhlmann**

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

# P3: MD Simulation of Polymer Networks: Polysiloxanes

Pascal Puhlmann and Dirk Zahn

**Polysiloxanes,** mainly known as silicones, are polymers whose molecules have a backbone chain of alternating silicon and oxygen atoms with additional organic functional groups (e.g. methyl, -CH3). This conformation gives silicones a wide range of outstanding properties such as chemical inertness, elasticity and water resistance, as well as exceptional stability at high and low temperatures. These and other material-specific properties have given silicones a wide range of applications, from lubricating greases and electrical cable insulation to biomedical applications.
Until now, we developed a MD force field based on quantum mechanics allowing bond breakages along the silicones backbone by describing the silicone-oxygen bond by a Buckingham potential instead of the usual harmonic potential [1]. This feature enables the bond breakages and bond reorganizations without preparation at sufficiently large distances and tensile force. The Si-O bonds of the backbone are much more vulnerable to mechanical induced stress than the Si-C bond. Therefore, the next step after the production of silicone oils, we studied with oscillatory compression/decompression runs the degradation process. This approach enabled us to assess bond breakage, reassembly and cyclization mechanisms in our molecular dynamics simulations [2].

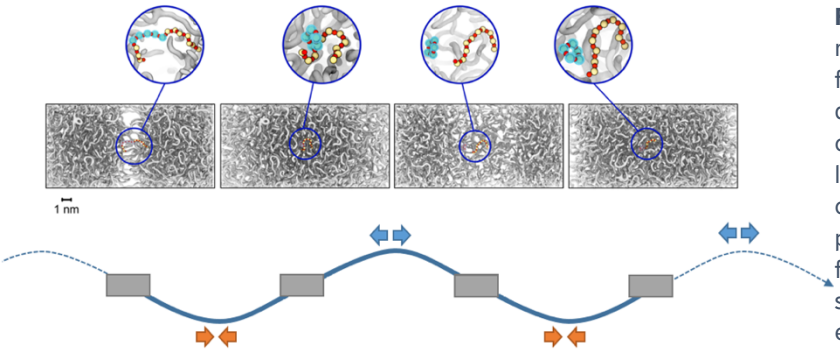


**Fig 1:** Exemplary series of snapshots from mechanical testing of the silicone oil formulation derived from 90/10 dimethylsilandiol/trimethylsilanol. Upon completion of subsequent half-cycles a linear silicone strand experiences coiling/elongation moves that eventually provoke Si-O bond reorganization in favor of extruding a cyclopentasiloxane species. Yet the reaction energy is not exactly zero, but (slightly) endothermic because of the intramolecular strain inhered to the ring formation. For better visibility only Si (yellow/cyan) and O (red) atoms are shown, whilst the remaining oil molecules are illustrated in grey, respectively.

We found under thousands of reaction events that all reactions follow the pattern of forming a 4-centered motif of Si-O bonds. In our testing models, which contain differently sized linear and (minor extends of) cyclic PDMS, we identified the formation of cyclic molecules.

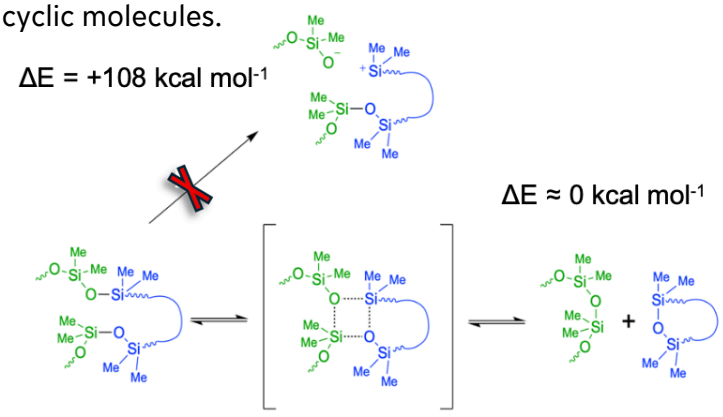


**Fig 2:** General mechanism for the degradation of PDMS strands. Undercoordinated forms of Si and O atoms are not observed, but the molecules may be temporarily overcoordinated followed by possible bond rearrangements. A cyclic transition state is formed at any position on the strand. It follows a shorten of the chain and the segregation of a cyclic siloxane product. As shown by the simple case of the system with only cyclic siloxane, in which enlargement occurs, this reaction is reversible. This suggests a kinetic driving force rather than a thermodynamical one. This reaction may happen within the same molecule or with other molecules after collision.

We found, the observed formation of small cyclic oligomers ([CH3)2SiO]x with x ≤ 12) as main product in experiments at elevated temperatures (~600–1000 K) is reasonable well reproduced by our simulation setup of mechanical testing.

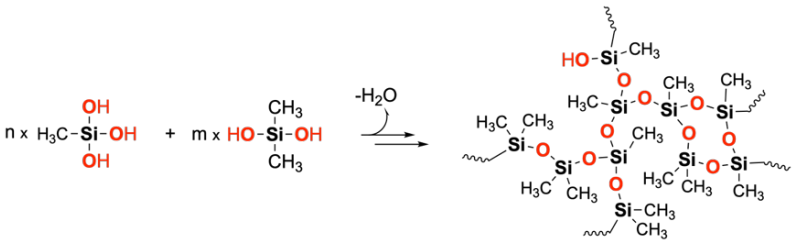

**Fig 3:** Reaction of dimethylsilandiol and methylsilantriol precursors yielding PDMS. Upon condensation reactions, water is removed from our models focusing on silicone resin formation.

With this procedure in mind, we refined our simulation protocol of [1] to feature the polymerization of silicone solids. We used the same method but in addition we used an energy term observed from QM calculation in [1] which accounts for the energy of the proton transfer and allowed only a 10 % error in our polymerization protocol. 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 [3].

With the help of graph theory, we reduced the network analyses to the interpretation of branched strands and finite loops, respectively. The former are characterized by interpenetrating loops and therefore exhibit a form of 'physical bonding', while percolating strands of covalently bonded -O-Si-O- strands seem to dominate the elastic properties like the Young's moduli. Further on, we identified the number density of percolating strands and the length of the shortest percolation as descriptors of the stiffness of the silicone resins studied. Our analysis revealed, both show major variation across nm scales subsets of the polymer network. We therefore conclude that capturing 3D homogeneous polymer networks require much larger simulation cells, ideally exceeding the 4 nm dimensions by at least one order of magnitude. Next, focus is on mechanical testing of the silicone resin.

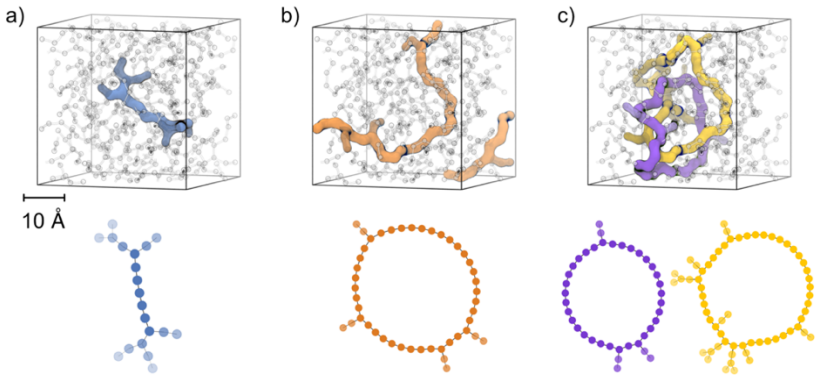


**Fig 5:** Structural analysis on an example system with 10% MMS-T content. Only Si atoms are shown. While all pictures refer to the same polymer network, different cutouts are highlighted. The rest of the system is grayed out. The lower panel equals graph theory. (a) typical sequence (blue) of bonding featuring linear parts as well as branching nodes. (b) percolation via head-to-tail connection of a selected -O-Si-O- strand (orange). While percolations involve the crossing of the periodic box boundaries, (c) illustrates finite loops within the simulation cell. The two rings are identified as two separate circles in graph theory (purple and yellow). While covalent -O-Si-O- strand percolations refer to chemically bonded bulk materials, finite loops may interpenetrate and thus give rise to physical bonding.

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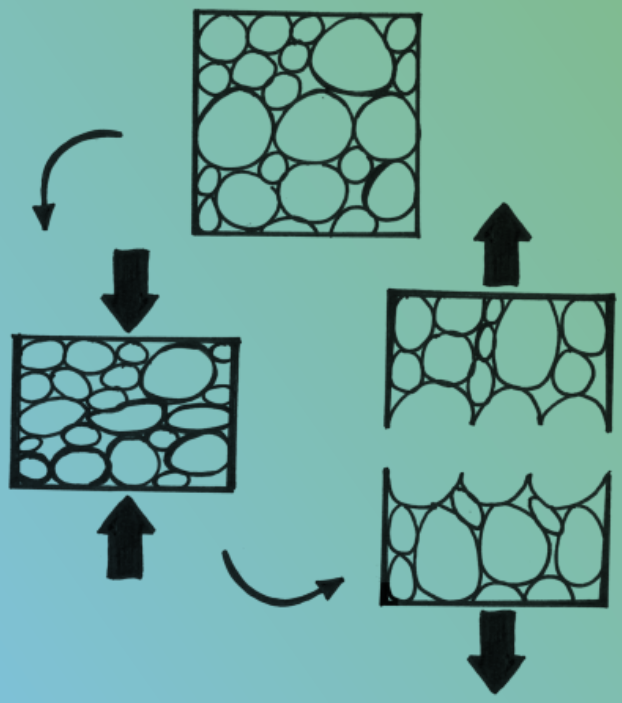

# P5

## COMPRESSIVE FAILURE IN POROUS MATERIAL

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**Prof. Dr. Michael Zaiser**
Materials Simulations
Department Material Science and Engineering

# P5: Phase-Field Simulation of Cracking Induced by Dendrite Growth in Solid-State Lithium Batteries: Starting from a Purely Mechanical Compressive Anti-Crack Scenario

Yuxin Luo and Michael Zaiser

interested in whether fluffy structures containing gaps can effectively arrest or trap crack propagation. And the prior work of Shegufta et al. [3], who employed peridynamic approach to study anti-crack behavior of porous materials, provides a valuable reference for validating our simulations. Anti-crack here denotes counterintuitive cracks that develop perpendicular Solid-state lithium batteries use lithium metal as anode and its electrolytes (SSE) is completely solid-state. This configuration endows them with higher energy density and enhanced safety compared with conventional lithium-ion batteries that have already been widely commercialized. As a highly promising next-generation battery, solid-state lithium batteries are well aligned with the growing demand for portable energy storage and the rapidly expanding electric vehicle market.

In commercial lithium-ion batteries, graphite is used as the anode, so that lithium ions do not directly deposit as lithium metal once reaching the negative electrode, but instead are intercalated into the graphite layers, effectively suppressing dendrite formation. However, In solid-state lithium batteries, uneven deposition of lithium ions on the anode surface can lead to the counterintuitive formation of lithium dendrites with concomitant cracking of SSE, despite the SSE possessing a mechanical strength greater than that of lithium metal.

According to the experimental results reported by Ning et al. [1], the mechanics governing the initiation and propagation of dendrite-induced cracking are different. When voids connected to the anode are fully filled with lithium metal during charging, subsequent lithium-ion deposition builds up pressure within these voids. Once this pressure exceeds the local fracture strength of SSE, crack initiation occurs. In contrast, the propagation of dendrite-induced cracks is governed primarily by the critical strain energy release rate. Lower compressive stack pressure can slow crack propagation, however, a certain level of stack pressure is still required in solid-state batteries to mitigate asperity contact at the lithium metal anode–SSE interface and to suppress void formation resulting from lithium stripping.

Many studies have explored strategies to inhibit dendrite cracking, such as adjusting the stack pressure, charging voltage, or by synthesizing new solid-state electrolyte (SSE) materials. From a mechanical perspective, Christian et al. [2] found that hierarchical structures can partially confine cracks near the interface. This effect is attributed to the gaps within the hierarchical structure, which can arrest crack propagation, so that even if crack initiation occurs, the crack remains localized within a limited region. Therefore, it raises the question of whether dendrite cracking could also be suppressed through the deliberate design of specific mechanical structures in the material.

From the above analysis, it can be observed that dendrite-induced cracks in solid-state lithium batteries tend to migrate during repeated charge–discharge cycles. The phase-field method is particularly suitable for studying such crack phenomena, as both crack initiation and propagation are captured spontaneously without the need to explicitly track crack paths.

The dendrite cracking problem is also inherently multi-physical, involving complex coupling between different governing equations, which places high demands on the robustness and efficiency of the numerical solver. For this reason, we first focus on developing a purely mechanical phase-field solver. Owing to the presence of stack pressure, the battery domain is subjected to compressive loading. In addition, we are to the applied compressive stress in highly porous materials. Consequently, we start from a purely mechanical compressive anti-crack scenario.

In phase-field fracture modeling, the decomposition of elastic strain energy is a crucial step that significantly influences the resulting crack path. There exist various decomposition methods. Among them, Miehe et al. proposed splitting the strain energy into tensile and compressive components, this strategy then has been widely adopted in tensile crack scenarios. As shown in the leftmost panel of Fig. 1, for a center crack under compressive loading that leads to the formation of anti-cracks, the Miehe decomposition fails to capture the phenomenon accurately. Therefore, we introduce a variable

$$\theta = 1 - \varphi_l^{e-}/\varphi_0^{e-}$$

the subscript $l$ denotes the lost compressive strain energy, while $0$ indicates the initial compressive strain energy. The total strain energy can then be expressed as

$$\varphi_d^e = g(\phi)[\varphi^{e+} + (1-\theta)\varphi^{e-}] + \theta\varphi^{e-}$$

Since the occurrence of anti-cracks requires a volumetric collapse within the porous material, compressive strain energy will also lose during this process, so in our case, $\theta = 0$, the resulting

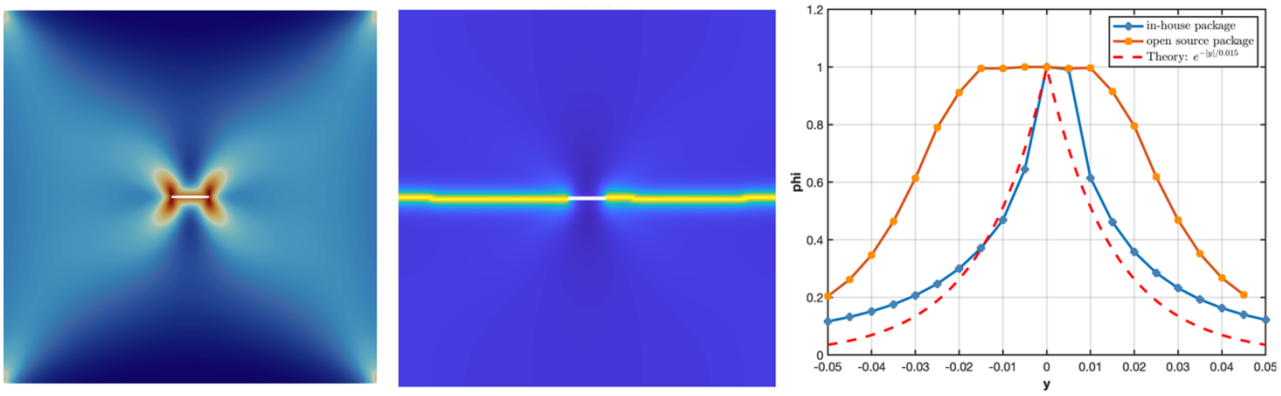


**Fig. 1:** From left to right: the crack pattern of a central crack under compressive loading using the Miehe phase-field model (PhaseFieldX [4]); the compressive crack pattern of the central crack without energy decomposition (in-house MATLAB package); and the crack phase-field profile.

crack pattern is shown in the central panel of Fig. 1. It is worth noting that we compared the results obtained using an open-source package based on FEniCS, a widely adopted solver within the phase-field community, with those from our in-house package. We found that, compared with the theoretical phase-field crack profile, the results computed by our in-house package are in closer agreement.

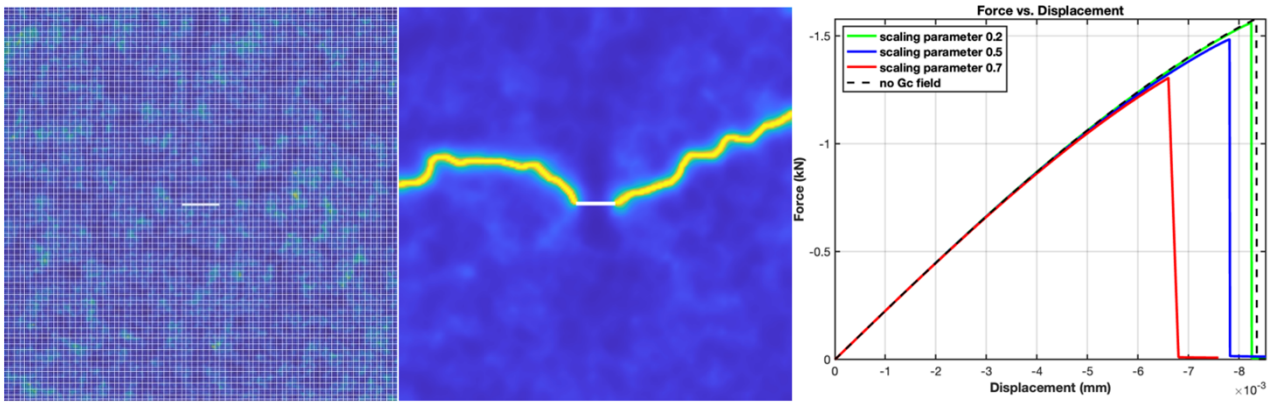


**Fig. 2:** From left to right: Gc field with a scaling parameter of 0.5; the corresponding crack pattern for a scaling parameter of 0.5; and force–displacement curves for various values of the scaling parameter.

As mentioned earlier, the critical energy release rate Gc significantly influences dendrite crack propagation. Therefore, we introduced a Gc field and employed a scaling parameter to control the degree of its randomness. To reduce mesh dependency, the Gc field was generated based on a Gaussian random field with spatial correlation. As shown in Fig. 2, the crack path tends to avoid regions with higher Gc values. And as the degree of randomness increases, the material strength is reduced. These observations are consistent with classical fracture mechanics.

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# P6

## FRACTURE IN THERMOPLASTICS: DISCRETE-TO-CONTINUUM


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**Lukas Laubert**

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# P6: Investigation of thermoplastic multiscale fracture mechanisms using large-scale MD simulations reaching up to the microscale

Eva Maria Richter, Felix Weber, Maximilian Ries and Sebastian Pfaller

Fracture in thermoplastics is a highly complex, fundamentally multiscale phenomenon, where nanometer-scale polymer chain movement drives micrometer-scale mechanics. A critical challenge remains in fully bridging these atomic (nano) and macroscopic (micro) length scales to connect molecular architecture to global failure properties. Traditional simulation methods are inherently limited in addressing this gap. Molecular Dynamics (MD) simulations can capture nanoscale events like chain sliding and bond breakage, but are computationally restricted to the nanoscale, making it impossible to cover the entire process zone. Conversely, continuum-based methods, such as the Finite Element (FE) method, are suitable for large material areas, but struggle to accurately depict fracture as they often reduce it to a mere separation of elements without reference to the underlying molecular mechanisms.

Numerous multiscale simulation techniques are being developed to bridge this gap, but their confident development and validation are hindered by a severe lack of suitable, high-fidelity benchmark data simultaneously spanning both the nano- and micro-regimes. The objective of this work is to directly address this critical data gap and offer new fundamental insights into the thermoplastic fracture process by utilizing a novel coarse-graining framework to perform large-scale Molecular Dynamics simulations. The study employs a novel coarse-graining framework that successfully upscales an established MD model of a Generic Thermoplastic Polymer (GTP) in

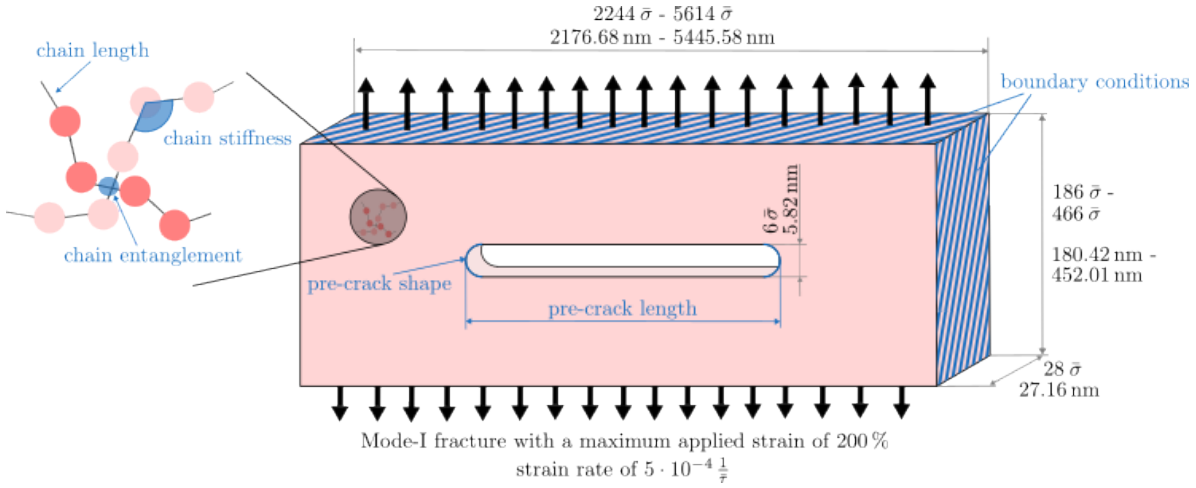


**Fig. 1:** Illustration of the simulated setups. All setups are flat three-dimensional cuboids that entail 30 million coarse-grained GTP superatoms. The following variables are varied and their influence on the fracture behaviour investigated (marked in blue): pre-crack length, chain length, chain stiffness, chain entanglement, pre-crack shape and boundary conditions. The exact sample sizes stem from the choice of material parameters and optimization regarding results. In all samples, a Mode-I loading is applied, reaching a maximum strain of 200 %. The strain rate is $5 \cdot 10^{-4} \frac{1}{\bar{\tau}}$.

LAMMPS [1]. This approach enabled the modeling of systems with up to 30 million coarse-grained superatoms, allowing simulations to cover multiple micrometers of material, significantly exceeding previous MD limits. This scale is necessary to accurately capture the formation of voids, the early stages of fibril growth, and crack propagation on the microscale while retaining nanoscale resolution. The system setup involves a Mode-I uniaxial tensile test, applying a load to small strips of atoms at the top and bottom of the cuboid, allowing the majority of atoms to move freely in response. A relatively high maximum strain of 200% is chosen since local strains in the fracture process zone exceed by far the global applied strain. The simulations are systematically varied to investigate the influence of key parameters on crack propagation, including boundary conditions, pre-crack length, and intrinsic material properties (chain length, chain entanglement, and chain stiffness).

A critical pre-study of smaller, fully periodic systems (~3 million superatoms) demonstrated the necessity of this large scale. These smaller systems consistently failed to exhibit crack propagation, showing only the widening of existing pre-cracks. This proved that for simulating highly localized fracture, the system size must be large enough to ensure that local process zone mechanics dominate over the global influence of the periodic boundaries, motivating the shift to the 30 million superatom systems. Post-processing and analysis were performed using OVITO Pro [2], including cluster analysis, bond breakage quantification, void visualization, and spatial binning of virial stress values. The analysis of the large-scale MD simulations revealed two major findings critical for multiscale modeling.

**1. The inactive "dead zone":** The study identified and characterized an inactive or 'dead' zone - an obstacle region that forms immediately between the sharp crack tip and the developing polymer fibrils. The existence of this zone, previously only hinted at [3], must be structurally overcome for sustained crack growth. In the investigated reference configuration, this inactive zone, measuring 533 nm at 25% applied strain, was eventually overcome at 175% applied strain, initiating crack propagation. Analysis of the stress state, specifically the ratio of the virial volumetric stress to the von Mises stress, showed that the inactive zone consistently held a value of 1. This uniformity strongly suggests a stress state where no further voids nucleate in this region. The dynamic interplay among the rupture zone (void formation), the inactive zone, and the pre-crack is therefore the core driver of fracture.

**2. Sensitivity to boundary conditions and domain size:** While the introduction of even a minor defect immediately made it energetically favorable for the surface to grow at the defect site, indicating that no minimal pre-crack length is necessary for crack initiation, the key finding is that crack propagation is primarily sensitive to the interplay between boundary conditions and simulation domain size. This sensitivity was confirmed by a decisive experiment using semi-periodic (shrink-wrapped) boundary conditions in the x- and y-direction, allowing for free lateral contraction, compared to the fully periodic reference setup. Under semi-periodic conditions, no rupture zone was identified, and crack propagation did not occur. This outcome suggests that when free lateral contraction is permitted, the material compensates for the applied strain by plastically flowing around the widening pre-crack, a process that is energetically more favorable than the formation of new void surfaces. Conversely, the fully periodic setup forces the material to generate new surfaces (voids or crack extension) to accommodate the large applied stretch under constrained lateral relaxation. In the end, these micrometer-scale molecular dynamics simulations successfully leverage a novel coarse-graining framework to generate robust, high-resolution benchmark data necessary for the confident development and validation of next-generation multiscale modeling techniques for thermoplastics. The generated insights and data is essential for bridging the atomic (nano) and macroscopic (micro) length scales to fully connect molecular architecture to global failure processes. The high-fidelity, microscale data on the fracture process zone will directly serve as the necessary benchmark for the extension of concurrent multiscale methods to cover fracture. Specifically, future work will integrate these findings into the Capriccio method, a domain-decomposition approach coupling Molecular Dynamics (MD) and the Finite Element (FE) method, to enable the simulation of crack propagation in systems with truly macroscopic dimensions and realistic boundary conditions.

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# P6: Modeling Brittle Fracture with the Capriccio Method

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In [1], we examine the predictability of the modeling framework developed in P6. Specifically, we show that the Capriccio method [2], which couples molecular dynamics (MD) with the finite element (FE) method, is capable of performing fracture simulations of amorphous materials that yield quantitatively plausible results. In the course of P6, it became clear that thermoplastic polymers, on which previous research activities have focused exclusively, pose a major challenge in terms of the required system dimensions due to their large fracture process zones. It is therefore desirable to reduce the complexity of such feasibility and sensitivity studies by investigating materials with smaller process zone sizes. Furthermore, the use of chemically specific, atomistic models derived from first principles in the MD domain enables the comparison of the calculated (fracture) mechanical quantities with experimental and analytical values. An overarching advantage of applying the Capriccio method to a different type of material is that conclusions can be drawn about the universality of the approach.

For this purpose, we apply the Capriccio framework to an atomistic model of silica glass [3]. First, we derive the elastic properties to be used in the FE domain from pure MD simulations. We then couple MD domains to surrounding FE domains to which we apply boundary conditions typical for fracture mechanical test setups, see Figure 1. By loading the samples with a surface traction $\bar{\mathbf{t}}$ applied to the boundary of the FE domain, the crack with a length of $a$ and a width of $L_x^{\mathrm{crack}}$ is caused to propagate through the MD domain. The latter consists of silicon (Si) and oxygen (O) atoms and is subject to Newtonian particle dynamics (ND) in its interior, while it is exposed to additional dissipative particle dynamics (DPD) terms in its outer part to regulate the temperature. The so-called anchor points, which are colored blue, play the role of information transmitters between the FE and MD domains. Different MD quantities in front of the crack tip are measured in an observation region with the in-plane dimensions $L_x^{\mathrm{obs}} = L_y^{\mathrm{obs}}$. Furthermore, the crack opening displacement $\delta$ is evaluated between the two purple points. The total width, length and thickness of the samples are labeled with $b, 2c$, and $h$, respectively. With this setup, we perform mode I, mode II, and mode III simulations on a rectangular plate (also referred to as a "strip") with an edge notch by applying far-field stresses and three- and four-point bending tests. Examples of deformed configurations of the

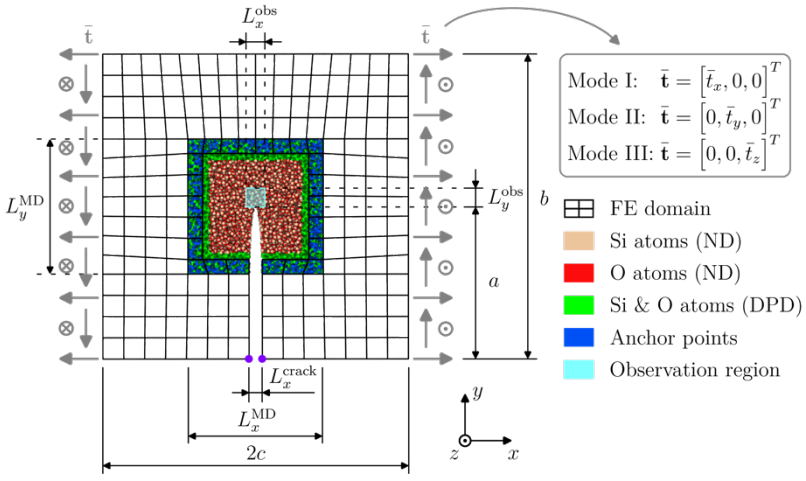


**Fig. 1:** Geometric specifications of the fracture simulations [1].

rectangular plate specimens are shown in Figure 2. These are realized by applying tension (mode I), in-plane shear (mode II) or out-of-plane shear (mode III) to the boundary of the FE domain.

To compare the results obtained in the simulations with experimental values, we derive the critical stress intensity factors $K_{ic}$ $(i = \mathrm{I}, \mathrm{II}, \mathrm{III})$ for the three fracture modes. Using tabulated formulas, the

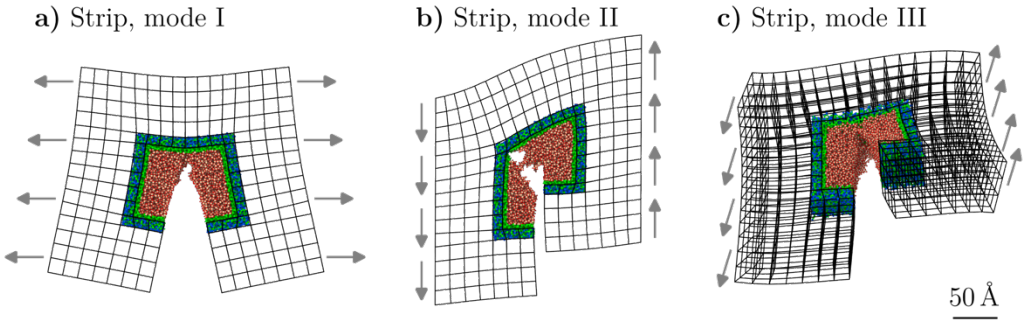


**Fig. 2**: Deformed configurations of a rectangular plate with an edge notch ("strip") applying a) mode I, b) mode II, and c) mode III conditions [1].

applied boundary conditions are translated into the currently applied stress intensity factors $K_i$. For instance, the stress intensity factor under mode I conditions for the strip under tension can be expressed as [4]

$$K_I = \frac{P}{b}\sqrt{\pi a}F,$$

where $P$ is the force exerted on the boundary of the FE domain and $F$ is a geometry factor that relates the crack length $a$ to the sample width $b$. By determining the point at which the crack starts to propagate based on the maximum virial stress measured in front of the crack tip, we thus obtain the critical stress intensity factors $K_{ic}$.

An important prerequisite for the evaluation of $K_{ic}$ is the applicability of linear elastic fracture mechanics (LEFM). LEFM assumes that plastic effects are limited to a sufficiently small area near the crack compared to the overall dimensions of the specimen [5]. By measuring the distribution of different strain measures in the atomistic samples, we show that these conditions are fulfilled in the present setups. Since the values for $K_{ic}$ are within a plausible range both in terms of experimental values and analytical considerations based on LEFM, we conclude that the Capriccio method is a powerful tool to apply arbitrary mechanical boundary conditions to MD specimens in a facile manner while upscaling the overall specimen dimensions, yielding quantitatively reasonable results. This is an important insight for future studies in P6 using the Capriccio method to investigate fracture in amorphous materials.

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## aP6: Overcoming hurdles in concurrent discrete-to-continuum coupling

Lukas Laubert and Sebastian Pfaller

Discrete-to-continuum coupling techniques are applied in non-affine mechanical loading analyses of particle-based models such as for analyzing fracture modes I, II, and III. Our contributions [1] and [2] investigated the Capriccio method, a state-of-the-art FE–MD coupling approach, focusing on strain inconsistencies between coupled domains under mechanical loading. They revealed that the coupled region experiences motion resistance, i.e., counteracting forces opposing spatial motion. [1] confirmed that conducting a larger number of smaller displacement increments alleviate this effect, while [2] showed that the anchor point (AP) stiffness—crucial for force transmission between domains—not only penalizes spatial domain mismatches but also suppresses motion across space, which inherently requires temporary mismatches. As a remedy, we introduce an additional coupling constraint that decouples the rigid-body motion of a confined MD region from its deformation-related movement. With this extension, strain inconsistencies in load cases involving asymmetric displacements of the coupling regions are reduced to levels comparable to simulations where the MD sample's center of mass remains practically stationary. Moreover, the extension rules out certain dynamic contributions in the MD region and restores the FE stiffness matrix singularity typical of purely static FE problems. A simple demonstration is the rigid-body translation of a sandwich system in which an MD sample is coupled to two FE layers on opposite sides. Using the original coupling scheme, Figure 1 (left) shows persistent strain accumulation,

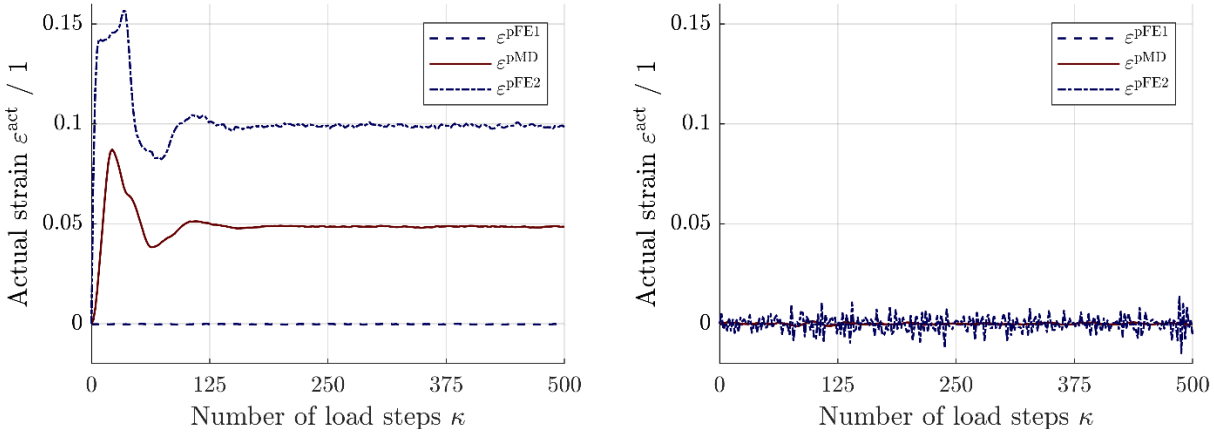


**Fig. 1:** Evolution of the average actual strain in each MD and FE domain under rigid body displacement using (left) the original Capriccio coupling scheme and (right) the rigid-body decoupling extension.

whereas the modified scheme in Figure 1 (right) eliminates it—at the cost of minor strain fluctuations in the FE domain, likely due to local force fluctuations in the MD region and slightly asymmetric AP spring distributions across the two coupling zones. Overall, this extension enables more accurate deformation and fracture studies, such as bending simulations, where the MD sample traverses large spatial distances.The introduced extension eliminates motion resistance related to rigid-body motion of the MD domain, but does not address contributions arising purely from deformation. To mitigate these effects, the AP stiffness concept must be refined. In the original Capriccio method, the AP stiffness not only binds MD particles to the FE mesh but also penalizes movement of the FE mesh from its previous position after the preceding iteration. This restricts the FE mesh from moving freely relative to the MD particles, promoting strain deviations—especially under Dirichlet boundary conditions.

To resolve this, the AP stiffness is divided into two components. During the MD run, the AP stiffness retains its original role, tightly coupling MD particles to the FE domain. During the FE run, however, it is replaced by a newly introduced molecular statics (MS) stiffness contribution. This MS stiffness can be chosen significantly smaller, allowing temporary separation between FE and MD domains

and thus reducing motion resistance. Moreover, the MS stiffness can be tuned to approximate the effective stiffness of the MD region during the FE run—particularly when combined with the earlier rigid-body decoupling extension. While this approach performs well in simplified 1D coupling tests, applying it to realistic MD scenarios becomes challenging when the AP-to-MD stiffness ratio is much greater than one. Tremendous local force and position fluctuations of the MD particles can induce unbalanced forces on the FE mesh, leading to skewed elements and early simulation failure unless stabilized by a rather high MS stiffness, thereby limiting the potential benefits of this approach.

Another coupling modification, which shows optimal performance in 1D models but faces similar stability challenges, involves redefining the FE coupling region as an interface. Here, spring attachments during the FE calculation act only on the interfacial nodes—analogous to the MS stiffness but localized at nodal points. This allows a more precise emulation of the MD region's effective stiffness, as the FE-coupling no longer spans a mixed-stiffness transition zone. The FE domain retains full stiffness across this region, which still contains MD particles, but the AP forces are projected solely onto the interface nodes. Figure 2 compares the strain evolution for identical 1D geometries using (left) the original Capriccio coupling with optimal parameters and (right) the new interface–interphase approach, which also includes the rigid-body decoupling extension.

In the original Capriccio method, improved results under optimal parameters require increasing the number of boundary-imposed displacement increments, i.e., a larger number of finer resolved

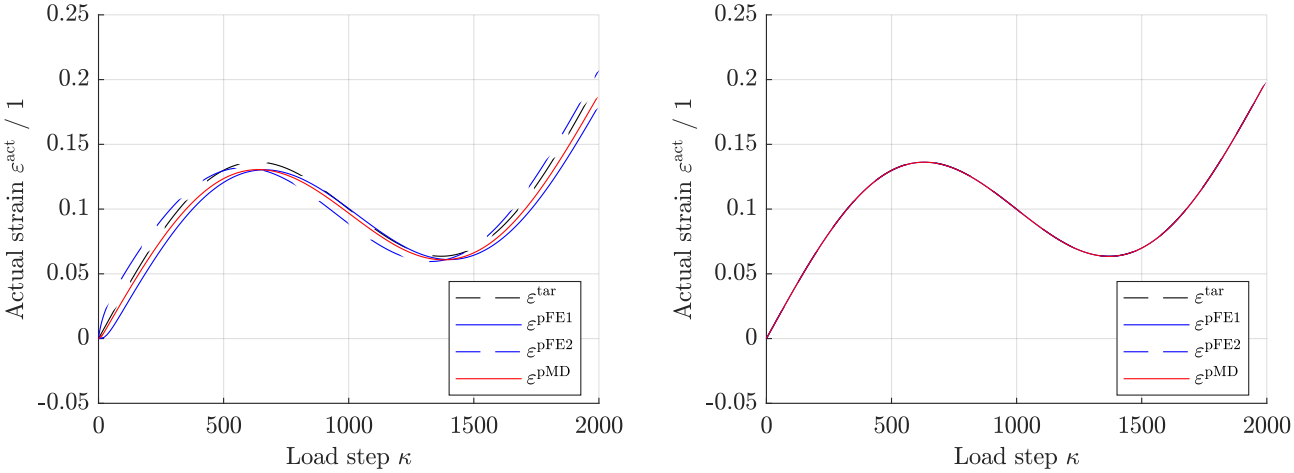


**Fig. 2**: Evolution of the actual strain in each MD and FE domain under one-sided Dirichlet loading, using (left) the original Capriccio coupling with optimal parameters and (right) the interface–interphase approach.

load steps, which raises computational cost. Moreover, the optimal parameter values depend on the chosen number of load steps. In contrast, the new hybrid interface–interphase approach only requires increasing the AP stiffness—or directly fixing MD particles to the FE domain position. Its performance remains unaffected by the load step resolution and the associated computational effort, although it still relies on a staggered solution scheme. As the new approach—pending further methodological extensions for 3D systems—is not yet stable for fully resolved 3D MD–FE coupling setups, further stabilization strategies for the FE nodes—without reintroducing motion resistance—are currently under investigation.

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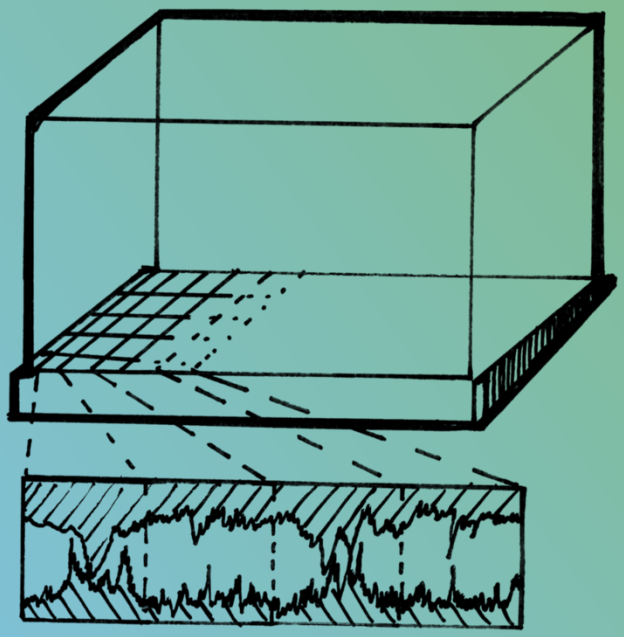

# P7

## COLLECTIVE PHENOMENA IN FAILURE AT COMPLEX INTERFACES

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# P7: Fracture at Interfaces of Architected Thin-Layer-Composites

Leon Pyka and Paolo Moretti

Graded and architected materials can be designed to adapt mechanical properties to the individual use case. For instance, hierarchically structured materials have shown enhanced work of failure and desirable adhesion and detachment properties. This material design falls within the realm of bionic engineering, as multiple examples of hierarchical microstructures can be found in nature, ranging from bone to the gecko foot [1,2,3].

Recent numerical studies have employed coarse-grained methods and network simulations to elucidate the mechanisms by which hierarchical arrangements confer greater resistance to fracture [5,6,7]. So far, project P7 has studied the effects of fracture phenomena in different bio-inspired thin-film structures. The employed network model represents the material as a set of connected nodes, enabling both fracture by edge removal and the generation of desired geometry. The gap structure leads to the localisation of failure exactly at the interface. In the presence of a notch at the interface, the work of fracture is higher than that of reference systems with similar numbers of connections [4].

Expanding upon these findings, exploratory studies were designed to model thin composite structures where a hierarchical, graded or reference structure is placed on a reference structure (Fig. 1).

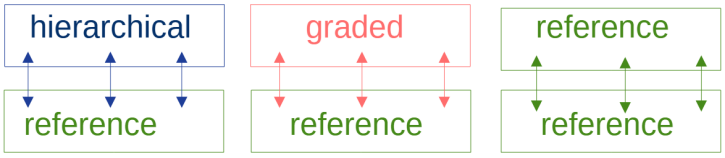


**Fig. 1:**: Schematic of the different tested thin composite structures.

The graded structure is designed so that the number of horizontal connections per layer is the same as in the hierarchical system, but the exact gap structure is dissolved. As this composite system of two structural types is symmetric, the localisation effect cannot be observed; therefore, more systems with different base-structure heights are tested.

In the case of different stiffnesses in the base reference structure, it is evident that for systems with pre-notches at the interface, the graded and hierarchical structures exhibit higher work of fracture than the reference system. The same holds for systems with different base-structure heights (offsets), as depicted in Fig. 2.

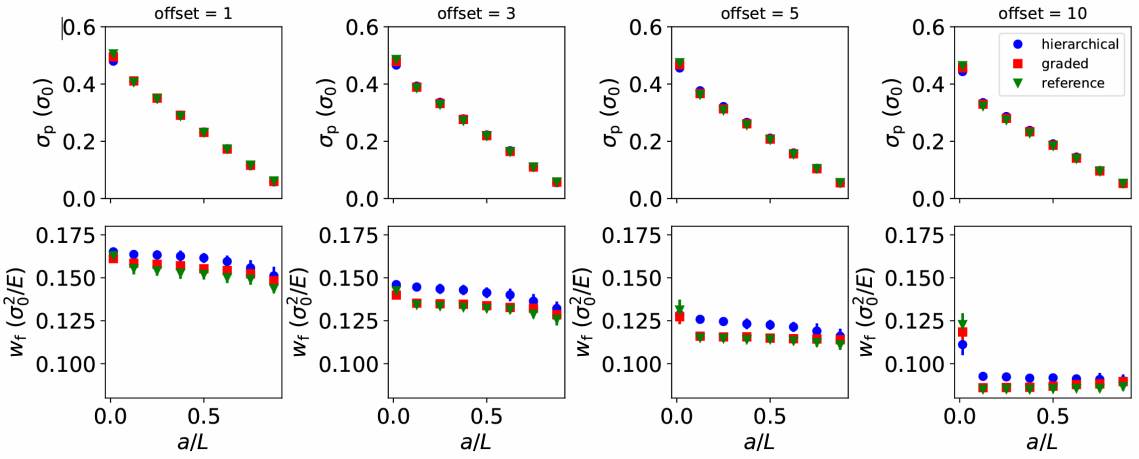


**Fig. 2:** Maximum strain $\sigma_p$ and work of fracture $W_f$ for systems of different base-structure heights (offset) with respect to pre-notch lengths a divided by structure length L.

The statistical simulations so far have provided the necessary evidence of the improved performance of the architected structures. Further investigations of the system's distribution of elastic energy and density of state aim to provide a generalised understanding of the behaviour and its underlying mechanisms, culminating in the observed improvements.
These investigations focus on elastic energy and the local density of states with eigenvalues near the lower spectral edge (associated with low-energy deformation modes). As evident from Fig. 3 an asymmetry is manifesting in the architected systems compared to the reference. But the most decisive influence is visible in the hierarchically structured systems. It shows higher energy in the stiffer bottom layer. The local density of states is affected by the gap structure in the hierarchical realisation, leading to differences in the density of eigenvalues associated with different energies. This evidence suggests that the underlying mechanisms are interlinked with the energy redistribution.

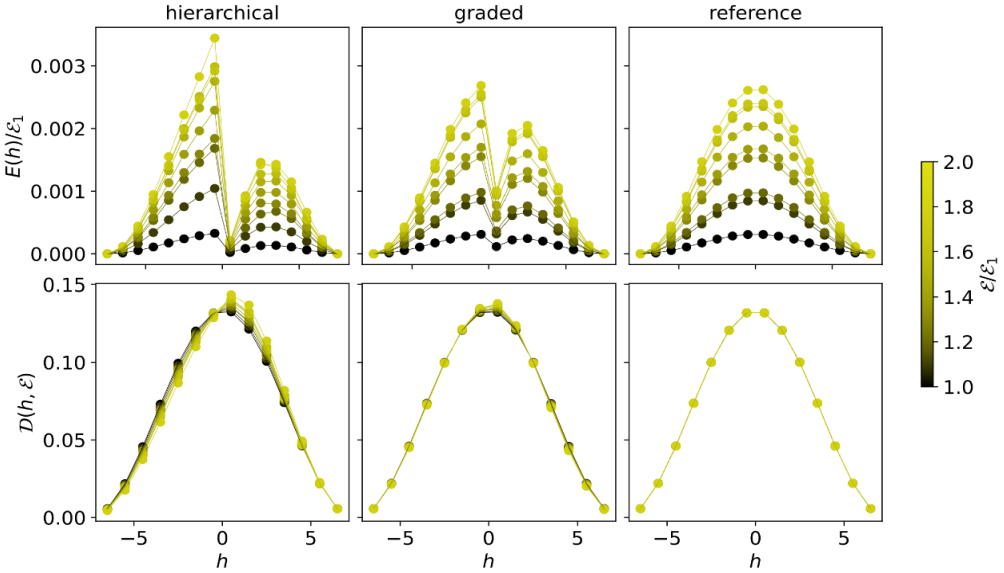


**Fig 3.:** Elastic energy and density of state for a composite system where the lower part of the composite is of higher stiffness.

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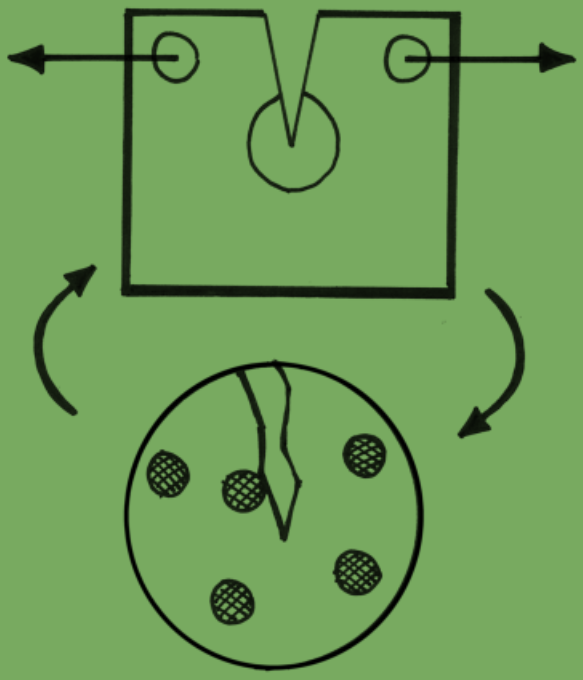

# P8

## FRACTURE IN POLYMER COMPOSITES: MESO TO MACRO


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**Lucie Spannraft**

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Applied Mechanics
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# P8: Efficient phase-field fracture simulations for fracture analysis in heterogeneous materials

Maurice Rohracker and Julia Mergheim

Project P8 investigates the influence of mesoscopic parameters on the macroscopic fracture properties of nanoparticle-reinforced polymers using homogenization methods. Typical mesoscopic parameters include the volume fraction and configuration of nanoparticle-reinforced structures. For mesoscopic simulations, an efficient fracture simulation framework is essential for a computationally feasible homogenization scheme. The phase-field fracture method is a popular approach for simulating fracture. However, it is computationally expensive, particularly for heterogeneous materials. In this method, the crack is approximated by a smeared field, known as the crack field, which is controlled by the length scale parameter $l_c$ (see Figure 1) and requires appropriate mesh sizes near the crack. Crack propagation is only correctly captured with small time

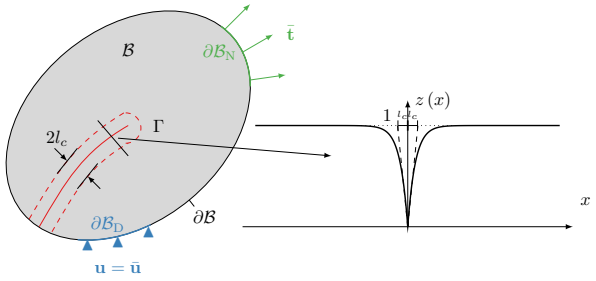


**Fig 1:** Smeared model of the phase-field fracture method.

step sizes. Additionally, minimizing the nonconvex functional leads to a fully coupled solution scheme for both the displacement field and the crack phase-field. These factors contribute to the high computational cost. Therefore, the development and implementation of performance enhancement strategies are necessary. The phase-field model for brittle fracture is based on Griffith's energy concept of fracture, the main developments of which are summarized in [1]. The solution of both fields can be obtained by finding $\mathbf{u} \in \mathcal{B} \rightarrow \mathrm{R}^{\mathrm{dim}}, \mathrm{z} \in \mathcal{B} \rightarrow [0,\,1]$, with $\mathrm{z} = 1 \Rightarrow$ intact and $\mathrm{z} = 0 \Rightarrow$ broken, s. t.

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

Three performance enhancement strategies are incorporated into the standard phase-field fracture model, as described in [2]. The residuum-based convergence criterion, commonly used as a convergence criterion in alternating minimization schemes, exhibits slow convergence during fracture time steps. Drawing on [3], a physically motivated ansatz for the convergence criterion, based on the fracture energy, the central quantity in these simulations, is introduced. In this approach, a time step is considered converged if the relative change in fracture energy falls below a specified tolerance. Various methods of adaptive spatial refinement (ASR) are compared in [4]. ASR constitutes the second performance enhancement strategy, where the phase-field threshold refinement criterion is applied. Apart from that, a repeating time step scheme is employed. Adaptive temporal refinement and coarsening further enhance the efficiency of the fracture simulation framework. Large time step sizes are initially used during the elastic loading regime. The time step size is refined, and the process repeated if significant changes in fracture energy are detected. Once the time step size is refined, coarsening is suspended until the initial time step is resolved. The solution process for a time step, incorporating all performance enhancement

strategies, is outlined in Figure 2. This approach ensures that crack propagation is captured This approach ensures that crack propagation is captured only on the finest mesh with the smallest time

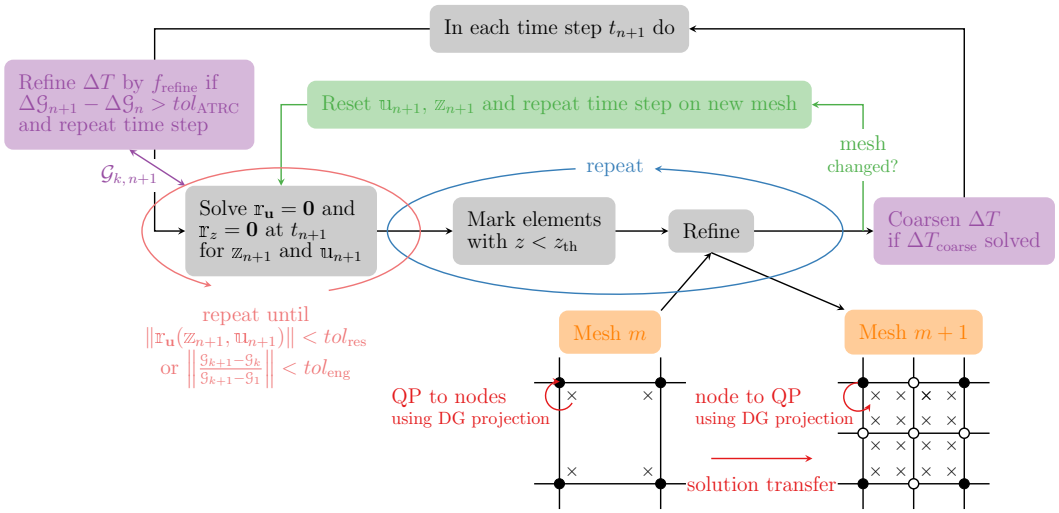


**Fig. 2:** Staggered solution scheme with all performance enhancement strategies.

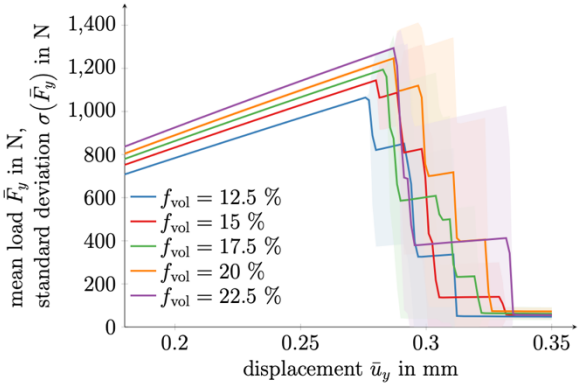


**Fig. 3:** Load-displacement curves of the multi inclusion double edge notch tension test.

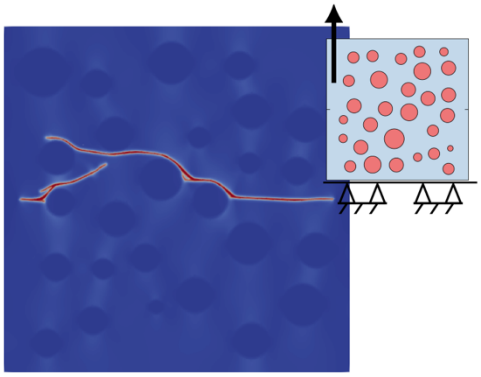

**Fig. 4:** Phase-field contour of the tension test of one configuration of the complex structure.

step size. The effectiveness of this enhanced simulation framework is demonstrated in [2] on a benchmark problem, where the parameters for the three strategies are calibrated independently. In this case, a highly accurate solution achieves a speedup of 3, while a more efficient solution attains a speedup of 17 with minimal loss of accuracy. The performance enhancement strategies are also applied to fracture simulations of heterogeneous structures. In these simulations, stiff silica particles of varying sizes are embedded in a weaker epoxy matrix with two notches, and a tensile load is applied. Four random configurations for each of the five different volume fractions, ranging from 12.5 % to 22.5 %, are generated and the fracture simulations are performed. Figure 4 shows the statistical load-displacement response of all simulations. An increasing volume fraction results in a stiffer response as well as a higher peak load. Different crack patterns are observed from the fracture analysis, as seen in Figure 4. Crack propagation initiates at one of the two notches, traverses the matrix material, circumvents the particles, or may arrest in front of a particle before continuing. These phenomena produce complex crack patterns that are highly dependent on the heterogeneous configuration. The application of performance enhancement strategies yields reliable physical results within reasonable computation times, enabling further investigations, such as the inclusion of particles of uniform size or defects.

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## aP8: Generalized mechanical interfaces at finite strains

Lucie Spannraft, Paul Steinmann and Julia Mergheim

Interfaces exist on various size scales in numerous materials relevant for many engineering applications. For instance, microscopic grain boundaries in polycrystalline metals or macroscopic adhesive bonds in, e.g., aircraft production, lightweight construction or sealing applications. Interfaces significantly impact the overall behavior by, both, increasing the strength but also acting as a weak link in case of decohesion. In many applications, anisotropic decohesion arises with interacting normal and shear damage modes. Further, the cohesive damage is affected by in-plane stretch and the corresponding membrane response from interface (in)elasticity. For anisotropic decohesion at finite strains, additional cohesive stresses are required to fulfill the balance of angular momentum at the interface, i.e.,

$$[\bar{\boldsymbol{P}}^{\mathrm{c}} + \bar{\boldsymbol{P}}^{\mathrm{m}}] \cdot \bar{\boldsymbol{F}}^{\mathrm{T}} + \boldsymbol{T}^{\mathrm{c}} \otimes [[\boldsymbol{\varphi}]]$$

with the cohesive and membrane Piola stresses $\bar{\boldsymbol{P}}^{\mathrm{c}}$ and $\bar{\boldsymbol{P}}^{\mathrm{m}}$, the cohesive tractions $\boldsymbol{T}^{\mathrm{c}}$, the interface deformation gradient $\bar{\boldsymbol{F}} \coloneqq \bar{\nabla}\bar{\boldsymbol{\varphi}}$, and the displacement jump $[[\boldsymbol{\varphi}]]$.

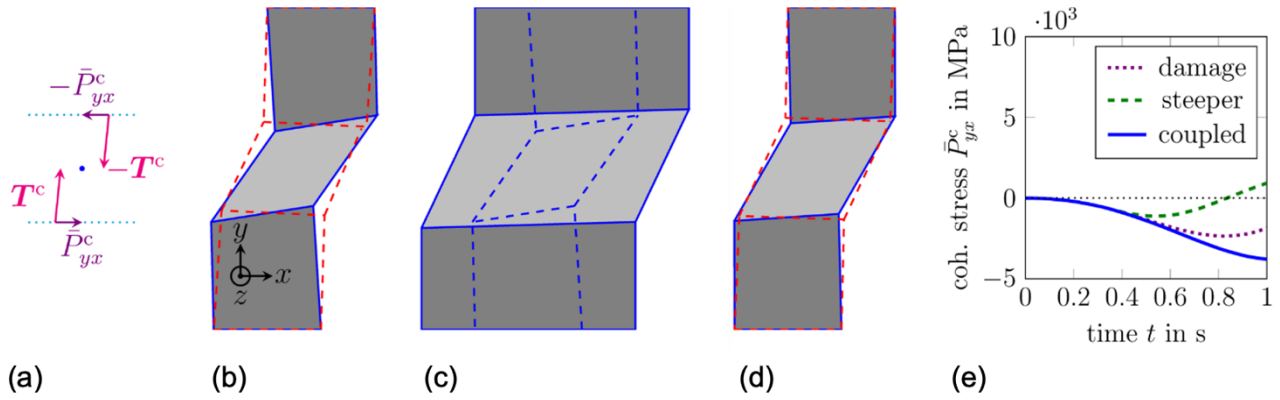


**Fig. 1:** (a) Schematic representation of cohesive tractions and stresses at a generalized interface with displacement jump. (b-e) Tension-shear tests at an interface (light gray) with cohesive anisotropy comparing $\bar{\boldsymbol{P}}^{\mathrm{c}}$ calculated (blue) and non-physical $\bar{\boldsymbol{P}}^{\mathrm{c}} \doteq \boldsymbol{0}$ (red). (b) Elastic interface. (c) Elastic interface w(solid blue)/wo(dashed blue) in-plane stretch. (d) Damage mode coupling. (e) Cohesive stress for different damage progressions and coupling corresponding to (d). Cf. [1,2].

When neglecting these shear like stresses, the cohesive tractions may cause non-physical rotations at the interface, which overall creates incorrect results, cf. Figure 1 (a,b). Different influences on the cohesive stresses can be observed in FEM simulations using our generalized interface model [2]. In-plane stretch (even when not accounting for a membrane formulation) reduces cohesive stresses by means of the interfacial determinant of the interface deformation gradient, i.e., the enlargement of the interface, compare Figure 1 (c). Cohesive damage initiation and progression (also due to damage mode coupling) affects cohesive anisotropy, and thus, the cohesive stresses. In general, cohesive damage reduces the stresses for constant or decreasing anisotropy, see Figure 1 (d,e).

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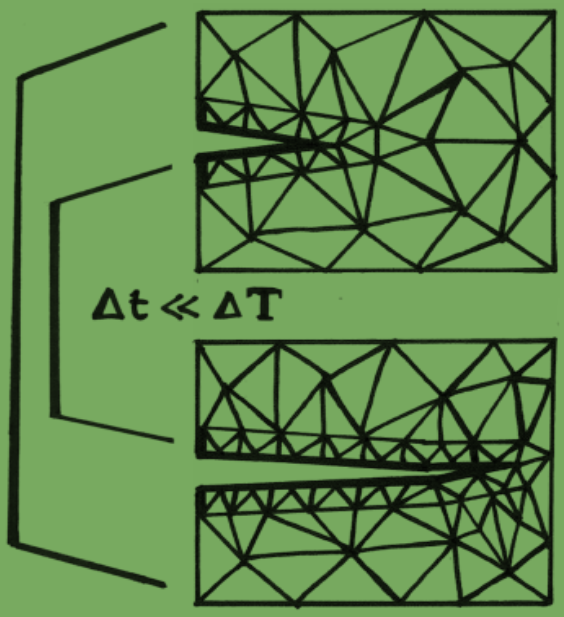


# P9

## ADAPTIVE DYNAMIC FRACTURE SIMULATION

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# P9: A discrete mechanics perspective on bond-based peridynamics

Prateek Prateek, Giuseppe Capocianco and Sigrid Leyendecker

Simulating fracture remains one of the most challenging problems in computational engineering. While Classical Continuum Mechanics (CCM) provides a powerful framework for modelling elastic deformation, its core mathematical requirement, i.e. the existence of continuous spatial derivatives fundamentally breaks down near a crack surface or tip. When a crack forms, the displacement field becomes discontinuous, rendering the standard CCM governing equations singular and unsolvable at the crack face. To circumvent this mathematical singularity techniques, such as the eXtended Finite Element Method (XFEM), which requires specialized enrichment functions to model displacement jumps, or Phase-Field Approaches, which smear the discontinuity over a finite width. These methods often increase computational overhead and introduce model-dependent parameters that complicate the simulation process.

In Project P9, we have adopted Peridynamics (PD), a fundamentally different, particle-based nonlocal formulation, to model crack initiation and propagation. In PD, a material point $\boldsymbol{x}$ interacts nonlocally with all other material points within a spherical finite neighbourhood $\mathcal{H}_x$ with a radius $\delta$, also known as it's horizon. Instead of forces being calculated based on the spatial derivative of the displacement field at a single point (as in CCM), they are computed by taking an integral to sum up all the interactions the point has with its neighbour, as shown in Figure 1. Since this interaction between certain points can be present or absent, fracture is an inherent part of the constitutive model itself, and the equations of motion remain mathematically well-posed and can still be solved. Several different formulations of PD exist, categorized by how the interaction force between points is calculated. We have concentrated our initial implementation and validation efforts on the Bond-

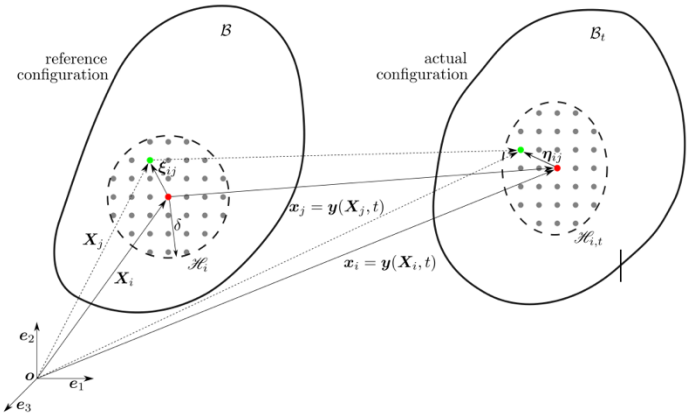


**Fig. 1:** Discrete PD body in the reference and actual configuration.

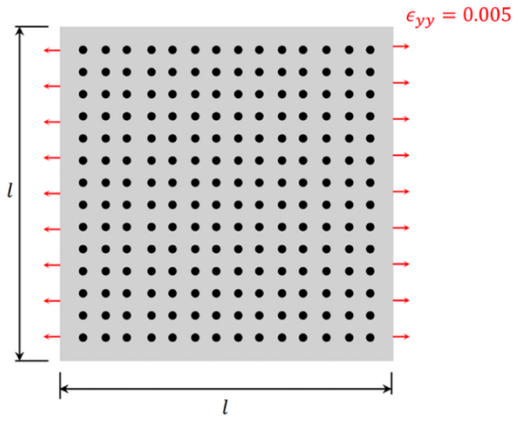


**Fig. 2:** Setup for elastodynamic study.

Based Peridynamics (BBPD) formulation. In BBPD, the force density that two material points exert on each other is parallel to the vector connecting the points. The resulting equations of motion are given by:

$$\rho\,\ddot{\boldsymbol{x}}(t) = \int_{\mathcal{H}_x} \boldsymbol{f}\left(\boldsymbol{x}'(t) - \mathbf{x}(t), \boldsymbol{X}' - \boldsymbol{X}\right) dV_{X'} + \mathbf{b}(\boldsymbol{X}, t),$$

Moving beyond standard time-integration schemes, a critical component of Project P9 is the development of structure-preserving Variational Integrators (VIs) specifically tailored for the PD formulation. The primary aim of employing VIs is to construct numerical methods that naturally conserve physical properties, such as energy and momentum, while accurately simulating the initiation and propagation of cracks in materials. By deriving the discrete equations of motion from a discrete Lagrangian, VIs provides superior long-term stability and accuracy compared to conventional schemes, which is crucial for complex, long-duration fracture simulations where subtle energy drift can lead to non-physical crack growth.

To investigate the performance of the variational integrators derived for bond-based PD, different discretization schemes were used to approximate the discrete Lagrangian, resulting in various explicit and implicit update schemes. Specifically, schemes such as the right-end rule, trapezoidal rule, and midpoint rule were utilized, where the right-end and trapezoidal rules lead to explicit schemes while the midpoint rule resulted in an implicit scheme. Figure [2] illustrates the setup of the elastodynamic study performed using these integrators: an initial displacement is applied on the left and right sides of the square discrete body, and the body is then allowed to oscillate freely.

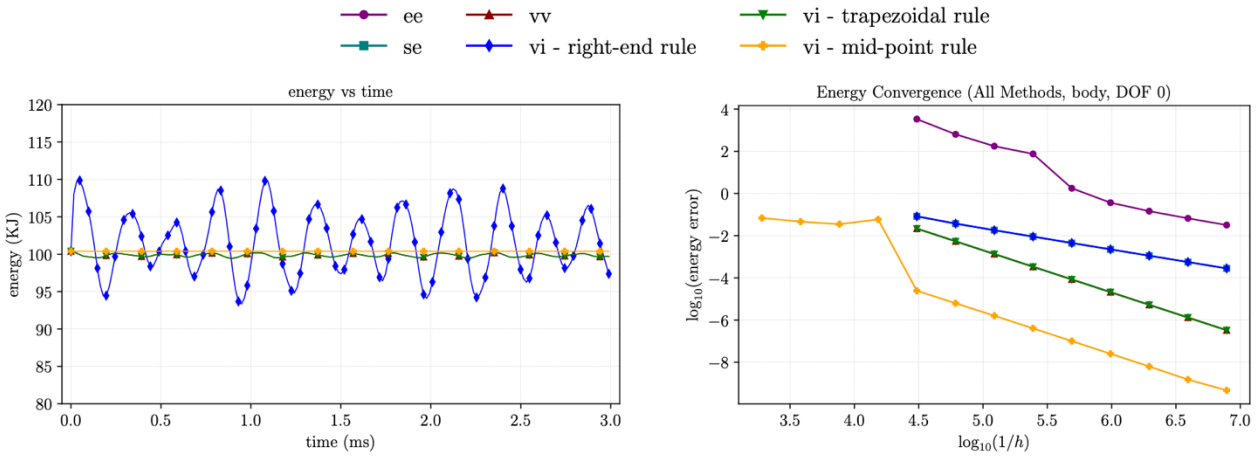


**Fig. 3:** Energy conservation plot (left) and energy convergence plot (right) for different numerical integration schemes

The convergence behavior of these integrators was rigorously investigated through this elastodynamic test, with the results highlighting significant differences in their long-term stability and accuracy. As shown in Figure [3], the implicit midpoint rule VI yields the lowest energy error for a given time-step size. The implicit midpoint-rule variational integrator, the trapezoidal rule, and the velocity Verlet (VV) method all achieve a robust second-order convergence rate. Notably, the VV and trapezoidal-rule curves coincide exactly, whereas the implicit midpoint rule consistently attains a substantially smaller energy error for any chosen time-step size. In contrast, both the right-end rule and the symplectic Euler method overlap perfectly, confirming a shared but less accurate first-order convergence rate. Taken together, these findings underscore the superior energy stability of variational integrators within the context of peridynamic simulations.

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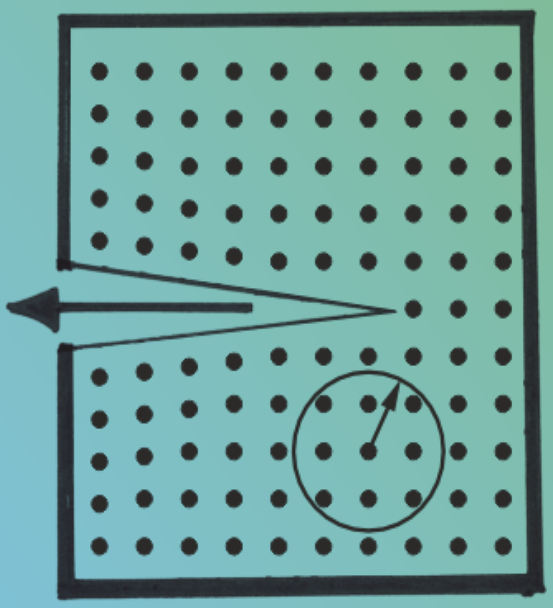

# P10

## CONFIGURATIONAL FRACTURE MECHANICS OF DISCRETE SYSTEMS


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# P10: Investigating neural network approaches for accelerating continuum-kinematics-inspired peridynamics simulations

Aditi Sharma, Ali Javili, Paul Steinmann

Continuum-kinematics-inspired peridynamics (CPD) is an alternative formulation of peridynamics and a geometrically exact framework proposed by Javili et al. [1]. In CPD, the numerical implementation requires discretising the continuum by a finite number of grid points, each occupying a finite volume in space; the interaction between these grid points is characterised by one-neighbour, two-neighbour and three-neighbour interactions within the horizon.

The most common numerical implementation adopts a mesh-free discretisation approach, wherein the domain is divided into uniformly spaced material points with a known volume in the reference configuration. Together, the points form a grid. The mesh-free implies that there are no geometrical relations between points. Moreover, each point in the grid interacts with others within a finite neighbourhood, known as the horizon, which defines the region of nonlocal influence. The material points interact with each other through bonds, and the mechanical response is defined at the bond level, rather than at a continuum point.

In CPD, the governing equations at each material point are expressed as integrals over the horizon. These equations are numerically evaluated at discrete collocation points. At each of these collocation points, the horizon integrals can be approximated with a quadrature relation using appropriate weighting coefficients. Here, the neighbouring points coincide identically with the quadrature points, and the accuracy of this numerical integration depends on the number of these neighbours. The numerical accuracy of the integration can be enhanced by increasing the number of neighbours present in the horizon of a point. This can be achieved by decreasing the grid spacing and keeping

the horizon size constant, which will increase the number of neighbours for each point. However, achieving this through a uniformly dense grid across the entire domain incurs significant computational cost [2].

Additionally, the nonlocal governing equations involve a single, double, and triple integral over the horizon for one-, two-, and three-neighbour interactions, respectively. The numerical evaluation of these integrals is computationally expensive as it must be performed repeatedly for each material point and at every deformation step, making large-scale simulations computationally prohibitive. Additionally, problems involving intricate fractures are computationally expensive, as the fracture path is heavily influenced by the discretisation level. A finer discretisation increases the number of material points and, consequently, the computational cost.

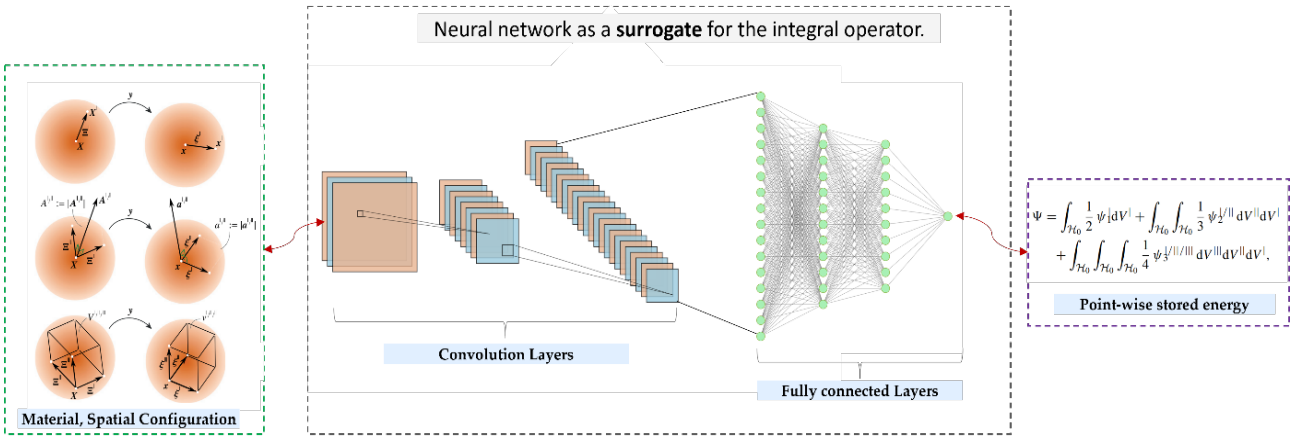


**Fig. 1**: The preliminary framework of the neural network as an integral operator in CPD.

The research aims to explore the feasibility of developing a surrogate neural network to approximate the integral operations in CPD. The goal is to train the network to predict the outcomes of one-, two-, and three-neighbour interaction based on representative data, thereby bypassing the need for explicit numerical integration in each iteration. Such a surrogate model could significantly reduce computation time while maintaining acceptable accuracy, making large-scale CPD simulations more accessible. The study will begin by generating high-fidelity datasets from numerical CPD simulations for one-, two-, and three-neighbour interactions. These datasets will then be used to train and validate neural networks that can reproduce the integration results. Finally, the surrogate model will be integrated into the CPD framework to evaluate its performance in terms of accuracy and computational efficiency. Figure 1 shows a preliminary outline of the planned neural network architecture.

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## P10 Damage in continuum-kinematics-inspired peridynamics

Marie Laurien, Ali Javili and Paul Steinmann

Peridynamics [1] is a nonlocal continuum formulation that naturally allows for discontinuities, such as cracks. Continuum-kinematics-inspired peridynamics (CPD) [2] extends the peridynamic framework to overcome the fundamental limitation of classical bond-based peridynamics, i.e., a fixed Poisson's ratio. Despite the potential of peridynamics for fracture modeling, CPD still lacks a comprehensive damage formulation. Therefore, the goal of this work [3] is the introduction of damage into the formulation of CPD. Here, nonlocal interactions between material points are captured via one-, two- and three-neighbor interactions, allowing to measure length, area and volume changes. For each type of interaction, a separate damage variable is employed, depending on the associated strain. For a two-dimensional problem, the damage parameters of the model are derived from the classical fracture energy in a semi-analytical procedure.
In order to assess the model's performance in predicting experimental outcomes, we performed a series of fracture experiments in our laboratory. Diagonally loaded square plates with center cracks of varying inclination angle are tested to study different fracture modes. PMMA was used to analyze brittle material behavior. The center precrack was introduced into the sample by, first, milling a crack and, second, sharpening the crack tip using a very thin saw. Figure 1 illustrates the test setup used in the tensile testing machine (left) and the experimentally observed crack paths (right).

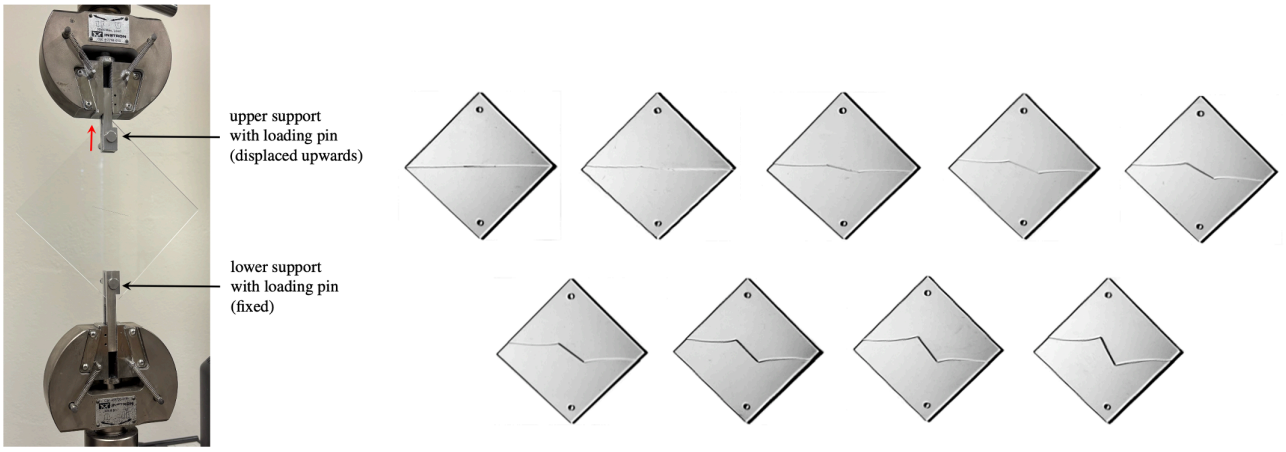


**Fig. 1:** Fracture experiment using a diagonally loaded precracked PMMA plate: Experimental setup (left) and resulting crack paths for varying precrack angles (right).

The numerical results were obtained using a 2D CPD model. As strong nonlinearities are introduced through brittle damage, an incremental damage algorithm is developed to solve the CPD equations. To this end, the damage is incorporated in a subincremental manner into the solution and a Newton-Raphson scheme is employed to solve the equations for a fixed damage state. This procedure substantially improves the convergence behavior.

The comparison of the experimental and the numerical results demonstrates the model's capability to capture the maximum loads and the crack paths. As an example, Fig. 2 illustrates the evolution of the CPD crack path and the corresponding experimental result.

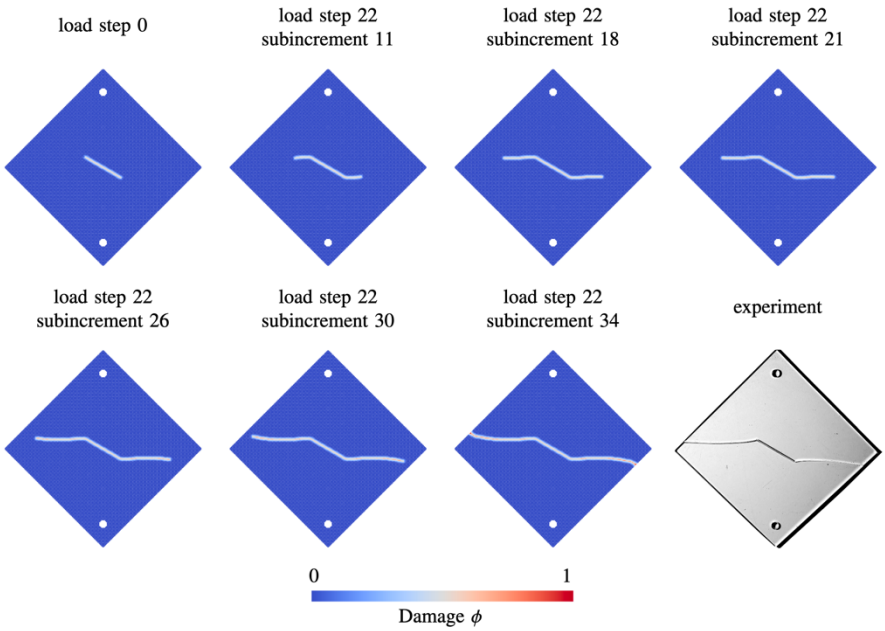


**Fig. 2:** Evolution of the crack path as predicted by the CPD model and comparison to the experimental result for an example crack angle. The CPD path is obtained stepwise due to the subincremental numerical procedure.

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

Anna Titlbach, Paul Steinmann, Michael Stingl, Areti Papastavrou and [1]Andrew McBride
[1] Glasgow Computational Engineering Centre, University of Glasgow

Vasquez-Sancho et al. and Núñez-Toldrà et al. [1,2] have emphasised the important role of the flexoelectric effect in the healing of microcracks in human bones. This effect describes the generation of an electric potential under unhomogeneous deformation, which is caused by the high stress gradients at the tip of a microcrack. The resulting electric field acts as a biological trigger, activating osteocyte activity and initiating the remodelling process. While the flexoelectric effect is well-known in physics and mechanics, research into its occurrence in human bone and its relevance to healing is still in its infancy.

Motivated by the fact that a deeper understanding of such regeneration mechanisms, made possible by accurate modelling and simulation, has considerable potential for further developing medical treatment strategies and innovative therapeutic approaches, we have developed a micromorphic modelling approach [4,5], that can be used to simulate the initial healing phase of microcracks, triggered by flexoelectricity. This is captured in our model by the increase of the nominal bone density. The finite element model is implemented using the open-source library deal.II. As a numerical example we consider a cantilevered, cracked bone sample that is subjected to strong bending, to induce unhomogeneous deformation and amplify stress gradients, see Figure 1.

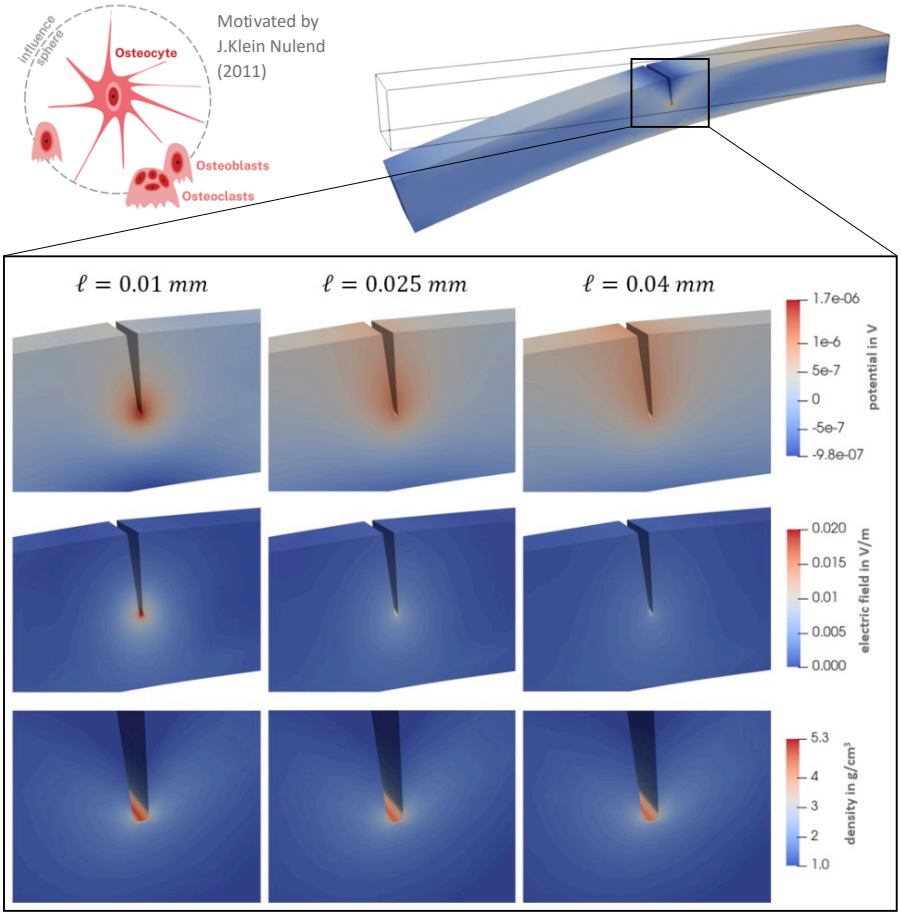


**Fig. 2:** Distribution of the electric potential, the electric field magnitude and the nominal bone density inside the cracked bone sample, showing variations in the micromorphic length scale; the schematic drawing at the top left shows the non-local nature of osteocyte mechanosensing [5], which is captured by the micromorphic length scale

A micromorphic length scale is introduced in our model to capture the size-dependent effects, which come along with microstructured materials, as well as the inherently nonlocal nature of osteocyte mechanosensing [5]. As can be seen in Figure 1, the length scale influences the localisation in which the electric potential appears around the crack tip. The more local the potential appears, the higher the electric field and density increase can be observed at the crack tip. Since we do not yet consider healing in our model in the form tissue formation (volumetric growth), but only in the form of density increase, these locally elevated density values indicate that healing will be initiated at this point.
In its current stage, the model is capable to reproduce the key biological stimulus for bone remodelling induced by flexoelectricity, which is captured through a localised increase in nominal bone density at the crack tip. However, calibration of the model parameters based on experimental data is the crucial next step in model development.
The highlights this year were, on the one hand, the publication of the above-mentioned research results in the Journal of Computational Methods in Applied Mechanics and Engineering under the title Modelling the flexoelectric effect in human bone—A micromorphic approach 446 (2025) 118234, and, on the other hand, my contributions at the ESBiomech in Zurich and at the XI. International Conference on Computational Bioengineering (ICCB) in Rome, see Figure 2. Moreover, I have gained valuable experience in teaching, which has greatly contributed to my personal and professional development and provides a deeply rewarding and enriching complement to my daily research work.

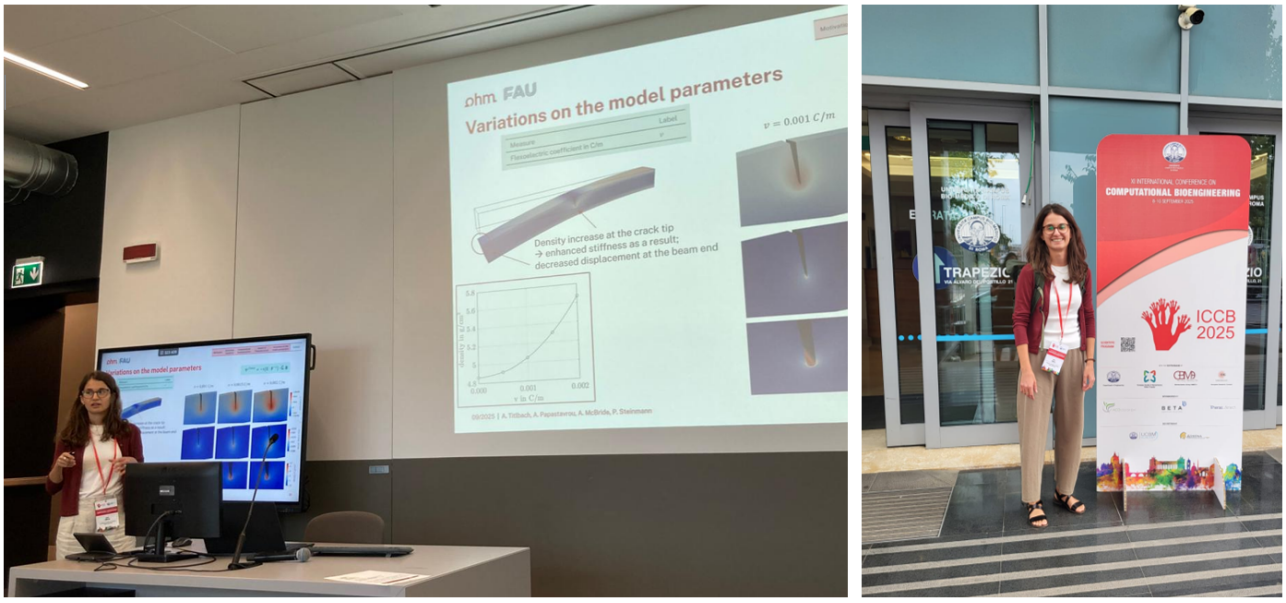


**Fig. 3:** Pictures taken during and after my presentation at the XI. International Conference on Computational Bioengineering – ICCB 2025 – from 8.-10. September 2025 in Rome.

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# P11

## FRACTURE CONTROL BY MATERIAL OPTIMIZATION

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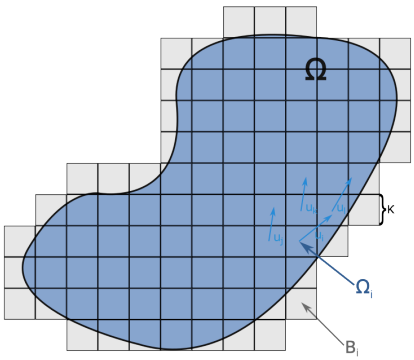
# P11: Research Report from April 2025 to December 2025

Max Zetzmann and Michael Stingl

Peridynamics is a relatively new approach to modeling problems encountered in the field of solid mechanics. It was originally introduced in the year 2000 by Silling in his seminal work [1]. In contrast to classical solid mechanics, which relies on partial differential equations, peridynamics reformulates the equations determining the displacement by focusing on the forces between points within a body determined by a given function f. In particular, this reformulation dictates that the equations of motion are expressed not through the spatial derivatives of u, but rather through an inherently non-local integral term whose integrand relies on finite differences of the displacement field, replacing the need for any spatial gradient. This shift in the mathematical formulation relaxes the regularity assumptions on the space of solutions, allowing displacements that exhibit spatial irregularities. In particular, solutions are now no longer required to have a weak derivative, as is usual in the classical theory. This, on the other hand, caused peridynamics to gain substantial traction in the domain of fracture modeling, where the presence of cracks and other defects naturally introduces discontinuities in displacement.

The original peridynamic model, the so-called bond-based model, first introduced by Silling in [1], provides a straightforward implementation that gained popularity due to its comparable numerical and theoretical simplicity and efficiency. However, this model has limitations, as it can only replicate a fixed Poisson's ratio, which led to the formulation of a more generalized model known as the state-based model. This generalization permits the modeling of materials with arbitrary values of bulk and shear moduli. A particularly noteworthy state-based model is defined in ([2], 5.3 Example 3). One should note that the bond-based model is a special case of this state-based model, meaning that results proven for this choice of the state-based model also naturally apply to the bond-based case.

The current focus of our research in the 3rd cohort of P11 deals with the linearization of the aforementioned state-based model, with the primary objective being establishing the convergence of the solutions of the discretized equations to the corresponding continuous solution under a general set of assumptions. Such a result has already been achieved for the linear static state-based model since the start of the 3rd cohort, which constitutes most of the work done so far.
The convergence therein is proven in two ways: first, within a general context that accommodates a broader range of input data, albeit requiring the precise evaluation of multiple integrals that form the constituents of the equations under consideration, and second, in a numerical context, where one-point quadrature is used to simplify these integrals, resulting in a feasible model for practical applications. As a trade-off, this numerical approach imposes stronger but still manageable assumptions on the input data and, most importantly, is restricted to the use of a specific weighting function. This particular choice for the weighting function, however, is widely seen in the literature and represents a “standard” choice.




To obtain the discretized equations, a version of a piecewise constant approximation is chosen with respect to a partition of the domain Ω resulting from intersections with (half-open) cubes tiling the surrounding space.
To derive an algebraic form, the basis functions for a given κ are then defined to be the characteristic functions corresponding to each element of the partition; the result is then a linear equation of the usual form

$$Ku = b.$$

As mentioned before, this approximation on its own still faces the issue that due to the inherently non-local formulation of peridynamics, each entry of the matrix B contains multiple nested integrals that are infeasible to compute in practice. This motivates the second approach to the convergence proof, which applies a quadrature rule to these integrals. This naturally requires stronger assumptions on the input data, namely the right-hand side and material parameters.
For our research, we require the material parameters to be almost everywhere locally L-Lipschitz continuous and bounded. Both of these requirements do not impose significant restrictions for practical purposes. The "almost everywhere" property allows discontinuities in both the right-hand side as well as the material properties, which is consistent with the overall compatibility of peridynamics with jumps in the displacement.
The proof of both convergence results builds on theory used for the well-posedness of the continuous equations, which has already been shown under general conditions in [5], [6]. The well-posedness was established through techniques comparable to those used in the classical theory of linear elasticity, employing the Lax-Milgram theorem to the bilinear form defining the variational equations on an appropriate Hilbert space based on $L^2(\Omega)^d$, which also realizes the boundary conditions. This was made possible by successfully proving the coercivity and boundedness of the aforementioned bilinear form. The coercivity specifically was attained similarly to the classical theory through a non-local Poincare-type inequality on this Hilbert space.
The convergence proof also makes use of the measure theoretical and topological properties of the set on which the input data jumps. Measure theoretical arguments and boundedness is used to control the terms on those discrete elements on which we don't have control over the input data, while the Lipschitz continuity is used everywhere else. The main idea is that the volume of all elements that we can't control vanishes as the discretization becomes arbitrarily fine. This immediately yields a density result for our choice of using a piecewise constant inner approximation. The convergence in the analytical case then directly follows, while for the model that employed one-point-quadrature, a uniform coercivity result and a convergence result for the discrete bilinear forms are additionally needed and subsequently proven.
We plan to submit these results in a paper around December 2025.
Steps towards future research have also been made by working on similar results for non-linear dynamic models including fracture.

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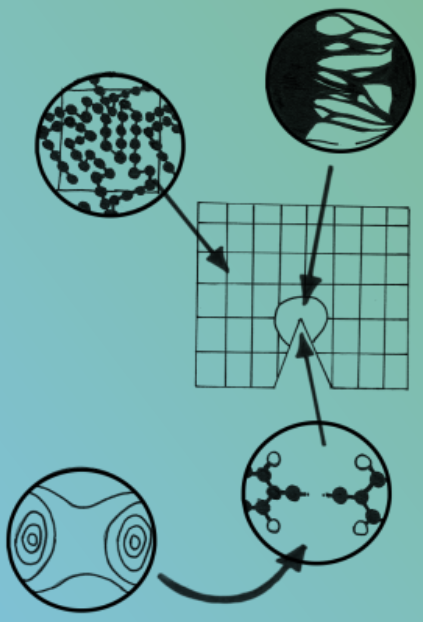

# P12

## QUANTUM-TO CONTINUUM MODEL OF THERMOSET FRACTURE

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# P12: Development of a coarse-grained molecular model of the cross-linked epoxy

György Hantal, Sebastian Pfaller and Ana- Sunčana Smith

To facilitate the ultimate goal of project P12, the direct coupling of the molecularly resolved cross-linked epoxy to a mechanically equivalent FEM model, part of our efforts have been dedicated to developing a simplified, coarse-grained model to be directly coupled through the Capriccio scheme. The application of coarse-graining serves two purposes: on the one hand, it allows to get rid of the irrelevant degrees of freedom and thereby to increase the size of the system, and on the other hand, by defining charge neutral interaction sites, this procedure generates only short-ranged (effective) interaction potentials, which eliminates, by construction, the problem of missing long-range interactions beyond the boundaries of the molecularly resolved model. The chosen interaction scheme was the Iterative Boltzmann Inversion technique [1] which allows to gradually refine bonded as well as non-bonded interaction potentials defined between any interacting beads. This technique aims at preparing a coarse-grained model that is equivalent to the fine-grained one from a structural point of view by assuring that both models produce the same equilibrium structural correlation functions. Initially, fine-grained molecular configurations were generated by running 5 different curing simulations, each of them reaching about 93-96% crosslinking degree. In the first step, a python script was prepared that takes the equilibrium configurations as well as the definition of the coarse-grained beads and the requested bonded and non-bonded interactions. The script then generates the initial guess (by Boltzmann inversion) of the interaction potentials in a tabulated form adapted for the GROMACS simulation software. A second script was also prepared that recomputes the structural correlation functions produced by the test simulations applying the guess potential. The recomputed correlation functions are then used to update the interaction potentials for the next round of test simulations. Figure 1 illustrates the definition of the coarse grained beads (Fig 1a) as well as the a coarse-grained bond stretching potential defined between the CB and CN beads (Fig 1b) corresponding to the distance distribution computed on the reference fine-grained configurations (Fig 1c). By the end of the year 2025, 6 rounds of iteration have been performed, which allowed us to converge the coarse-grained bonded interaction potentials (bond stretching and bending). Additional rounds of iterations are currently being run to obtain also the (28) non-bonded interactions which are known to take longer to converge. In the next step, the equilibrium linear elastic properties (isotropic Young's modulus and Poisson's ratio) will be determined in preparation for the scale-bridging Capriccio coupling between the particle-based and continuum epoxy models.

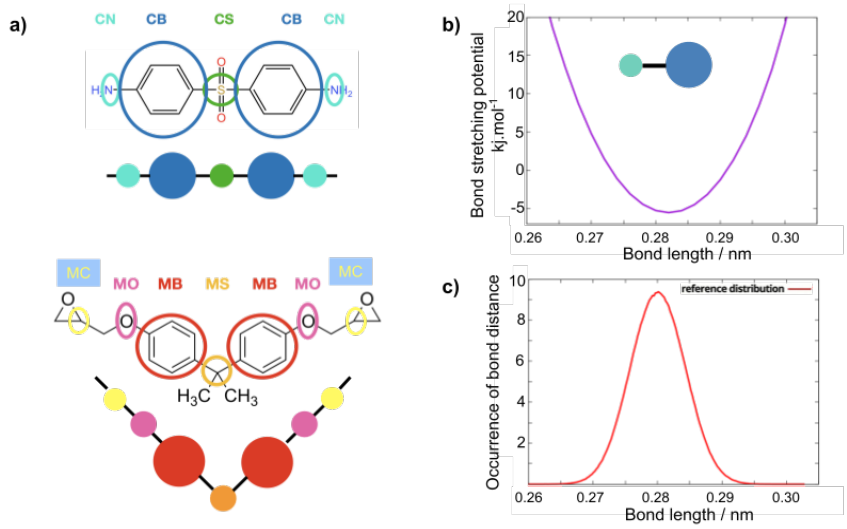


**Figure 1:** Illustration of the coarse-graining procedure: Definition of the coarse grained beads (a), coarse-grained bond stretching interaction potential between the CB and CN beads (b) corresponding to the reference bond distance distribution function (c).

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# aP12: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 develop a chemically accurate and physically robust description of bond formation during epoxy curing, enabling predictive modeling of network structure and, ultimately, fracture behavior. In the current phase of the project, the focus is on understanding how local chemical environments influence curing reaction energetics and incorporating these effects into a high-fidelity curing protocol for epoxy thermosets. Previous studies have demonstrated that curing reaction dynamics directly impact network morphology and material properties [1].

Earlier stages of the project relied on gas-phase quantum chemical calculations to parameterize curing reactions. However, significant discrepancies between gas-phase activation energies and experimentally inferred values motivated the explicit inclusion of environmental effects. To address this, we employed QM/MM (ONIOM) calculations, treating a ~30 Å region around the reaction site explicitly to capture steric constraints, electrostatic screening, and hydrogen bonding interactions from the surrounding polymer matrix. This approach provides activation barriers that are representative of in-situ curing conditions and suitable for direct comparison with experimental data.

Using an automated workflow, reaction events extracted from reactive molecular dynamics simulations are systematically identified and subjected to a posteriori QM/MM analysis. This workflow enables consistent construction of QM/MM models and high-throughput extraction of activation energies and local structural descriptors, providing a statistically meaningful dataset spanning hundreds of curing events.

Analysis of the QM/MM results revealed a broad distribution of activation energies, with many barriers substantially higher than gas-phase estimates. Importantly, a subset of reactions exhibited significantly reduced activation energies. Structural analysis showed that these low-barrier outliers consistently coincided with the presence of hydrogen bonding near the reacting epoxy site, indicating a stabilizing effect of hydrogen-bonded configurations. Based on this observation, a modified curing protocol was developed in which reaction events are conditioned on predefined hydrogen-bonding geometrical criteria. This allows systematic control over hydrogen-bonded reaction environments and enables direct assessment of their influence on curing dynamics.

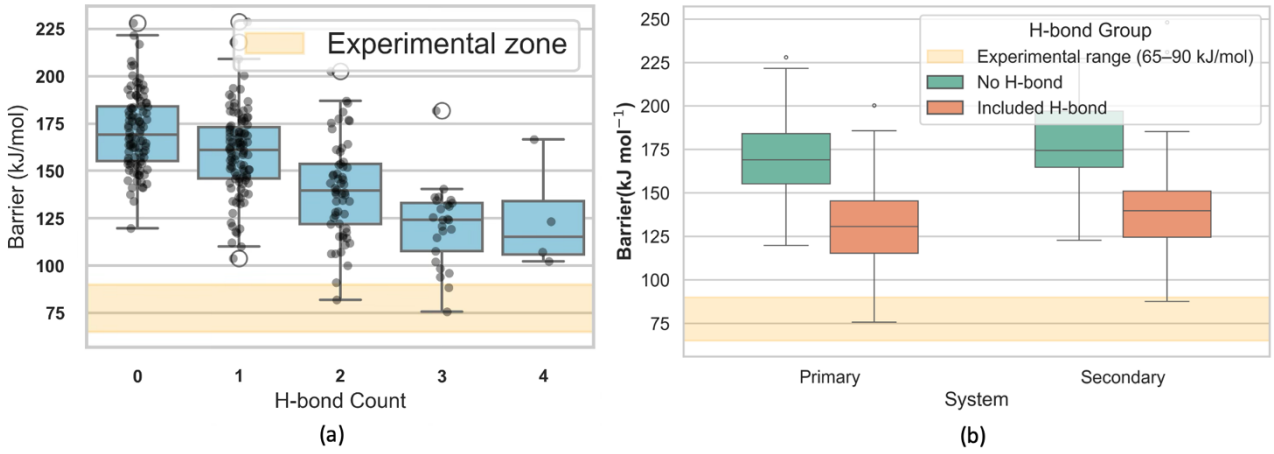


**Fig. 1**: (a) Barrier height decreases systematically with stronger and multiple H-bonds (b) Barrier height decreases for both curing reactions.

**Conclusions, main achievements, and outlook**

At the current stage of the project, the primary achievement is the establishment of a reliable and automated framework for analyzing curing reaction energetics in epoxy thermosets under realistic environmental conditions. By combining reactive molecular dynamics simulations with a posteriori QM/MM calculation, we are now able to systematically evaluate activation energies for a large number of individual curing events while explicitly accounting for the surrounding polymer environment.The QM/MM analysis has revealed a broad distribution of activation energies that differs substantially from gas-phase estimates, highlighting the importance of environmental effects during curing. In particular, the presence of hydrogen bonding near reactive sites has been identified as a recurring structural feature associated with deviations from average activation energies as shown in Fig 1(a) and Fig 1(b). The implementation of hydrogen-bond-based criteria into the curing protocol represents an important methodological development. This approach enables controlled generation of curing events under specific local environments and provides a systematic way to probe how hydrogen bonding may influence curing dynamics. At this stage, the protocol serves as an exploratory tool to assess trends rather than as a finalized parametrization strategy.In parallel, an initial data-driven analysis framework has been established to relate QM/MM-derived activation energies to local structural descriptors. Models were constructed using combinations of geometric parameters and hydrogen-bond-related descriptors to assess their influence on predictive performance. The inclusion of hydrogen-bond descriptors leads to a systematic improvement in model predictions, providing a quantitative indication that hydrogen bonding carries relevant information for describing variations in activation energies. Robustness analyses indicate that predictive performance depends sensitively on model complexity. While the inclusion of additional descriptors improves interpolation accuracy, excessive parametrization can reduce model stability and generalizability. These observations highlight a balance between capturing relevant physical interactions and avoiding overparameterization. Ongoing work therefore focuses on applying additional statistical and robustness-based methods to refine the descriptor set and to identify representations that are both physically interpretable and transferable. Moving forward, the immediate focus will be on consolidating the hydrogen-bond-conditioned curing simulations and quantifying their influence on reaction statistics across different stages of cure. Subsequently, graph-theoretical methods will be applied to the resulting polymer networks to characterize loop formation and connectivity, providing a foundation for linking curing chemistry to network topology. These developments will support the longer-term objective of integrating chemically informed curing dynamics into fracture modeling of epoxy thermosets.

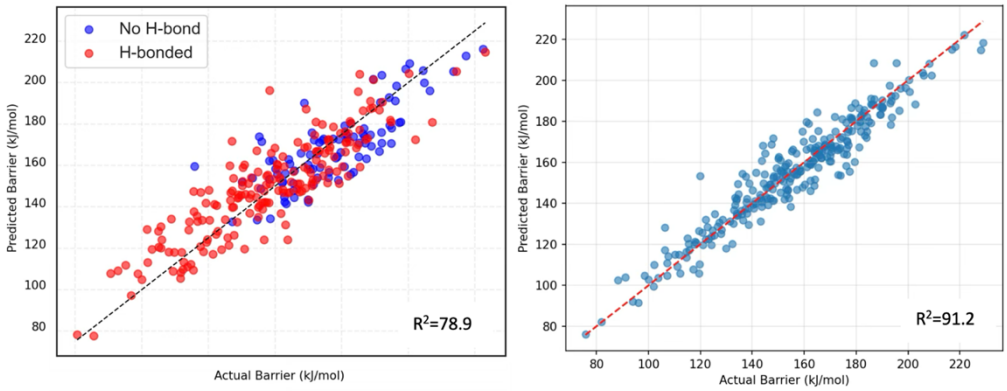


**Fig. 2:** (a) Model with only geometrical descriptor (b) Model with both hydrogen strength parameter and geometry parameter.

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## aP12: Multiscale Simulation of Strain-Induced Bond Breakage in Crosslinked Epoxy Networks

Barışcan Arıcan, Christian Wick, György Hantal and Ana-Sunčana Smith

Fracture initiation in crosslinked epoxy resins is governed by covalent bond rupture occurring within a mechanically loaded and chemically heterogeneous polymer network [1]. In this project, a multiscale simulation approach is developed to study such processes by dynamically coupling large-scale molecular dynamics (MD) deformation with local quantum-mechanical calculations.
As an example system, we investigate a highly crosslinked DGEBA/DDS epoxy network, which is subjected to uniaxial tensile deformation using MD. Due to the covalent nature of the crosslinks in the epoxy thermoset system, we expect homolytic bond scission as the dominant mechanochemical response to large tensile forces [1]. Since the nature of classical molecular force fields does not account for bond-breaking processes, we adopt the following scheme to induce quantum-mechanically informed bond scission into the simulations: During deformation, selected backbone bonds are continuously monitored as potential rupture candidates. When a bond reaches a critical deformation state, a local reaction zone is extracted (Figure 1) and evaluated using a QM/MM calculation based on the ONIOM method [2]. The quantum calculation is performed in the presence of the surrounding strained environment, allowing mechanical and electrostatic interactions from the polymer network to be retained during rupture assessment. If bond cleavage is confirmed, the molecular topology is updated automatically, followed by a short stabilization phase, after which mechanical loading continues.

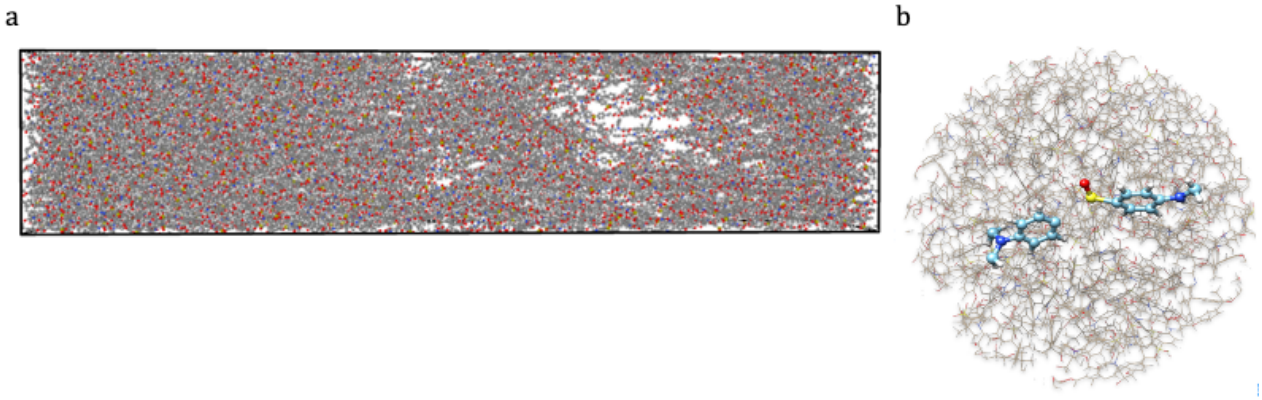


**Fig. 1:** (a) Uniaxially strained DGEBA/DDS epoxy network during deformation, showing damage morphology after multiple rupture events. (b) Representative ONIOM QM/MM subsystem around a rupture candidate; the QM region is embedded in an MM environment (electrostatic embedding).

Several multiscale approaches to strain-induced bond breaking have been proposed in recent years [3]. In many of these methods, bond rupture is ultimately determined using simple geometric indicators, which are not sufficient to capture the quantum-mechanical nature of bond cleavage, and the associated quantum-mechanical calculations are performed on isolated or weakly embedded clusters. As a result, the influence of the local chemical and mechanical environment on bond rupture is only partially captured. In the present framework, rupture decisions are instead based on electronic structure information obtained from ONIOM QM/MM calculations that explicitly embed the quantum region within the surrounding polymer network.

Bond rupture is diagnosed using quantum-mechanical indicators derived from the electronic structure of the QM region. In particular, the emergence of spin contamination, reflecting the admixture of higher-spin states into the broken-symmetry wavefunction, is used as an indicator of homolytic bond cleavage. This criterion provides a physically motivated signal of bond scission that goes beyond purely geometric measures.

Following bond scission, chemically consistent capping fragments are introduced to terminate the newly formed chain ends. These fragments are constructed using a block-chemistry fragmentation scheme [4], which preserves charge neutrality and maintains electrostatic consistency after topology changes, enabling seamless continuation of the MD simulation.

A major outcome of this work is the implementation of a fully automated simulation driver that integrates mechanical deformation, ONIOM-based QM/MM rupture assessment, topology modification, and post-reaction stabilization into a single workflow. The framework enables stress–strain simulations of large crosslinked epoxy networks (127k atoms) up to complete rupture, and can access strain rates down to 108s-1 (Figure 2), with each individual bond-breaking event validated at the QM/MM level and stored together with detailed information on the surrounding molecular environment, providing a rich dataset for correlating macroscopic mechanical response with microscopic rupture processes.

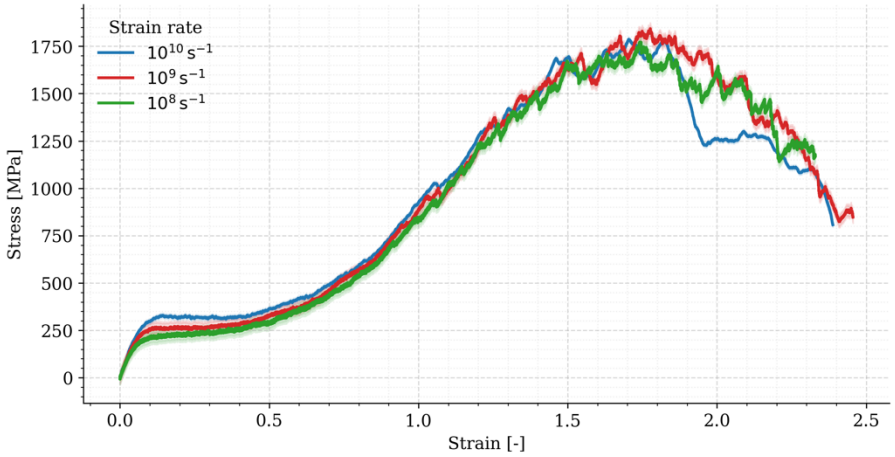


**Fig. 2**: Mean stress–strain response of the crosslinked DGEBA/DDS epoxy network obtained from continuous tensile deformation simulations at three applied strain rates ($10^{10}$, $10^{9}$, and $10^{8}$ $s^{-1}$). Solid lines show the mean curves; shaded bands indicate variability across independent trajectories.

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# P13

## FRACTURE IN ROCKS: FROM SINGLE GRAINS TO SEISMIC SCALE


**Javad Karimi**

**Bakul Mathur**

**Ruaridh Smith**

**Prof. Dr. rer. nat. Daniel Köhn**
Tectonics
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# P13: Microstructural Controls on Rock Fracture: Porosity Effects and Riedel Shear Nucleation

Javad Karimi, Bakul Mathur and Daniel Koehn

## Introduction

Rock microstructure exerts a fundamental control on deformation, determining stress concentration, fracture nucleation, and permeability evolution [1]. While tensile failure is critical in hydraulic fracturing, shear localization, specifically the formation of Riedel shears is central to fault zone evolution and reservoir sealing capacity [2], [3]. However, standard numerical models often rely on idealized spherical particles, failing to capture the geometric complexity of natural rocks required for accurate fault prediction. This report presents progress on two fronts to address this limitation: (1) quantifying the effect of porosity and grain packing on fracture mode using Discrete Element Method (DEM) simulations of Brazilian tests, and (2) developing a workflow integrating image segmentation and the Elle platform to model realistic Riedel shear formation in sandstone.

## Methodology

### DEM Framework and Brazilian Tests

Mechanical simulations were conducted using the YADE DEM framework [4]. The rock matrix was represented by the 'CpmMat' (Cohesive Particle Model), which captures brittle failure via bond breakage, linear elasticity, and frictional plasticity. Granular assemblies with porosities of 10%, 20%, and 30% were generated by adjusting grain size distributions. These were subjected to diametral compression to simulate tensile splitting.

### Image Segmentation and Elle Integration

To move beyond idealized sphere packings, a custom image segmentation algorithm was developed to process optical thin sections. The code uses thresholding and watershed segmentation to separate grain boundaries and pore spaces. The segmented data is imported into the Elle numerical platform to reconstruct the exact grain topology. This realistic geometry is mapped into YADE to simulate the kinematic evolution of Riedel shears under direct shear, ensuring natural grain angularity is preserved.

## Results: Porosity Effects on Fracture Pattern and Mechanical Response

Simulations of the Brazilian tests revealed a fundamental transition in failure morphology governed by initial porosity.

### Fracture Patterns

A distinct contrast was observed between low and high porosity samples. Low-porosity specimens (10%) exhibited a highly brittle failure mode: damage nucleated centrally and rapidly coalesced into a single, narrow through-thickness tensile crack aligned with the loading axis. Conversely, high-porosity specimens (30%) developed a diffuse damage band. Fracture clusters nucleated at multiple pore boundaries throughout the central zone, forming a broad network of microcracks rather than a clean fracture (Figure 1). This confirms that increased void space promotes distributed energy dissipation.

### Mechanical Response

The mechanical data correlated directly with the fracture patterns. Low-porosity samples displayed a smooth, monotonic stress increase leading to a distinct peak and catastrophic softening. In contrast, high-porosity samples displayed pronounced stress oscillations and a multi-peak response. These fluctuations are attributed to sequential local failure events where cracks arrest at

pores, causing temporary stress relaxation. The porous structure acts as a series of crack arrestors, leading to a pseudo-ductile global response despite the brittle nature of the constituent grains.

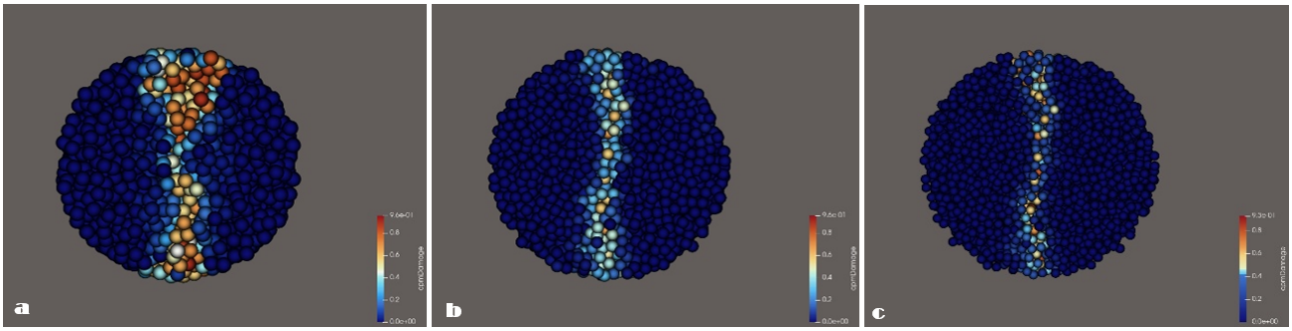


**Fig. 1:** Failure patterns of samples with varying porosities: (a) 30% (diffuse), (b) 20%, and (c) 10% (localized).

### Ongoing Work: Modeling Riedel Shears with Elle

Current research focuses on applying the Elle-YADE coupling to investigate shear zone evolution under direct shear conditions.

### Segmentation Implementation

Thin sections of sandstone have been successfully processed using the custom segmentation code. The algorithm identifies grain contacts and pore geometries acting as stress concentrators. The resulting digital microstructures successfully capture the angularity and interlocking of natural grains, which are lost in standard spherical DEM packings.

### Riedel Shear Nucleation

Preliminary results suggest that the realistic grain angularity preserved by the segmentation process alters the internal friction angle required to initiate Riedel shears. Our simulations indicate that natural, angular grains promote earlier localization of R-shears compared to spherical assemblies due to enhanced interlocking. Future work will quantify the precise orientation of R-shears relative to the shear vector under varying degrees of cementation.

### Conclusion

This research highlights the critical role of microstructure in rock failure. The completed Brazilian tests demonstrate that high porosity promotes diffuse, oscillatory failure, while low porosity favors localized brittle fracture. Furthermore, the integration of image segmentation and Elle establishes a robust method to simulate Riedel shears within realistic grain geometries. This workflow bridges the gap between petrographic observation and geomechanical modeling, offering improved predictions for fault evolution in heterogeneous reservoirs.

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# P13: Modeling of fragmentation and fracturing processes in deformation bands

Bakul Mathur and Daniel Koehn

The primary objective of this research is to develop a physically motivated multiscale numerical framework to investigate deformation band initiation and localization in porous granular rocks. Deformation bands form in response to localized compaction and shear in sandstones and sediments, leading to porosity reduction, grain crushing, and progressive mechanical weakening [1,2]. While previous work focused on single-grain fracture mechanisms, the current study advances the framework by explicitly coupling inter-particle bond breakage with intra-granular grain crushing. This coupled approach allows the investigation of how cement degradation, grain unconfinement, and stress redistribution interact to localize deformation at the mesoscale. The broader objective is to describe how distributed grain-scale damage progressively localizes into deformation bands, forming a basis for future upscaling to fault-scale and reservoir-scale models.

**Microscale Modeling**: At the microscale, this project builds on earlier work on single-grain fracturing using polyhedral particles in the discrete element framework YADE [3]. Individual grains are represented as rigid polyhedra subjected to internal stress evaluation based on contact forces. Grain fracture initiation is governed by a combination of Mohr–Coulomb–Weibull (MCW) failure criterion[4] and contact line stress criterion[5]. MCW combines a stress-based failure envelope with statistical size effects through Weibull scaling. The contact line stress criterion involves splitting the grain along critically stressed contact lines.

**Mesoscale Modeling**: The main scientific advance of this year is the coupling of inter-granular bond breakage with intra-granular grain splitting at the mesoscale. Cementation between grains is modeled using bonded contacts, while grains themselves are allowed to fracture under elevated local stresses. Each bonded contact is represented by linear normal and tangential springs,

$$F_n = k_n \delta_n, \qquad \mathrm{F}_t = k_t \delta_t$$

and fails according to a coupled normal–shear elliptical criterion:

$$\left(\frac{F_n}{\sigma_n^{\mathrm{eff}}}\right)^2 + \left(\frac{\| \mathrm{F}_t \|}{\tau^{\mathrm{eff}}}\right)^2 \geq 1$$

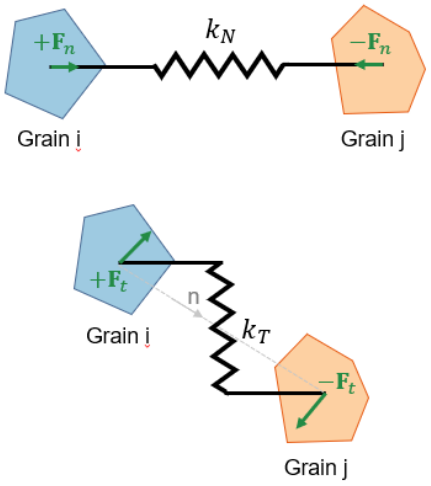


**Fig. 1:** Normal and tangential bonded-contact model between neighboring grains. The normal interaction is represented by a linear spring with stiffness $k_N$, transmitting normal force $F_n$between grains iand j. The tangential interaction is modeled by a tangential spring with stiffness $k_T$, transmitting shear force $F_t$..

Bond strength is made length-dependent, with bond length acting as a proxy for local porosity. Longer bonds represent wider pore throats and weaker cementation, while shorter bonds correspond to stronger confinement. Effective strengths are scaled as

$$\sigma_n^{\mathrm{eff}}, \tau^{\mathrm{eff}} = (\sigma_n^0, \tau^0)\, g(L)$$

where $g(L)$is a decreasing function of bond length. This allows damage to localize naturally in porous regions without prescribing deformation bands. Grains that lose all cement bonds are assumed to become mechanically weakened due to loss of lateral confinement and their effective strength is reduced. Grain splitting therefore occurs preferentially in regions of prior bond damage, producing localized multiparticle crushing zones.

This coupled formulation enables deformation bands to emerge from micro-mechanical interactions between bond degradation and grain fracture, rather than from imposed geometrical constraints.

**Large scale modeling**: Large-scale modeling is planned as a future extension of this work. The present mesoscale formulation provides a physically grounded constitutive basis for upscaling grain-scale damage mechanisms into continuum descriptions of deformation bands. Planned directions include homogenization of grain-scale damage variables into band-scale weakening laws, coupling DEM-derived constitutive responses with continuum or FEM models, and investigation of band interaction, spacing, and growth under varying stress paths.

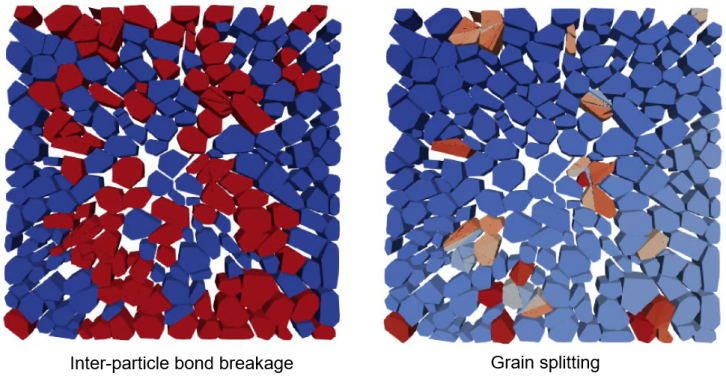


**Fig. 2:** Coupled inter-granular bond breakage and intra-granular grain splitting. Left: spatial distribution of broken inter-particle bonds, highlighting preferential bond damage in initially porous regions of the assembly. Right: resulting grain splitting events, showing that intra-granular fracture localizes predominantly within zones of prior bond loss

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# aP13: Modelling energy systems in faulted and fracture Media

## Spatial fracture network analysis through fingerprints, clustering and upscaled permeability tensors

**Ruaridh Smith, Daniel Koehn and Rahul Prabhakaran**

**Research motivation and objectives:** Fractures play are key components within naturally fractured reservoirs which can influence fluid flow within subsurface energy systems such as hydrocarbon or geothermal resources. As such understanding the organisation and interactions of these networks is vital for the exploration, development and production from these systems. Within Germany geothermal energy is becoming a popular renewable energy source with major projects have primarily been focused on southern Bavaria where high heat flows have been observed at depth [1,2]. However there has been limited research on the potential geothermal resources in the north where low permeable reservoirs (carbonates) have been identified in increased heat flow regions controlled by granitic intrusions [e.g., 3,4]. Low permeable reservoirs such as the units observed in northern Bavaria rely on fractures to increase flow and provide efficient pathways for fluids. Therefore, understanding the characteristics of these features is vital for further exploration.

A major challenge in the exploration of the reservoirs in northern Bavaria is the limited research and studies on the subsurface geology and corresponding fracture networks, especially compared to the south where there are abundant data and analysis available [5]. Thus, there remains a gap in the research required in the north to constrain the fracture networks and model their influence on the subsurface permeability. Surface geology such as outcrop analogues can be used to image and extract information of fracture networks that are present in geological formations at depth which can be subsequently integrated into subsurface models and simulations.

The main objective of this research is to model fracture networks that are present in northern Bavaria and develop methods to integrate data from outcrop to the subsurface into large-scale fracture flow models. As part of this overall aim, a secondary investigation is presented to better understand how fractures vary spatially and across scales to assess the effect on network permeability.

**Methodology:** To assess the variation in the fracture networks, we apply two main analyses on 2D network data collected from several sites across northern Bavaria, located along the Franconian Alb using drone, LiDAR and photogrammetry.

We first used a fingerprinting method (fig. 1a) which represents networks using spatial graphs. Using MATLAB scripts, this method is a combination of block areas and shape factors and quantifies the network based on the areas between fractures rather than the fractures themselves. The three bin areal probability distributions are plotted against the shape factors (0 to 1) to uniquely define the fingerprint (Fig. 1b). A secondary analysis is then also applied to the fracture network. We use analytical aperture modelling based on tectonic stress (fig. 1c) and integrate this

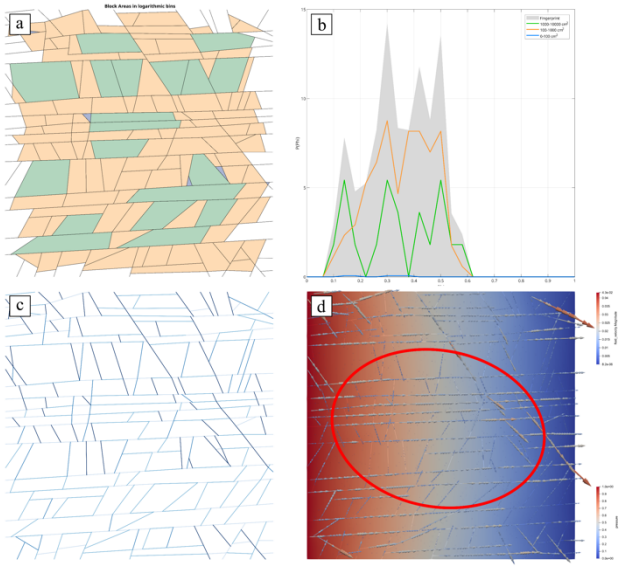


**Fig. 1:** Fracture analysis and upscaling workflow showing a) network fingerprint, b) distribution of block area and shape factors, c) aperture modelling and d) 2D fluid flow simulation on a fracture network.

information into 2D numerical fluid flow simulations using the MOOSE Framework to upscale the fracture network permeability (fig. 1d). We then apply a hierarchical clustering using R on all 25 fractured sections for both the fingerprint and permeability analysis to assess variability between the sections which are then represented on a dendrogram diagram.

**Analysis and clustering of networks:** Initial analysis of the fingerprints and the distribution of block size and shape factor show variation between fracture traces across both quarries with the different block sizes varying between and within sections. Faults captured within the fracture traces seem to also play a role in influencing the fingerprints distribution, affecting both block size and shape. Clustering analysis shows inter-quarry variation to be relatively low with a level of variation at or below 1.0, however some outlying sections were identified. When comparing between quarries (fig.2), the variation becomes more challenging with sections from the different quarries clustering together. Several sections that contain faults from both quarries cluster together, however clear similarities are more unclear.

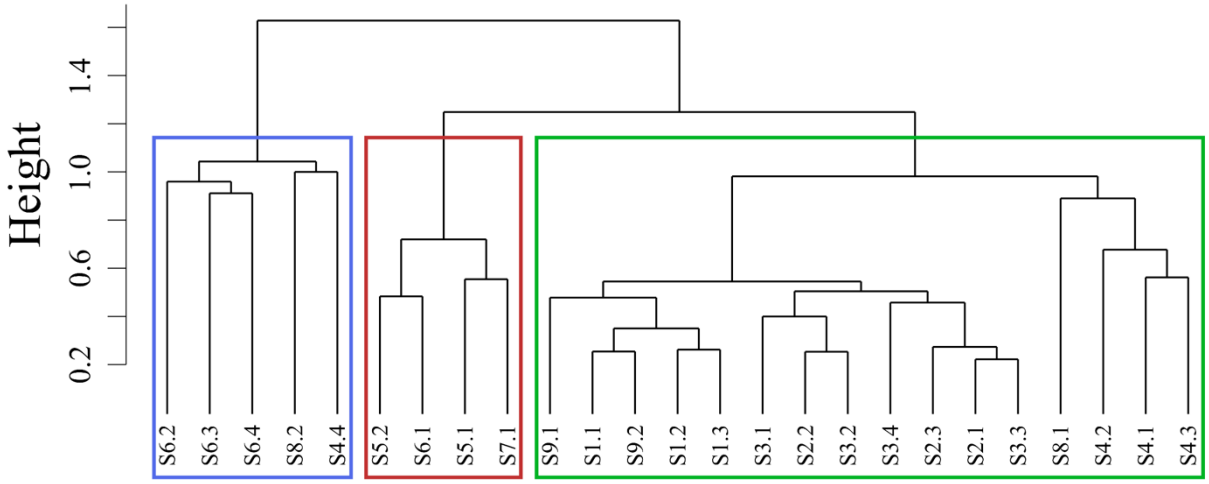


**Fig. 2:** Dendrogram showing the hierarchical clustering of the fingerprinting analysis for all sections from both quarries.

The results from the 2D permeability highlighted the influence of both large-scale faults on the tensor orientation and small connected fractures. Furthermore, sections were identified in both quarries that had influence on long horizontal fractures. The clustering of the tensors also showed similarities between sections based on their captured orientation with tensors from the NW-SE sections presenting a more anisotropic horizontal flow compared to the isotropic subvertical flow from the sections orientated NE-SW.

**Discussion and future work:** The approach and methodology we applied to assessing the variation of fractures is quite novel with the application of spatial graph theory to the networks. The influence of faults to the network and subsequently the permeability is consistent with previous work on the structural geology of the region [6]. It was also found that since the there was a clear clustering difference between the two section orientations

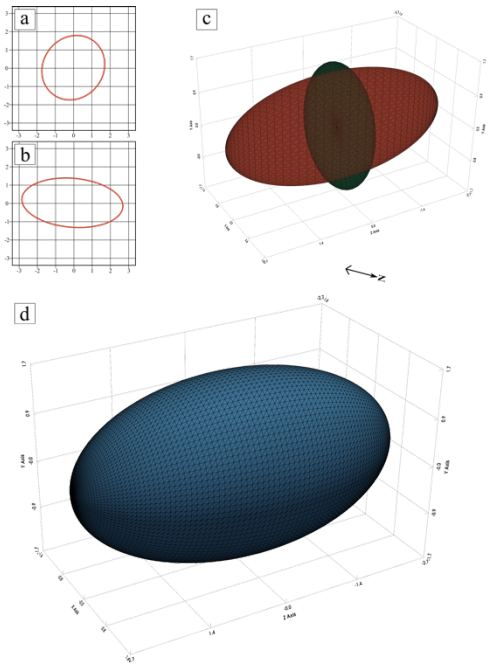


**Fig. 3:** 3D permeability tensor realisation obtained from sections orientated a) NE-SW and b) NW-SE. c) 2D tensors projected in 3D space. d) Calculated upscaled 3D tensors

of permeability we could estimate a 3D permeability tensor of the region (fig. 3).
Through averaging the 2D tensors for both section orientations (fig. 3a&b), we can combine these two tensors in 3D space (fig. 3c) and calculate an ellipsoid representing the 3D permeability. This orientation also generally aligns with the main structural features in the region indicating flow could be strongly influenced by the large-scale and observable structures in the basin.
Further collaborations within the FRASCAL group (P1) are in continued development concerning the simulation of small-scale mineralisation processes along fault planes observed in outcrops which form mirror-like surfaces.

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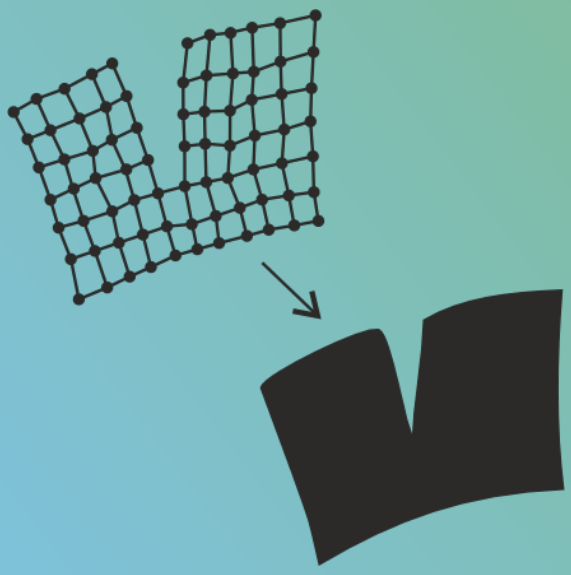

# P14

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

**Ba Duc Duong**

**Prof. Dr. Manuel Friedrich**
Applied Analysis
Department of Mathematics

## P14: Quasistatistic/Dynamic crack growth: atomistic to continuum

Ba Duc Duong and Manuel Friedrich

In last years, P14 has published some interesting results related to the behavior of atomistic and discrete models and their convergence towards a continuous one, for example in [4]. To summarize, the main principle introduced in [3] is to use energy minimization to tackle so called free discontinuity problems. To justify the convergence of the atomistic result to the continuous one, the standard tool in this context is to prove Gamma-convergence of the atomistic model towards the continuous one. Concerning this subject, we can view [2] as a breakthrough result. However, this result does not address the issue of time evolution yet. Considering this detail comes with some hurdles, where [1] laid the first ideas to include the time component, many of which are still relevant today. The study of an atomistic model and its convergence towards a continuous one was a significant part of the second cohort of P14 and culminated in the papers [4] and [5].

The last paper in the second cohort, however, touched on a slightly different subject. As is often the case in numerical applications, one analyzes discretized versions of a certain model to see whether they can be approximated, which will be discussed in more detail below. In cooperation with Vito Crismale, it was shown in [6] that it is possible to consider a discretized version of the Griffith energy with an adaptive mesh, which also Gamma-converges to the regular one. In this vein, we want to dive a bit deeper into the topic of approximations during the third cohort.
To elaborate a bit, the strict continuous models for fracture, for example given by [3] contain a minimization of some crack set, which is mathematically described by the $\mathcal{H}^{d-1}$-measure of the jump set of a function. It is known that for simulations, this model only has limited applicability as the jump measure is very hard to treat numerically. Therefore, there is a need for suitable approximation models. A popular approach to approximate fracture, also used in the FRASCAL community, is the phase-field approach developed by [9]. This paper was groundbreaking in that it transformed a minimization problem with originally a single variable into an approximation scheme with two variables. Incorporating time is also quite cumbersome in this case and has been solved by [8] albeit for the special case of anti-planar shear, where it is possible to consider the full gradient and not just the symmetrized gradient as is usual in the description of the stiffness tensor. Another approximation method introduced by [7] is eigenfracture. In [7], they proved a Gamma-convergence result, which justifies the approximation scheme from an analytical viewpoint. There remains just one crux as is often the case, the time component is completely missing in their consideration, in fact it was “beyond the scope” of their work.

Solving this issue was the main project for this year. Following the ideas of [8], we first need to find a consistent time-dependent formulation for the eigenfracture model. More precisely, such a model should have the following properties: (1) Irreversibility (2) Minimization of a time-dependent version of the eigenfracture energy given in [7] (3) Energy balance.
To do this, we formulate an iterative scheme for a (suitably chosen) time-discretization. Existence for this is usually established using the direct method, which we also took advantage of. This means that our method results in a model that is discretized in space and time.
The next step is to analyze the limit as the time discretization parameter goes to zero. This step already involves a couple of subtleties. As the functions we defined do not attain the necessary convergence properties to simply go to the limit pointwise for all times, we must first treat the time convergence on a dense subset of the time interval. By this we mean that we only take a limit on a countable subset of the time interval and can recover the remaining time steps via a (second) limiting process. But this procedure does not come without difficulties. It turns out that this process together with irreversibility significantly complicates defining a crack set for the limit in time. Additionally, it is not clear from the beginning that the limit in time is also an energy minimizer for

eigenfracture. We managed to grasp most of these problems quite quickly as they naturally arise in related work as well.
With this method, we showed that there exists a minimizer for each scale we want to do eigenfracture on. We will denote this pair by $t \mapsto (u_\varepsilon(t), \gamma_\varepsilon(t))$. The next step, which is usually the more interesting one, is to analyze the limit $\varepsilon \to 0$ and whether it converges to the formulation given in [3] or not. Many aspects of this have been tackled in related papers in similar settings, where we only had to slightly adapt known methods. The core issue in such problems though is always that we have to show stability of the limiting function. This step is usually where the novelty lies, since it works differently for each type of model. Our case was not the exception, which meant that we had to find a way to show this.
The core idea was laid out in [1], where the jump-set transfer for the normal Griffith energy was introduced. We had to transfer this jump-set transfer to the eigenfracture setting. This presents several challenges. In [1], one aspect is the fact that we create a surface where we add a small portion of area. Ideally, one would simply take the construction given there and plug it into the eigenfracture setting. The problem is that in the eigenfracture setting, the small area can translate to a possibly huge neighborhood, which is how fracture is penalized in the energy. Ensuring that we can do an alternative construction such that we can also control the neighborhood was the main challenge.
To summarize the procedure, we first slightly alter the hypersurface given in [1]. Afterwards, we differentiate between the added portions that are close to the original surface and the ones that are further away. One can show that slightly increasing the original surface is not too expensive, which covers the portions close to the original ones. For the other parts, we can calculate that with the alteration, the energy contribution is small enough.

In conclusion, this approach yields a suitable result for a time-evolution variant of eigenfracture. We plan to finalize the publication, first for the anti-planar case, in the beginning of 2026. Since the arguments are strictly geometrical, we strongly believe that extending the approach onto the full vectorial one is quite straightforward and is an idea for a future endeavor. Additionally, we have mentioned the paper [8], which is also an open problem for the full vectorial case. On this issue, we have already discussed ideas on how to tackle it and hope that we can also make progress on this in 2026.

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# 3. Publications

The FRASCAL publications for 2025 are listed below with the corresponding abstract and the assignment to their respective projects. The acronyms in brackets behind the authors have the following meaning:

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

The FRASCAL community had a total of **14 publications** in 2025. Datasets can be published on the zenodo platform - with or without an associated text-based publication. A total of **8 datasets** were published here in 2025.

## P1 | Chemistry at the crack tip

Mörsel S., Ritterhoff C. L. (PhD), Kellner R., Meyer B. (PA) and Hirsch A.
**N-Heterocycle-Substituted Hexa-peri-Hexabenzocoronenes with Windmill Architectures**
In: Chemistry – A European Journal (2025), Vol 31
DOI: 10.1002/chem.202403124


„We describe the synthesis and computational investigation of *N*-heterocycle-substituted hexa-*peri*-hexabenzocoronenes (HBCs). Following our method for the preparation of thioether-substituted HBCs, we prepared pyrrole-, indole-, carbazole-, and 1H-benz[g]indole-substituted HBCs from the corresponding fluorinated precursors under microwave irradiation. A series of polysubstituted benzoindole-HBCs with windmill architectures was also synthesized using the polyfluorinated HBC analogs, and the substituent effects on the electronic properties of the HBC core were investigated. Similar to the thioether substituted HBCs, the nature of the heterocycle does not influence the optoelectronic properties of the HBC core. The attachment of multiple benzoindole substituents leads to a bathochromic shift of the absorption and emission spectra, comparable to our previous studies. Due to the circular arrangement of the benzoindole moiety, the attachment of multiple substituents results in the presence of multiple conformers at room temperature. The rotation barrier can be overcome by heating the compounds to 323–333 K. Additionally, the investigation of the relaxed geometries shows two π-stacking motifs within the conformers.“

Oleszak C. , Ritterhoff C. L. (PhD), Meyer B. (PA) and Jux N.
**β-meso-Fused pyrene-porphyrin scaffolds with panchromatic absorption features**
In: Organic & Biomolecular Chemistry(2025), Issue 4
DOI: 10.1039/D4OB01447B


„The π-extension of porphyrins with pyrenes through the β-*meso*-fusion of five-membered rings is demonstrated. Three architectures resulting from combining up to two porphyrins and pyrenes were obtained straightforwardly in good overall yields. Although significantly planarized, the molecules retain excellent solubility and processability. Spectroscopic characterization and density-functional theory calculations reveal intriguing absorption features.“

Oleszak C. , Ritterhoff C. L. (PhD), Schulze E. J., Hirsch A., Meyer B. (PA) and Jux N.
**A synthetic methodology towards π-extended porphyrin-rylenediimide conjugates**
In: RSC Advances (2025), Issue 2
DOI: 10.1039/D4RA08045A


"In this work, we present a straightforward synthetic route for the preparation of functionalized β-*meso*-fused porphyrins, which are subsequently connected to rylendiimides. The resulting donor–acceptor-type conjugates exhibit intriguing optical properties, such as panchromatism and profoundly bathochromically shifted absorption curves. A better understanding of the molecules' electronic structure was gained through density-functional theory calculations, which unveiled small HOMO–LUMO gaps."

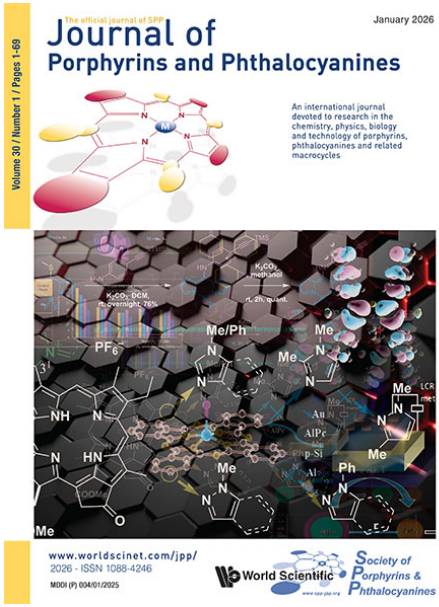
Oleszak C. , Ritterhoff C. L. (PhD), Meyer B. (PA) and Jux N.
**Manchromatic PAH-Porphyrin Hybrids with a Step-Wise Increasing π-System**
In: ChemistryOpen (2025), Volume 14, Issue 3
DOI: 10.1002/open.202400481


“The rational synthesis of three *β-meso*-fused porphyrins with a step-wise increasing π-system size is presented. The synthetic route, which introduces a five-membered ring between the macrocycle and an aromatic fragment, is modular in its nature and proceeds straightforwardly. The well-soluble conjugates have intriguing optical properties, namely bathochromically shifted and flattened absorption curves. Density functional theory (DFT) calculations provide insights into the electronic structure and transitions, unveiling small HOMO-LUMO gaps.”

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

**A helical porphyrin-nanographene with an extended aromatic network**

In: Journal of Porphyrins and Phthalocyanines (2025), Volume 29, No. 03n04
DOI: 10.1142/s1088424625500440

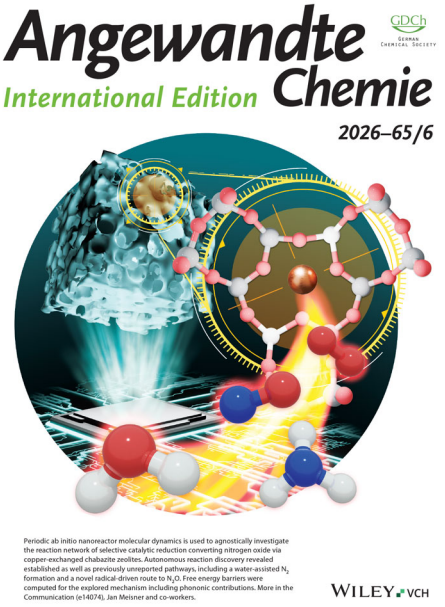



„Presented is a straightforward synthetic methodology toward a porphyrin-based “N-doped” nanographene that includes a chiral element. This central element is a “defective” hexa-*peri*-hexabenzocoronene (HBC) resembling π-extended [5]-helicene, which is fused to two porphyrins via five rings in a β-*meso* fashion. The conjugate shows excellent processability and exhibits fascinating photophysical characteristics, which were probed using optical spectroscopy and density functional theory calculations.“

Schulze E. J., Mack E. A., Ritterhoff C. L. (PhD), Borucu U., Meyer B. (PA), Guldi D. M. and Hirsch A.

**Multidirectional Charge Separation in Self-Assembled Aggregates of Perylenebisimide-Porphyrin Bola-Supra-Amphiphiles**

In: Angewandte Chemie International Edition (2026), Volume 29, No. 03n04
DOI: 10.1002/anie.202523324




„We report on the synthesis of a hydrogen-bond mediated bola-type supra-amphiphile and assembly thereof in water. The assembly is based on amphiphilic porphyrins and hydrophobic perylenebisimdes (PBI), which both form the resulting bola-form solely through the H-bonding motif, which is shielded by the assembly of the chromophores itself. The amphiphilic porphyrin was functionalized, on one hand, with a cyanuric acid and, on the other hand, with an oligo carboxylate dendron as polar head group. Two Hamilton receptors were linked to the PBI on each imide position. Assembly was achieved by lyophilizing solutions of both components in water/THF mixtures, followed by redispersion in pure water yielding stable suspensions. Cryogenic transmission electron microscopy (cryo-TEM) and dynamic light scattering (DLS) reveal a spherical morphology with diameters ranging from 15 – 100 nm. Once formed, the assemblies showed broadened absorptions and quenched PBI-centered fluorescence. Using time-resolved absorption spectroscopy, the nature of the fluorescence quenching was confirmed to be either charge separation, by which the porphyrin donates an electron to the PBI, or symmetry breaking charge separation, by which π-π stacked PBIs donate and accept electrons. Denaturation of the supra-amphiphile went hand-in-hand with a reinstation of the PBI fluorescence and suppression of charge separation.“

## P3 | Fracture in polymer composites: nano to meso

Puhlmann P (PhD). and Zahn D. (PA):
**Molecular Mechanisms of Silicone Network Formation: Bridging Scales from Curing Reactions to Percolation and Entanglement Analyses**
In: Polymers (2025), 17 (19)
DOI: 10.3390/polym17192619

polymers

"The curing of silicone networks from dimethylsilanediol and methylsilanetriol chainbuilder–crosslinker precursor mixtures is investigated from combined quantum/molecular mechanics simulations. Upon screening different crosslinker content from 5 to 15%, we provide a series of atomic-resolution bulk models all featuring 98–99% curing degree, albeit at rather different arrangement of the chains and nodes, respectively. To elucidate the nm scale alignment of the polymer networks, we bridge scales from atomic simulation cells to graph theory and demonstrate the analyses of 3-dimensional percolation of -O-Si-O- bonds, polydimethylsiloxane branching characteristics and the interpenetration of loops. Our findings are discussed in the context of the available experimental data to relate heat of formation, curing degree and elastic properties to the molecular scale structural details—thus promoting the in-depth understanding of silicone resins."

## P6 | Fracture in thermoplastics: discrete-to-continuum

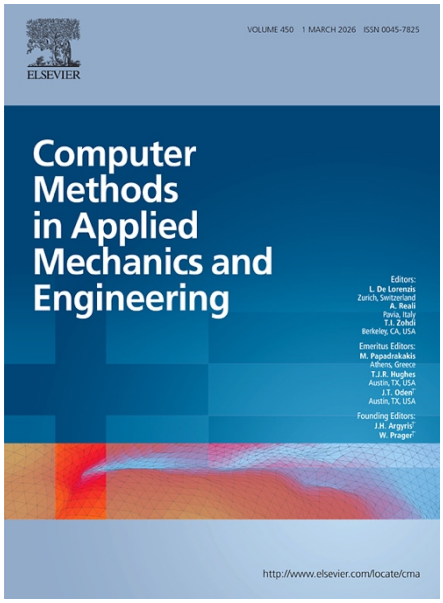
Dötschel V., Richter E. M. (PhD), Possart G., Steinmann P. (PA) and Ries M. (PDR):
**Reactive coarse-grained MD models to capture interphase formation in epoxy-based structural adhesive joints**
In: European Journal of Mechanics – A/Solids (2026), Vol. 116
DOI: 10.1016/j.euromechsol.2025.105801


„Adhesive joints offer a superior strength-to-weight ratio compared to conventional fastening methods, making them essential for achieving cost-efficiency and sustainability goals. The adherends influence the adhesive in their immediate vicinity, creating regions with altered microstructures. These regions, known as interphases, exhibit material properties that differ from those of the bulk adhesive and are not fully understood from an engineering perspective. To address this issue, we introduce a novel coarse-grained molecular dynamics (CGMD) model for adhesive joints, which aims to study the interphase formation and its resulting properties at the molecular level. We utilize a reactive epoxy model from the literature for the adhesive and implement matching aluminium substrates, along with the necessary adherend-adhesive interaction parameters. The resulting adhesive joint model allows us to investigate the formation of the adhesive's microstructure during the curing process and the mechanical properties of the joint. We conduct a parameter study on the adherend-adhesive interaction parameters, unravel the role of grafting bonds and their distribution, and examine the impact of the adhesive's thickness. Additionally, we identify an interphase based on variations in the local microstructure, estimate its size, and determine the influencing parameters. In this first contribution, we demonstrate the capabilities of our model in evaluating the mechanical behavior of the interphase, which is crucial for gaining a better understanding of adhesive joints."

Laubert L. (aPhD), Weber F. (PhD), Detrez F. and Pfaller S. (PA):
**Approaching and overcoming the limitations of the multiscale Capriccio method for simulating the mechanical behavior of amorphous materials**
In: International Journal of Engineering Science (2025), Vol. 217
DOI: 10.1016/j.ijengsci.2025.104317


"The Capriccio method is a computational technique for coupling finite element (FE) and molecular dynamics (MD) domains to bridge their length scales and to provide boundary conditions typically employed in large-scale engineering applications. Earlier studies showed that strain inconsistencies between the coupled domains are caused by the coupling region's (bridging domain, BD) resistance to spatial motion. Thus, this work examines influences of coupling parameters on strain convergence in Capriccio-coupled setups to study the mechanical behavior of solid amorphous materials. To this end, we employ a linear elastic 1D setup, imitating essential features of the Capriccio method, including force-transmitting anchor points (AP), which couple the domains via linear elastic springs. To assess the effect of more complex interactions in 3D models versus 1D results, we use an interdimensional mapping scheme, allowing qualitative and quantitative comparisons. For validation, we employ both an inelastic polystyrene MD model and a predominantly elastic silica glass MD model, each coupled to a corresponding FE material description. Our 1D results demonstrate that decreasing the conventionally high AP stiffness, along with other less significant measures, diminishes this motion resistance, revealing an optimal ratio between the material stiffness of the coupled domains and the cumulative AP stiffness. The 3D silica setup confirms that these measures ensure decent domain adherence and sufficiently low strain incompatibilities to study the mechanical behavior of elastic models. However, these measures turn out limited and may not ensure sufficient accuracy for studying the deformation and fracture behavior of Capriccio-coupled inelastic models. To overcome this, we employ a modified coupling approach, revising the Capriccio method's AP concept by introducing a much lower so-called molecular statics stiffness during the FE calculation and a higher AP stiffness during only the MD calculation. Initial results on the 1D setup indicate that essential coupling limitations can be overcome, albeit with the risk of oscillatory strain amplifications depending on the BD's design. This novel approach may enable a more accurate analysis of the mechanical behavior of coupled inelastic amorphous materials. We recommend evaluating its performance in 3D alongside additional methodological extensions. Overall, our results outline the current limitations of the Capriccio method and lay the groundwork for its targeted extension to study the mechanical behavior and, in particular, fracture phenomena in inelastic amorphous materials.

Laubert L. (aPhD), Weber F. (PhD) and Pfaller S. (PA):
**Assessing the Capriccio method via one-dimensional systems for coupled continuum-particle simulations in various uniaxial load cases using a novel interdimensional comparison approach**
In: Computer Methods in Applied Mechanics and Engineering (2025), Vol. 439
DOI: 10.1016/j.cma.2025.117817




„This contribution investigates sources of insufficiencies observed with the Capriccio method for concurrent continuum-particle coupling using a novel comparison technique. This approach maps the deformation states of three-dimensional (3D) coupled domains into a concise one-dimensional (1D) representation, which allows for a separate evaluation of the domain strains in a unified representation, enabling facile comparisons of the domain states during deformation. For the investigation, we employ both a 1D coupled system resembling the most relevant features of the full 3D Capriccio method as well as a corresponding 3D setup. Our analysis explores interactions between different material models in finite element (FE) and molecular dynamics (MD) domains. Based on various load cases studied in the 1D setup, we identify a resistance of the coupling region to spatial movement as the fundamental cause of strain convergence problems when applying the staggered solution scheme. Using the developed mapping approach, examination of the corresponding 3D setup reveals that these strain inconsistencies are even exacerbated by adverse relaxation effects in viscous MD models, particularly when coupled to a corresponding viscoelastic–viscoplastic FE model, leading to divergence from optimal strain. Our findings confirm that smaller strain increments in combination with larger load step numbers significantly improve strain convergence in all domains. Overall, this indicates the need for detailed sensitivity analysis of coupling parameter influences to reduce the identified motion resistance of the coupling region. Based on promising results in 1D, we further recommend exploring monolithic solving schemes for 3D systems to achieve optimal strain convergence for all types of Capriccio-based coupled particle and continuum material models. Moreover, our systematic approach of system definition and interdimensional comparison may serve as a model to assess other domain-decomposition coupling techniques.“

## P8 | Fracture in polymer composites: meso to macro

Rohracker M. (PhD), Kumar P. (PDR), Steinmann P. (PA), Mergheim J. (PA):
**Efficient phase-field fracture simulations for fracture analysis in heterogeneous materials**
In: Computational Mechanics (2025), Vol. 290
DOI: 10.1016/j.ijsolstr.2023.112641

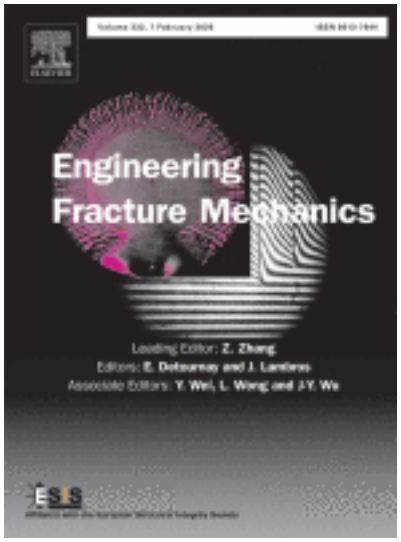

“Fracture in heterogeneous materials with complex microstructures poses significant challenges due to the intricate interactions between material heterogeneities and crack propagation. The phase-field method for brittle fracture has emerged as a particularly suitable and powerful simulation technique for addressing these challenges, offering a robust framework for capturing complex crack paths, branching, and coalescence of multiple cracks. The method, however, has notable drawbacks that can hinder its application to real-world simulations. Key limitations include its computationally intensive nature, driven by the need for fine spatial discretizations to resolve the smeared crack phase-field, small time step sizes for accurate crack detection, and slow convergence of staggered solution schemes during critical load steps. These challenges are addressed by proposing a combination of three complementary techniques to enhance both the performance and robustness of the phase-field fracture simulations: adaptive spatial refinement to focus computational effort near fractures, physically motivated convergence criterion to improve solver efficiency, and adaptive temporal refinement and coarsening to optimize time step sizes dynamically. The goal is to achieve efficient simulations without compromising physical accuracy, enabling reliable fracture modeling in heterogeneous microstructures. This study investigates the elastic and fracture responses of materials with varying microscopic properties, such as filler volume fraction and inclusion sizes.”

## P10 | Configurational Fracture | Surface Mechanics

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

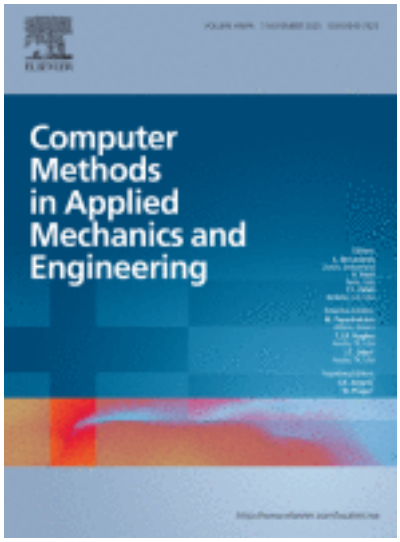
**A damage formulation for continuum-kinematics-inspired peridynamics to capture fracture experiments**

In: Engineering Fracture Mechanics (2026), Vol. 332
DOI: 10.1016/j.engfracmech.2025.111784




“Peridynamics (PD) is a nonlocal continuum formulation that naturally allows for discontinuities, such as cracks. It has therefore become attractive in the field of fracture modeling. Continuum-kinematics-inspired peridynamics (CPD) is a novel peridynamic reformulation that overcomes the fundamental limitation of classical bond-based PD, i.e. a fixed Poisson’s ratio. The novelty of this work is (i) the introduction of damage into the formulation of CPD and (ii) the comparison of the numerical results with fracture experiments conducted as a part of this study. In CPD, nonlocal interactions between material points are captured via one-, two- and three-neighbor interactions, allowing to measure length, area and volume changes. For each type of interaction, a separate damage variable is employed, depending on the associated strain. For a two-dimensional problem, the damage parameters of the model are derived from the classical fracture energy. In order to assess the model’s performance in predicting experimental outcomes, a series of fracture experiments is performed. Diagonally loaded square plates with center cracks of varying inclination angle are tested to study different fracture modes. The results demonstrate the model’s capability to capture the maximum loads and the crack paths observed in the experiments. This is the first contribution that integrates theory, computation and experiment within the framework of CPD.“

Titlbach A. (aPhD), Papastavrou A., McBride A. and Steinmann P. (PA):
**Modelling the flexoelectric effect in human bone—A micromorphic approach**
In: Computer Methods in Applied Mechanics and Engineering (2025), Vol. 446
DOI: 10.1016/j.cma.2025.118234




„Excessive habitual loading can cause microcracks in cortical bone, which are self-repaired through remodelling. The flexoelectric effect—electric potential generation due to inhomogeneous deformation—plays a key role in coordinating cellular healing activities. Based on McBride et al. (2020) and Titlbach et al. (2023), we propose a micromorphic framework that incorporates nonlinear electroelastic and flexoelectric contributions into the constitutive equations to determine the electric potential at a microcrack tip and, crucially, its impact on bone healing, which is captured through changes in nominal bone density. The framework is assessed using a prototypical cracked cantilever bone sample. Results demonstrate the model's ability to capture enhanced growth due to the flexoelectric effect and is complemented by a detailed analysis of the relevant material parameters."

## P12 | Quantum to continuum Model of Thermoset Fracture

Gayen, R., Vugrin L., Thang Z., Hantal G. (PhD), Halasz I., Smith A.-S. (PA):
**Deciphering Ball Milling Mechanochemistry via Molecular Simulations of Collision-Driven and Liquid-Assisted Reactivity**
In: Angewandte Chemie International Edition (2025), Vol. 64, Issue 50
DOI: 10.1002/anie.202505263


“Mechanochemistry by ball milling proceeds through a series of discrete, high-energy collisions between milling balls and the sample, yet the molecular-level processes that govern the resulting chemical and physical transformations remain poorly understood. In this study, we develop a molecular dynamics simulation protocol to investigate a model mechanochemical reaction between potassium chloride (KCl) and 18-crown-6 ether, both under dry conditions and in the presence of water as a liquid additive. Our simulations reveal that the reaction is initiated by collision-induced fragmentation of the KCl crystal into individual ions. This process occurs when the absorbed energy per ion pair during a collision exceeds the crystal's cohesion energy. We further show that the addition of a small amount of water facilitates the formation of complexes between potassium ions and 18-crown-6 molecules. However, excessive water content stabilizes the reactants instead, thereby suppressing complex formation. These findings highlight a non-linear relationship between liquid additive concentration and the reaction outcome. Our approach offers a molecular-level perspective on mechanochemical reactivity, providing valuable insights that could guide the rational optimization of milling conditions—particularly the targeted selection and dosing of liquid additives—to improve reaction efficiency.”

## 3.1 Dataset publications on Zenodo

Laubert L. (aPhD):
**One dimensional framework imitating the Capriccio method for coupling the finite element method with particle-based techniques**
Software
DOI: 10.5281/zenodo.7924399

Laubert L. (aPhD):
**Framework for projecting displacements of particles and nodes resulting from Capriccio method coupled deformation simulations to a one dimensional representation**
Software
DOI: 10.5281/zenodo.7924405

Laubert L. (aPhD), Weber F. (PhD) and Pfaller S. (PhD):
**Assessing the Capriccio Method via One-dimensional Systems for Coupled Continuum-Particle Simulations in Various Uniaxial Load Cases using a Novel Interdimensional Comparison Approach – data set**
Dataset
DOI: 10.5281/zenodo.7924405

Laubert L. (aPhD), Weber F. (PhD) and Pfaller S. (PhD):
**Approaching and overcoming the limitations of the multiscale Capriccio method for simulating the mechanical behavior of amorphous materials – data set**
Dataset
DOI: 10.5281/zenodo.13768063

Laubert L. (aPhD):
**FEMDcoupler: Preparing models for FE-MD coupling**
Software
DOI: 10.5281/zenodo.17094376

Rohracker M. (PhD), Kumar P. (PDR), Steinmann P. (PA) and Mergheim J. (PA):
**Efficient phase-field fracture simulations for fracture analysis in heterogeneous materials**
Dataset
DOI: 10.5281/zenodo.15425026

Laurien M. (PhD), Javili A. and Steinmann P. (PA):
**A damage formulation for continuum-kinematics-inspired peridynamics to capture fracture experiments**
Dataset
DOI: 10.5281/zenodo.15583097

Titlbach A. (aPhD), Papastavrou A., McBride A. and Steinmann P. (PA):
**Modelling the flexoeletric effect in human bone - A micromorphic approach**
Dataset
DOI: 10.5281/zenodo.15968102

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

The following is a tabular list of academic activities that took place in 2025 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 | Azad Kirsan

| from \| to | Name of conference | Location | Title of own poster |
|---|---|---|---|
| 17.03.2025<br>21.03.2025 | DPG Frühjahrstagung Regensburg 2025 | Regensburg | **Talk:** Free Energy Calculations of Electrolyte Decomposition Reactions on Lithium Battery Electrodes. |
| **Name** | **Supported researcher** | **Course \| field of study** | **Tasks relating to FRASCAL** |
| **Weiss**, Alexander | Azad Kirsan, P1 | Theoretical Chemistry | Generating structures for the dataset used in the training of a Li2O machine-learned interatomic potential using CPMD |
| **Student** | **Supervisor \| Date** | | **Topic** |
| **Stephani**, Pauline | Azad Kirsan \| 14.05 | | **Project theses:** Determination of diffusion coefficients and power spectra of electrolytes and ions in lithium metal batteries. |
| **Sell,** Marlene | Azad Kirsan \| Start: 01.09 | | **Master theses:** Development of a machine-learned interatomic potential for electrolytes in lithium metal batteries. |

### P1 | Christian Ritterhoff

| from \| to | Name of conference | Location | Title of own poster |
|---|---|---|---|
| 16.03.2025<br>21.03.2025 | DPG Frühjahrstagung Regensburg 2025 | Regensburg | **Talk:** The influence of strain-induced ferroelectricity on the fracture of oxide perovskites. |
| 31.03.2025<br>02.04.2025 | Molecular Modeling Workshop | Erlangen | **Talk:** The influence of strain-induced ferroelectricity on the fracture of oxide perovskites. |
| 25.08.2025<br>28.08.2025 | Psik 2025 | Lausanne | **Poster:** Modern Software Techniques for Fast-Fourier Transforms (FFTs) on Today's High Performance Computing (HPC) Architectures. |
| 08.10.2025<br>10.10.2025 | Woman in Science | Erlangen | **Poster:** Modern Software Techniques for Fast-Fourier Transforms (FFTs) on Today's High Performance Computing (HPC) Architectures. |
| **from \| to** | **Institute visited** | **Local supervisor** | **Research activities performed and skills acquired during stay** |
| 24.11.2025<br>28.11.2025 | ICAMS, Ruhr University Bochum | Ralf Drautz | Preparation for an application to the Walter-Benjamin Program of the DFG |
| **Sell,** Marlene | Azad Kirsan \| Start: 01.09 | | **Master theses:** Development of a machine-learned interatomic potential for electrolytes in lithium metal batteries. |

## P5 | Yuxin Luo

### Research stay

| from \| to | Institute visited | Local supervisor | Research activities performed and skills acquired during stay |
|---|---|---|---|
| 31.08.2025 - 30.09.2025 | Southwest Petroleum University | Prof. Mingiun Yang | Anticrack simulation with phase field fracture method |

## P6 | Eva Richter

| from \| to | Name of conference | Location | Title of own presentation |
|---|---|---|---|
| 07.04.2025 11.04.2025 | GAMM 2025 | Poznan, Poland | **Talk:** A „Capriccio light“ approach to study the capabilities of multiscale fracture simulations of thermoplastics. |
| **Name** | **Supported researcher** | **Course \| field of study** | **Tasks relating to FRASCAL** |
| **Roy**, Sohini | Eva Richter, P6 | Mechanical Engineering | A parameter study to investigate the influence of chain length, angle potential and degree of entanglement on the fracture behaviour of a generic thermoplastic polymer model. |
| **Van de Goor,** Joshua | Eva Richter, P6 | Mechanical Engineering | Investigation and improvement of the coupling in the Capriccio light approach, focusing on the interface between a GTP (generic thermoplastic polymer) lattice and GTP molecular chains. |
| **from \| to** | **Institute visited** | **Local supervisor** | **Research activities performed and skills acquired during stay** |
| 27.09.2025 - 08.11.2025 | Processing and Performance of Materials, Department of Mechanical Engineering, Eindhoven University of Technology, Netherlands | Frederik van Loock | Experiments and investigation regarding crazing and shear bands in annealed polycarbonate; experimental counterpart and extension to simulations regarding fracture of thermoplastics. |
| **Date** | **Name of the award** | | **Short description** |
| 27.11.2025 | NAFEMS DACH Student Award 2023/2024 | | For my Master thesis “A ‘Capriccio light’ approach to study the capabilities of multiscale fracture simulations of thermoplastics” in the category of material science and structural mechanics. The award is aimed at students who have completed a thesis (Bachelor, Master, etc.) in the field of calculation and simulation within an area of engineering sciences and to support gifted students and motivate them for further activity in the field of calculation and simulation in engineering sciences. At the same time, this also acknowledges the importance of academic institutions for the further development of numerical simulation in teaching and research. |

## P6 | Felix Weber

| from \| to | Name of conference | Location | Title of own presentation |
|---|---|---|---|
| 27.03.2025<br>28.03.2025 | Meeting of ESIS TC8 and DVM-Working group Simulation | Munich | **Talk:** Concurrent Molecular Dynamics-Finite Element Fracture Simulations of Amorphous Materials |

## P6 | Lukas Laubert

| from \| to | Name of conference | Location | Title of own presentation |
|---|---|---|---|
| 21.07.2025<br>24.07.2025 | 18th U.S. National congress on computational mechanics | Chicago, USA | **Talk:** Evaluating the coupling quality of domain decomposition methods. |
| 17.09.2025<br>19.09.2025 | 8th ECCOMAS Young Investigators Conference | Pescara, Italy | **Talk:** Evaluating the coupling quality of domain decomposition methods. |

| Collaborating Institution | Research topic | Researchers involved |
|---|---|---|
| Institut de Chimie et des Matériaux paris-Est at the Université paris-Est Créteil Val de Marne | BIO ART | Agustín Ríos De Anda<br>Stephanie Chedid |
| Laboratoire Modélisation et Simulation Multi-Échelle at the Université Gustave Eiffel | BIO ART | Fabrice Detrez<br>Moussa Lamamra |
| Department of Polymer Engineering at the Universität Bayreuth | BIO ART | Denise Schweser |
| Aerospace and Mechanical Engineering Department at the University of Liége | Continuum constitutive modeling | Ujwal Kishore Jinaga<br>Mohib Syed Mustafa |
| PULS Group FAU | Molecular simulations | Christian Wick<br>György Hantal<br>Sampanna Pahi<br>Bariscan Arican |
| Institute of Materials Simulation | Network model simulations | Christian Greff |
| Vernery Research Group at the College of Engineering and Applied Science | Molecular and network model simulations | Saleh Assadi, Zachary White |

## P7 | Leon Pyka

| from \| to | Name of conference | Location | Title of own presentation |
|---|---|---|---|
| 16.09.2025<br>19.09.2025 | 8th ECCOMAS Young Investigators Conference | Pescara, Italy | **Talk:** Tuning Fracture Behaviour in Architected Composite Materials. |
| **Name** | **Supported researcher** | **Course \| field of study** | **Tasks relating to FRASCAL** |
| Saba Taheri | Christian Greff<br>Leon Pyka | Computational Materials Science | Developing tests and expansions of a Python library as a framework for network simulations. |

## P8 | Maurice Rohracker

| from \| to | Name of conference | Location | Title of own presentation |
|---|---|---|---|
| 17.09.2025<br>19.09.2025 | 8th ECCOMAS Young Investigators Conference | Pescara, Italy | **Talk:** Efficient Phase-Field Fracture Simulations for Fracture Analysis in Heterogenous Materials |
| **Supervised Student** | | **Topic** | **Supervisor \| Date** |
| Frank, Sebastian (Master thesis) | | Numerische Bruchmodellierung von viskoelastisch-viskoplastisch gekoppelten Phasefeldansätzen | Maurice Rohracker 29.09.2025 |
| **Student assistant** | | **Course/ field fo study** | **Tasks relating to FRASCAL** |
| Shastry, Aaniruddha P. | | Computational Engineering | Extension and maintenance of the inhouse python toolbox RVEGen for generating geometry and meshes of RVEs |

## aP8 | Lucie Spannraft

| from \| to | Name of conference | Location | Title of own presentation |
|---|---|---|---|
| 17.02.2025<br>12.02.2025 | GFKT 2025 | Cologne, Germany | Participation only |
| 13.05.2025<br>16.05.2025 | CMCS 2025 | Paris, France | **Poster:** Generalized interfaces modeling adhesives and their failure |
| 14.11.2025<br>17.11.2025 | 9th China International Bonding Technology | Beijing, China | **Talk:** Generalized interfaces modeling adhesives and their failure |

## P9 | Prateek Prateek

| from \| to | Name of conference | Location | Title of own presentation |
|---|---|---|---|
| 26.08.2024<br>30.08.2024 | ECCOMAS 18th Thematic Conference on Computational Plasticity | Barcelona, Spain | **Talk:** A discrete mechanics perspective on bond-based peridynamics. |
| **from \| to** | **Institute visited** | **Local supervisor** | **Research activities performed and skills acquired during stay** |
| 12.05.2025<br>-<br>23.05.2025 | Lehrstuhl für Festkörüermechanik | Kerstin Weinberg | Focused on in-depth technical discussions and collaborative work on numerical modelling, structure-preserving time integration, and dynamic fracture in peridynamics-based simulations. |

## P10 | Marie Laurien

| Supervised Student | Topic | Supervisor \| Date |
|---|---|---|
| Sharma, Aditi<br>(Master thesis) | Adaptive grid refinement for fracture modelling in peridynamics. | Marie Laurien<br>02.05.2025 |

## aP10 | Anna Titlbach

| from \| to | Name of conference | Location | Title of own presentation |
|---|---|---|---|
| 06.07.2025<br>08.07.2025 | EDB Conference | Zurich, Switzerland | **Poster:** Exploring flexoelectric phenomena in human bone through a micromorphic continuum modelling framework. |
| 08.09.2025<br>10.09.2025 | ICCB Conderence | Rome, Italy | **Talk:** Modelling the Flexoelectric Effect in Bone: Numerical study of its influence on bone density growth at microcracks |
| **Partner institute** | | **Researchers involved** | **Research topic** |
| GCEC, University of Glasgow | | Anrew McBride | Modelling and Simulation of the flexoelectric effect in human bone using a coupled micromorphic approach. |

## P11 | Max Zetzmann

| Student assistant | Course/ field fo study | Tasks relating to FRASCAL |
|---|---|---|
| Schindhelm, Jonas | Continuous Optimization | Providing an overview of the existing literature in response to questions related to or stemming from research on the mathematical aspects of peridynamics. |

## P12 | György Hantal

| from \| to | Name of conference | Location | Title of own presentation |
|---|---|---|---|
| 31.08.2025<br>05.09.2025 | Conference of the European Molecular Liquids Group | Héviz, Hungary | **Talk:** Experimental-simulation investigation of the Effects of Inert Gases on the Properties of Imidazolium-Based Ionic Liquids. |

## aP12 | Sampanna Pahi

| from \| to | Name of conference | Location | Title of own presentation |
|---|---|---|---|
| 31.03.2025<br>02.04.2025 | MMWS | Erlangen | **Talk:** What is the impact of covalent-network formation on the curing kinetics of thermosets? |
| 24.07.2025 | GS EAM | Erlangen | **Talk:** What is the impact of covalent-network formation on the curing kinetics of thermosets? |
| 08.09.2025<br>14.09.2025 | AIMAT Summer school | KIT | **Talk:** What is the impact of covalent-network formation on the curing kinetics of thermosets? |
| 21.11.2025<br>22.11.2025 | CMSSP | Erlangen | **Talk:** Mechanistic Modeling of Epoxy Reaction Barriers using Geometric and Hydrogen Bond Descriptors. |
| **Date** | **Name oft he award** | | **Short desciption** |
| 24.07.2025 | Best poster award | | Awarded the best poster award by EAM with a cash prize of 250 Euros |
| 21.11.2025 | Best oral presentation award | | Awarded the best oral presentation award by the Physics department of Presidency University, Kolkata |

## aP12 | Bariscan Arican

| from \| to | Name of conference | Location | Title of own presentation |
|---|---|---|---|
| 16.03.2025<br>21.03.2025 | DPG Spring Meeting | Regensburg | **Talk:** Integrating chemistry into modeling fracture in cured epoxy resins under mechanical stress. |
| 31.03.2025<br>02.04.2025 | MMWS | Erlangen | **Talk:** Integrating chemistry into modeling fracture in cured epoxy resins under mechanical stress. |
| 24.07.2025 | GS EAM | Erlangen | **Talk:** Integrating chemistry into modeling fracture in cured epoxy resins under mechanical stress. |

## P13 | Javad Karimi

| from \| to | Name of conference | Location | Title of own presentation |
|---|---|---|---|
| 17.09.2025<br>19.09.2025 | Young Investigators Conference 2025 | Pescara, Italy | **Talk:** The Role of Grain Packing and Pore Distribution in Fracture Evolution of Rocks |
| **Partner Institute** | **Researchers involved** | | **Research topic** |
| Aristotle University of Thessaloniki | Javad Karimi, Daniel Koehn, Vasilios Melfos, Tarantola Alexandre | | Structural geology and tectonics of Northern Greece |

## P13 | Bakul Mathur

| from \| to | Name of conference | Location | Title of own presentation |
|---|---|---|---|
| 17.09.2025<br>19.09.2025 | Young Investigators Conference 2025 | Pescara, Italy | **Talk:** Contact-Anisotropy-Driven Microscale Splitting: A Polyhedral DEM Grain Fracture Model |

## P14 | Ba Duc Duong

| from \| to | Name of conference | Location | Title of own presentation |
|---|---|---|---|
| 08.09.2025<br>12.09.2025 | Frontiers in Calculus of Variations and Applied Analysis | Munich | Participation only |
| 24.09.2025<br>26.09.2025 | Hyperbolic Problems in Nürnberg 2025 | Nürnberg | Participation only |
| 29.10.2025<br>31.10.2025 | Bsverlangen | Erlangen | Participation only |

# 4. Qualification program

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, Special Seminars and Soft Skills Trainings. As a new cohort started the qualification program in 2025, we were able to draw on our full resources again.

### FRASCAL Mini Lectures

The Mini Lecture program 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 2025:

#### March 14 | Prof. Yamakou | Neural networks & machine learning

The lecture covered fundamental concepts in data science, including data preprocessing, exploratory analysis, and modeling. It provided an overview of machine learning techniques, highlighting supervised and unsupervised learning approaches. Neural networks were introduced, explaining their structure, activation functions, and training process. The session emphasized practical applications and the role of data-driven decision-making in various fields. (*Text: Prateek*)

#### March 21 | Dr. Maximilian Ries | pgfplots

In the Special Seminar, Dr.-Ing. Maximilian Ries introduced the participants to the LaTeX package 'pgfplots'. By going through three examples step-by-step, the participants learnt to use basic and advanced techniques in terms of generating scientific diagrams that are publication-ready. Furthermore, individual questions and problems could be addressed. Therefore, by working through the seminar, a template was obtained by each participant which proved to be a great starting point for respective individual projects. (*Eva Richter*)

#### March 28 | Prof. Paul Steinmann | Introduction to tensor calcus

Prof. Steinmann gave the Mini Lecture 'Introduction to Tensor Calculus' for interested members of FRASCAL. Starting with descriptive explanations concerning affine point and

vector spaces and associated operations, such as the scalar product and triple scalar product.
We discussed examples of use cases for engineering applications, such as the role of the triple vector product in calculations of the kinetic energy of a rigid body. In the last part, Prof. Steinmann provided an overview of topics related to tensor calculations, such as the dyadic product, eigenvalues and calculation of determinants. Practical examples in mechanics, such as the determination of the principal stresses of the stress tensor, supported the information. (*Text: Leon Pyka)*


*Picture: Paul Steinmann*

### April 4 | Prof. Paul Steinmann | Introduction to continuum mechanics

Professor Steinmann began his Mini Lecture, 'Introduction to Continuum Mechanics (ICOME),' by building upon concepts introduced in the previous Mini Lecture on tensor calculus. Hence, a mathematical operations toolset, such as dyadic products and tensor derivatives, was recapitulated. In the central part, Lagrangian and Eulerian mechanics were discussed, emphasising that both approaches are congenial and the respective measures can be transformed into one another. An overview of the respective balance and constitutive equations was provided, culminating in thermo-dynamic consideration of the continuum. (*Text: Leon Pyka*)

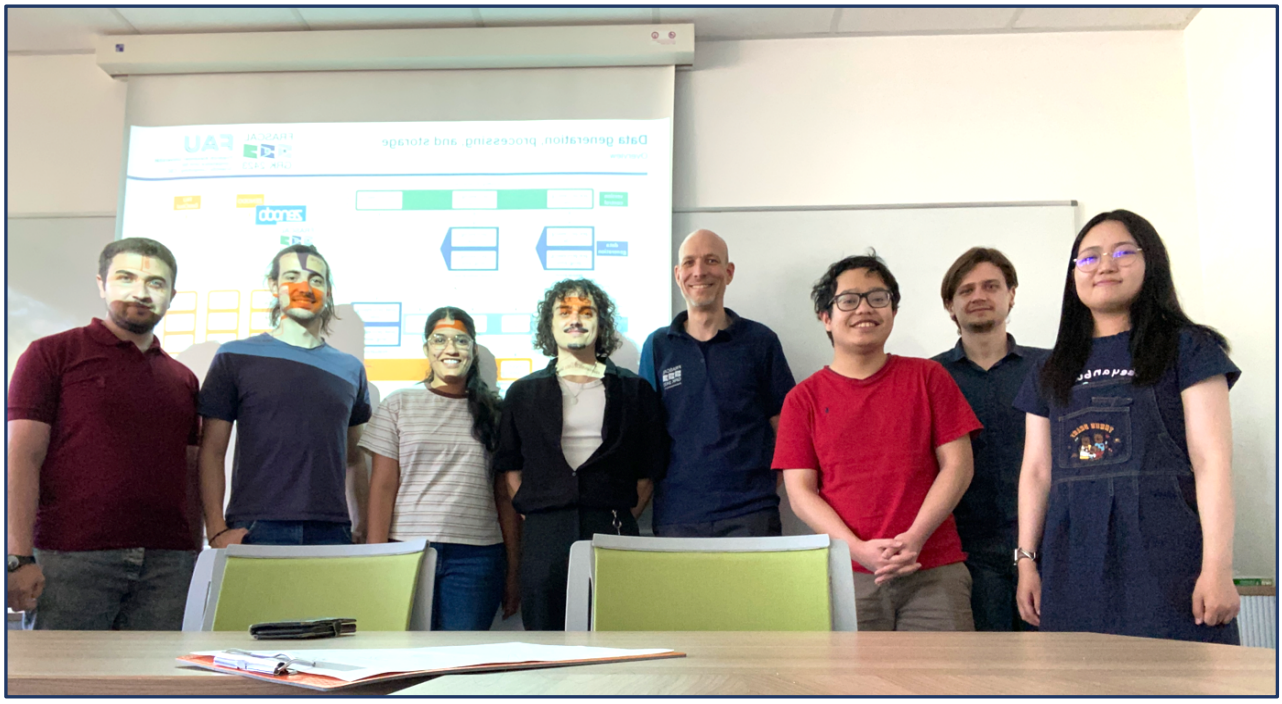
### June 13 | Dr. Paolo Moretti | Failure of disordered materials

The first part of this course begins with the size effect in materials and Griffiths' fracture theory, introducing the widespread presence of fluctuation phenomena in material properties and thereby highlighting the significance of applying statistical physics to the study of material failure. Using the example of percolation, Dr. Paolo Moretti explored whether the concept of continuous phase transitions can be applied to fracture processes, leading to the scale invariance in certain material properties during failure. He then systematically presented the mechanical foundations of network models, including constitutive equations, failure criteria and the incorporation of strength fluctuations

through various probability distributions. In the second part, through concrete coding examples, Dr. Moretti demonstrated how to construct network mesh by programming, and also the underlying theory of boundary operators and discretized computations. (*Text: Yuxin Luo)*

### June 20 | Dr. Sebastian Pfaller | Introduction to FRASCAL's research data management

In today's FRASCAL minilecture, Dr. Pfaller discussed Research Data Management and the importance of proper data storage. Key aspects included a thorough introduction to the different types of data a computational researcher may encounter, distinguishing between usable code/programs, input data, raw output data, and processed data. To store these various types in accordance with the FAIR principles, Dr. Pfaller presented various online storage systems, ranging from our own FRASCAL server (nas) to the European OpenAIRE project (Zenodo), and explained when to use each service. Finally, the lecture concluded with a brief overview of several copyright licenses and fitting examples of their usage.



*Picture: Sebastian Pfaller*

### July 27 | Prof. Michael Stingl | Introduction to mathematical optimisation

We look at optimisation and some applications related to FRASCAL projects. In the beginning, we introduce the necessary mathematical basics concerning optimisation as well as the two motivating examples we will apply optimisation on, namely topology optimisation in truss models and peridynamics. Concerning the mathematical concepts, we first try to derive necessary conditions concerning local minimisers, particularly the KKT-conditions. In the second part, we turn to convexity and algorithms used in optimisation. We also have a concrete toy implementation of cracks in peridynamics. Lastly, we take a glimpse at optimisation in stochastic models. (*Text: Ba Duc Duong*)

### October 17 | Dr. Capobianco & Dr. Sato | Introduction to numerics

The lecture began with a discussion on nonlinear systems, where Dr. Capobianco introduced several variants of the Newton–Raphson method. He explained how each method is formulated, their respective advantages and disadvantages, and in which situations one should choose which kind of nonlinear solver. Following that, the topic moved to initial value problems. Dr. Capobianco illustrated the Euler method, the implicit Euler method, and more advanced combined schemes using clear and intuitive examples. He also demonstrated how to evaluate the error and convergence of these methods, emphasizing the importance of stability in numerical solutions. Before the lunch break, Dr. Sato took over and provided an introduction to Gaussian elimination and LU decomposition, which he continued to discuss in greater detail during the afternoon session. He also elaborated on QR decomposition, explaining the concept through practical examples. (*Text: Javad Karimi*)

### October 31 | Prof. Julia Mergheim | Introduction to homogenisation

After covering the basics of continuum mechanics and motivating the need for homogenization approaches, analytical methods including the Mori-Tanaka method and the self-consistent method were introduced and compared with numerical approaches. The lecture was complemented by interactive computer exercises - one illustrating the difficulties in selecting an appropriate RVE and the other comparing the different analytical homogenization methods discussed. (*Text: Max Zetzmann*)

### November 14 | Soheil Firooz | Introduction to peridynamics

Mini-lecture entitled “Fundamentals of Local and Non-Local Continuum Mechanics: Theory, Material Modelling and Computational Aspects”. In this lecture, classical continuum mechanics fundamentals, material modelling and the computational implementation using FEM were covered. The struggles in local theory were highlighted, providing the motivation for adopting the nonlocal theory. Subsequently, peridynamics, as a non-local continuum approach, was explained. The lecture detailed continuum-kinematics-inpired peridnamics, including one-neighbour, two-neighbour and three-neighbour interaction models. Material modelling and computational implementation aspects in this framework were also discussed. Finally, several numerical examples were presented. The speaker also showed programming code examples to better illustrate the concept for both formulations. (*Text: Aditi Sharma*)

**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.

Two special seminars were held in 2025. Prof. Wolfgang Bangerth from Colorado State University and Prof. Eran Bouchbinder from the Weizmann Institute of Science could be engaged for the special seminar days.

**Special seminars 2025**

| Date | Title | Lecturer |
|---|---|---|
| 5 September | Supporting complex simulations with open source finite element | Prof. Wolfgang Bangerth |
| 8 December | Topological defects and multi-plane crack interactions in materials failure | Prof. Eran Bouchbinder |

## FRASCAL Seminars

In each lecture period one qualification day is reserved for a FRASCAL seminar, which is mandatory for the doctoral researchers. Within the framework of this seminar, recent developments in the doctoral and associated doctoral projects are presented as talks of 20 - 30 min duration, including a 5 - 10 min discussion. Based on these seminars, the doctoral and associated doctoral researchers can evaluate the progress of the doctoral project in comparison to the other projects together with the mentoring team.
Both FRASCAL Seminars 2025 took place at the LTM. This year, the presentations formed a symbiosis between the 2nd and 3rd cohort.

## 11th FRASCAL Seminar Program

## 12th FRASCAL Seminar Program


### TOPZ

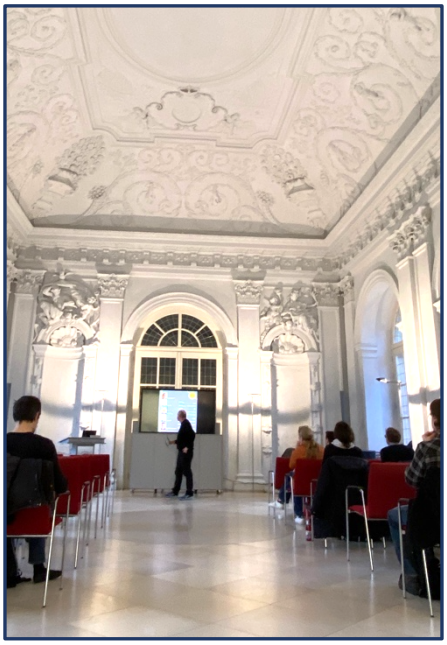
The digital format called FRASCAL TOPZ (Topical Overview Presentation Zoomposium), for which we meet once a week during the semester, was used for an informal get-together in ZOOM, where the PAs, the spokespersons, the doctoral and associated doctoral researchers, the postdoc, and the scientific coordinator were present. The latest scientific progress and open questions from one to two doctoral projects were briefly presented and jointly discussed. FRASCAL TOPZs provides 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. And to everyone's delight, with the start of the new cohort in 2025, more doctoral researchers are participating again!

### 4th FRASCAL Symposium

On November 20st, the FRASCALis met again in the Oragnerie to enjoy exciting presentations by invited (and FAU internal) scientists.

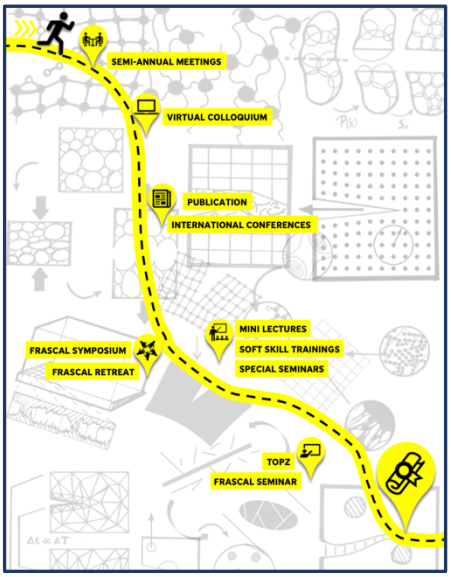
**Tristan Baumberger** from the Université Paris Cité opened the event with a talk on „*Length- and time-scales of crack growth in a polymer hydrogel*„. After a short coffee break, P13-PA **Daniel Köhn** took over with an interesting presentation on "*Fractures across scales from microstructures to mid ocean ridges*". The most exciting talk for all those in the audience who normally work in well-tempered laboratories or offices was given by **Nina Kirchner** from Stockholm University. As a glaciologist, she works in her icy

research station, taking the audience with her to this fascinating environment during her talk entitled "*Fractures in northern icy environments: challenges for glaciological and cryospheric research*". After their excursion into the cold, everyone enjoyed lunch before returning to the moderate climate of FAU. There, former FRASCLi **Wuyang Zhao** gave a presentation on "*Microscopic mechanisms of plasticity and fracture in glassy polymers*". **Miguel Ángel Moreno-Mateos** rounded off the symposium and spoke about "*Advances in soft fracture (and cutting) mechanics*". Thank you to everyone involved for a successful event and the enjoyable discussions!

# 5. Selected Highlights

2025 was a year full of activity, as there were not only numerous events, but also new FRASCALis who gained a lot of experience as part of the qualification program. The selection of highlights for 2025 is therefore slightly larger.




## 5.1 Welcome 3rd cohort!

At the beginning of March, the third generation of FRASCALIs was officially welcomed. In addition to chic portrait photos, there was a detailed briefing for everyone to help them find their way through the jungle of the qualification program. During the course of the year, it became clear that this new generations is highly motivated and committed, contributes wonderfully, and that everyone is giving their all for the FRASCAL community!

## 5.2 Eva`s research stay in netherlands

From September 27th to November 8th, Eva Maria Richter completed a six-week research stay with the group of Assistant Professor Frederik van Loock, which is embedded within the Processing and Performance (P&P) of Materials group at the Department of Mechanical Engineering at Eindhoven University of Technology (Netherlands). In the context of the group's strong experimental focus, Eva collaborated closely with PhD student Daniel Reitmair, conducting experiments that investigated the nature of shear bands and crazing in annealed polycarbonate. This stay proved highly valuable, offering an additional, essential experimental perspective that significantly complemented Eva's ongoing simulation-based work on thermoplastic materials. Furthermore, attending the weekly P&P group meetings and additional seminars fostered a deep and exchange with other researchers, sparking new ideas

for her own simulations and leading to further progress. Sebastian Pfaller also visited the group for several days to gain insight into their work. Eva also took the time to balance the successful research activities with various enr iching trips to explore the city and surrounding areas, providing an opportunity to experience Dutch culture. In conclusion, this six-week research stay was truly successful and fruitful. Sincere gratitude is expressed to Frederik van Loock and all colleagues at TU/e for making this such a special and enjoyable time!

*Text & Pictures @ Eva Richter*

## 5.3 FRASCAL Retreat

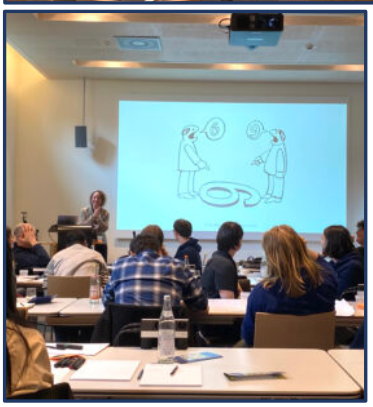
From 8th to 9th of May the FRASCALis went with a promising retreat program to Waischenfeld. Our bus trip started in beautiful weather and with almost punctual but highly motivated travelers.

**GET TOGETHER & FRASCALIZE**

After arriving and letting the coffee machine run hot for the first time, the 2nd cohort took the floor and reported on their respective FRASCAL journey. It was really nice to see that many also benefited from the FRASCAL community on a personal level. Advice to the next cohort was also very much appreciated! Afterwards, the FRASCALis of the 2nd cohort presented their demonstrators and ideas for the previous „Long Night of Science“ in order to inspire the FRASCAL newcomers for their science communication.

**WORKSHOP: MASTER YOUR INTERNATIONAL TEAMWORK**

In a very interactive workshop, Dr. Iris Wangermann introduced all FRASCALis – whether PA, PhD or coordination – to the world of international communication. With amusing games and lots of teamwork, it was a wonderful way to get a feel for different cultures and how to deal with unfamiliar rules and values. After the barbecue, not everyone went to bed early in order to be in high



spirits for the next day of the retreat. According to some rumors, music was played until the early hours of the morning.

**POSTERSLAM**

Next morning it was the 3rd cohort's turn: starting with a small pitch, everyone presented their scientific project as part of their FRASCAL PhD journey. Afterwards, there was enough time for an intensive discussion at the posters. Everyone who had to answer the tricky questions of the scavenger hunt was also encouraged to do so. Once again, all participants were highly motivated – but only one could win...

**CAREER PATHS**

Before the well-deserved lunch break, PD Dr. Sebastian Pfaller outlined what an academic career could look like. Thank you for the insight into your interesting academic development!

**HIKE**

Highly motivated and well-energized, the FRASCALis set off on a challenging hike. One highlight followed the next – but everyone kept going until the end, but had to cope with the experience with ice cream or beer.

**CLOSING**

As a crowning finale, Prof. Steinmann honored the dedication of our FRASCALis of the second cohort, as many are on the home stretch and it was their last retreat. New representatives were also elected for the next cohort – congratulations to Leon an d Ba Duc!

## 5.4 Start-up workshop @ Zollhof


Curious and full of expectation, a horde of FRASCALis and EBMers entered the elegant halls of the ZOLLHOF in Nuremberg on May 20th. We were greeted in a relaxed atmosphere by Prof. Dr. Kathrin Möslein, Vice President Outreach at FAU, who introduced us to the idea behind the collaboration between FAU and ZOLLHOF as one of Germany`s leading tech incubators. After the various research projects have been explained, Matthias Trost presented his path of funding a start-up and briefly mentioned intellectual property, working relations between scientists/engineers and business people, as well as, financing options. Dr. Judit Klein discussed, i.a., the ranking of viability, feasibility and desirability, which was counterintuitive for many engineers who wanted to focus on the feasibility and development of a technology first, rather than checking the actual market need and viability beforehand. After watching a video introducing a new technology, groups of three developed their three best and worst ideas for promoting that technology. The three worst were discarded and each group had to develop a need, solutions and values for one of the worst ideas from another group. This exercise showed how differently each group evaluated their ideas, how the group interacted and how easy/hard it was to break away from their original best ideas and work with the „bad" idea. The very interesting and productive workshop ended with a tour of the Zollhof building.

*Text: Andrea Dakkouri-Baldauf, Lucie Spannraft & Anna Donhauser*

## 5.5 Lange Nacht der Wissenschaften


On October 25, it was that time again: every two years, FAU and other scientific institutions in Erlangen, Nuremberg, and Fürth present their research to the broader public. Of course, FRASCAL also took part and demonstrated fracture behavior at three interactive stations. Using pretzel sticks, scissors, and flour, visitors were able to experience hands-on how fractures develop and behave on different scales. The highly coveted FRASCAL bags, which were given out as a reward after completing the stations, were already gone before the official end of the Lange Nacht. Many thanks again to all FRASCALis involved in helping and supporting us !


## 5.6 Doctoral Degrees

In 2025 two FRASCALis completed their doctoral journeys. **Angel Santarossa** (aP4) received his doctoral degree for his thesis on "*Experimental research and enhancement of granular gripping systems*". **Joscha Seutter** (P14) completed his doctorate on May 22 on the topic of *"Passage from Atomistic-to-Continuum for Quasistatic Crack Growth".*

Defense of Angel Santarossa`s doctoral thesis.
Picture @ www.mss.tf.fau.de