Friedrich-Alexander-Universität
Erlangen-Nürnberg

# Annual Report 2022

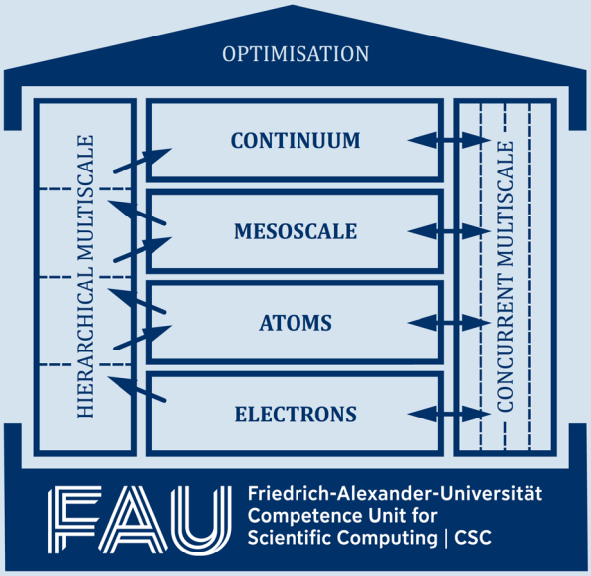
of the Research Training Group GRK 2423

FRASCAL

GRK 2423

# Fracture across Scales:

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



**Impressum**

**Spokesperson:**
Prof. Dr. Paul Steinmann
Institute of Applied Mechanics
Dep. of Mechanical Engineering
Friedrich-Alexander-Universität Erlangen-Nürnberg
Egerlandstraße 5
91058 Erlangen
Phone: +49 (0)9131 85 28502
Fax: +49 (0)9131 85 28503
E-Mail: paul.steinmann@fau.de
www.ltm.tf.fau.eu

**Coordination:**
Dr. Andrea Dakkouri-Baldauf
Competence Unit for Scientific Computing, CSC
Friedrich-Alexander-Universität Erlangen-Nürnberg
Martensstraße 5a
91058 Erlangen
Phone: +49 (0)9131 85 20782
Fax: +49 (0)9131 85 20785
E-Mail: andrea.dakkouri@fau.de
www.csc.fau.eu
www.frascal.fau.eu

# Preface

2022 marks a special year for FRASCAL: in January, the second cohort of doctoral researchers started with full steam, and already the first FRASCAL retreat in spring showed that the temporal overlap with the first cohort led to extraordinarily positive synergies. From the summer onwards, the preparation of the renewal application for the second funding phase of FRASCAL was on the agenda; the doctoral researchers contributed with great enthusiasm, so that the application and report could be submitted to the DFG on time in the autumn. The winter was then all about preparing for the upcoming on-site visit and was richly filled with numerous activities by the entire FRASCAL team. In parallel, many doctoral researchers from the first cohort submitted their dissertations, some of which have already been defended. FRASCAL was also able to edit a special issue of the international peer-reviewed Elsevier journal "Forces in Mechanics" with numerous manuscripts, which provide a great overview of the fantastic scientific work on "Fracture across Scales". Looking back, 2022 is a year full of activities and successes for FRASCAL!

Erlangen, December 2022

Paul Steinmann

# Content

# 1 General Information

## 1.1 Title in German and English

Skalenübergreifende Bruchvorgänge:

*Integration von Mechanik, Materialwissenschaften, Mathematik, Chemie und Physik*

Fracture across Scales:

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

## 1.2 Participating researchers

**Spokesperson:**
Prof. Dr.-Ing. Paul Steinmann

**Co-spokesperson:**
Prof. Dr. rer. nat. Michael Stingl

**Doctoral researchers' spokesperson:**
Paras Kumar (until April 2022)
Felix Weber (since May 2022)

**Doctoral researchers' gender representative:**
Nosaibeh Esfandiary (until April 2022)
Maurice Rohracker (since May 2022)

*Table 1: Participating supervisors*

| Principal Advisors (PAs) | Chair, Department, Work Address | Contact Data (Tel / Fax, Email, Web) | 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, 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, ltd.tf.uni-erlangen.de | Computational Dynamics |
| **Mergheim**, Julia, Prof. Dr.-Ing. | Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen | +49 9131 85-28 505 / -503, julia.mergheim@fau.de, www.ltm.tf.fau.eu | Computational Mechanics |
| **Meyer**, Bernd, Prof. Dr. rer. nat. | Computational Chemistry, Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen | +49 9131 85-20 403 / -404, bernd.meyer@fau.de, chemistry.nat.fau.eu/ccc/groups | Surface Science |
| **Moretti**, Paolo, Dr. | Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth | +49 911 65078-65 071 / -066, paolo.moretti@fau.de, matsim.techfak.uni-erlangen.de | Complex Microstructures |
| **Pfaller**, Sebastian, PD Dr.-Ing. habil. | Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen | +49 9131 85-28 507/ -503, sebastian.pfaller@fau.de, www.ltm.tf.fau.eu | Scale Coupling Methods |
| **Pöschel**, Thorsten, Prof. Dr. rer. nat. | Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraße 3, 91058 Erlangen | +49 9131 85-70 501, thorsten.poeschel@fau.de, mss.cbi.fau.de | Granular Media |
| **Smith**, Ana-Sunčana, Prof. Dr. rer. nat. | Theoretical Physics, Dep. of Physics, Cauerstraße 3, 91058 Erlangen | +49 9131 85 70 565 / -518, smith@physik.uni-erlangen.de, puls.physik.fau.de/ | Soft Matter |

| | | | |
|---|---|---|---|
| **Steinmann**, Paul, Prof. Dr.-Ing. | Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen | +49 9131 85-28 501 / - 503, paul.steinmann@fau.de, www.ltm.tf.fau.eu | Continuum Mechanics |
| **Stingl**, Michael, Prof. Dr. rer. nat. | Mathematical Optimisation, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen | +49 9131 85-67 141 / -20785, michael.stingl@fau.de, mso.math.fau.de | Optimisation |
| **Zahn**, Dirk, Prof. Dr. rer. nat. | Theoretical Chemistry, ComputerChemistryCenter, Nägelsbachstr. 25, 91052 Erlangen | +49 9131 85-20 205 / 404, dirk.zahn@fau.de, chemistry.nat.fau.eu | Condensed Matter |
| **Zaiser**, Michael, Prof. Dr. rer. nat. | Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth | +49 911 65078-65 060 / -066, michael.zaiser@fau.de, matsim.techfak.uni-erlangen.de | Statistical Mechanics of Materials |

*Table 2: Postdoctoral researcher*

| Post Doc | Chair, Department, Work Address | Contact Data (Tel / Fax, Email, Web) | Research Area |
|---|---|---|---|
| **Wick**, Christian, Dr. rer. nat. | Theoretical Physics, Dep. of Physics, Cauerstraße 3, 91058 Erlangen | +49 9131 85 70 566 / -518, christian.wick@fau.de, puls.physik.fau.de/ | Quantum-to-Continuum Model of Thermoset |

*Table 3: Doctoral researchers*

| Doctoral Researchers | Chair, Department, Work Address | Contact Data (Tel / Fax, Email, Web) | Research Area |
|---|---|---|---|
| **Bauer**, Christof | Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen | +49 9131 85-28 508 / -503, christof.bauer@fau.de www.ltm.tf.fau.eu | Fracture in Thermoplastics: Discrete-to-Continuum |
| **Esfandiary**, Nosaibeh | Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth | +49 911 65078-65 065 / -066, nosaibeh.esfandiary@fau.de, matsim.techfak.uni-erlangen.de | Collective Phenomena in Failure at Complex Interfaces |
| [1]**Canbolat**, Utku | Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraße 3, 91058 Erlangen | +49 9131 85-70 490 / -518, utku.canbolat@fau.de, mss.cbi.fau.de | Large Scale Simulations for Fragmentation of Granular Materials |
| [1]**Greff**, Christian | Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth | +49 911 65078-65 063 / -066, christian.greff@fau.de, matsim.techfak.uni-erlangen.de | Tuning Adhesion Properties of Hierarchical Materials |
| [1]**Igel**, Lennart | Mathematical Optimisation, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen | +49 9131 85-67 083 / -20785, lennart.g.igel@fau.de, mso.math.fau.de | Fracture Control by Material Optimisation |
| [1]**Jadhav**, Deepak Balasaheb | Applied Dynamics, Dep. of Mechanical Engineering, Immerwahrstraße 1, 91058 Erlangen | +49 9131 85-61 002 / -011, deepak.jadhav@fau.de, ltd.tf.uni-erlangen.de | Adaptive Dynamic Fracture Simulation |
| **Konrad**, Julian | Theoretical Chemistry, ComputerChemistryCenter, Nägelsbachstr. 25, 91052 Erlangen | +49 9131 85-20 425 / -404, julian.konrad@fau.de chemistry.nat.fau.eu | Fracture in Polymer Composites: Nano to Meso |

[1] 2nd cohort of FRASCAL

| Doctoral Researchers | Chair, Department, Work Address | Contact Data (Tel / Fax, Email, Web) | Research Area |
|---|---|---|---|
| **Kumar**, Paras | Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen | +49 9131 85-20 323 / -503, paras.kumar@fau.de, www.ltm.tf.fau.eu | Fracture in Polymer Composites: Meso to Macro |
| **Lakshmipathy**, Tarakeshwar | General Material Properties, Dep. of Mat. Science and Engineering, Martensstraße 5, 91058 Erlangen | +49 9131 85-27 486 / -504, tara.ll.lakshmipathy@fau.de, gmp.ww.uni-erlangen.de | Atomistics of Crack-Heterogeneity Interactions |
| [1]**Laurien**, Marie | Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen | +49 9131 85-64 407/ -413, marie.laurien@fau.de www.ltm.tf.fau.eu | Continuum-kinematics-inspired peridynamic modelling of fracture |
| [1]**Mathur**, Bakul | Tectonics, Dep. of Geography and Geosciences, Schlossgarten 5 91054 Erlangen | +49 1765 78 24271 bakul.mathur@fau.de, www.gzn.nat.fau.eu | Fragmentation and Fracture in Geological Rocks |
| **Müller**, Tobias | Computational Chemistry, Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen | +49 9131 85-20 421 / -404, tobias.tm.mueller@fau.de, chemistry.nat.fau.eu/ccc/groups | Chemistry at the Crack Tip |
| **Phansalkar**, Dhananjay | Applied Dynamics, Dep. of Mechanical Engineering, Immerwahrstraße 1, 91058 Erlangen | +49 9131 85-61 019 / -011, dhananjay.phansalkar@fau.de, ltd.tf.uni-erlangen.de | Adaptive Dynamic Fracture Simulation |
| **Ritter**, Jonas | Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth | +49 911 65078-65 064 / -066, jonas.ritter@fau.de, matsim.techfak.uni-erlangen.de | Compressive Failure in Porous Materials |
| [1]**Ritterhoff**, Christian | Computational Chemistry, Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen | +49 9131 85-20 421 / -404, christian.ritterhoff@fau.de chemistry.nat.fau.eu/ccc/groups | Chemistry at the Crack Tip |
| [1]**Rohracker**, Maurice | Applied Mechanics, Dep. of Mechanical Engineering, Paul-Gordan-Str. 3, 91052 Erlangen | +49 9131 85-64 410 / -413, mau.rohracker@fau.de, www.ltm.tf.fau.eu | Fracture in Polymer Composites: Meso to Macro |
| [1]**Seutter**, Joscha | Modeling and Numerics, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen | +49 9131 85-67 215 / - 67 225, joscha.seutter@fau.de, mso.math.fau.de | Discrete-to-Continuum Passage for Variational Fracture Models |
| [1]**Shegufta**, Shucheta | Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth | +49 911 65078-65 065 / -066, shucheta.shegufta@fau.de, matsim.techfak.uni-erlangen.de | Failure in Porous Materials |
| **Singh**, Sukhminder | Mathematical Optimisation, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen | +49 9131 85-67 048 / -20785, sukhminder.singh@fau.de, mso.math.fau.de | Fracture Control by Material Optimisation |
| **Velasco Sabogal**, Ali Mauricio | Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraße 3, 91058 Erlangen | +49 9131 85-70 506, mauricio.as.velasco@fau.de, mss.cbi.fau.de | Fragmentation in Large Scale DEM Simulations |
| [1]**Weber**, Felix | Applied Mechanics, Dep. of Mechanical Engineering, Paul-Gordan-Str. 3, 91052 Erlangen | +49 9131 85-64 410 / -413, felix.w.weber@fau.de, www.ltm.tf.fau.eu | Multiscale Fracture of Thermoplastic Polymers |

*Table 4: Associated doctoral researchers*

| Associated Doctoral Researchers | Chair, Department, Work Address | Contact Data (Tel / Fax, Email, Web) | Research Area |
|---|---|---|---|
| **Atila**, Achraf | General Material Properties, Dep. of Mat. Science and Engineering, Martensstraße 5, 91058 Erlangen | +49 9131 85-27 468 / -504, achraf.atila@fau.de, gmp.ww.uni-erlangen.de | Crack nucleation and propagation in anisotropic oxide glasses |
| **Esfandiary**, Samaneh | Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth | +49 911 65078-65 063 / - 066, samaneh.esfandiary@fau.de, matsim.techfak.uni-erlangen.de | Robustness and failure of brain activity patterns |
| **Hiemer**, Stefan | Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth | +49 911 65078-65 062 / -066, stefan.hiemer@fau.de, matsim.techfak.uni-erlangen.de | Machine Learning of Failure of Disordered Materials |
| **Hosseini**, Seyyed Ahmad, Dr.-Ing. | Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth | +49 911 65078-65 065 / - 066, ahmad.hosseini@fau.de, matsim.techfak.uni-erlangen.de | Modelling Fracture of Hierarchically Structured Materials |
| **Marzulli**, Valentina | Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraße 3, 91058 Erlangen | +49 9131 85-70 498 / -518, valentina.marzulli@fau.de, mss.cbi.fau.de | Mechanical characterization of granular materials |
| **Ries,** Maximilian | Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen | +49 9131 85-67 619/ -503, maximilian.ries@fau.de, www.ltm.tf.fau.eu | Multiscale Simulation of Amorphous Polymers |
| **Santarossa**, Angel | Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraße 3, 91058 Erlangen | +49 9131 85-70 482, angel.santarossa@fau.de, mss.cbi.fau.de | Crack Front Segmentation in I+III Mixed Mode Loading |
| **Schmidt**, Ina, Dr.-Ing. | Faculty of Mechanical Engineering Kesslerplatz 12 90489 Nürnberg | ina.schmidt@th-nuernberg.de | Computational Bone Remodelling |
| **Smith**, Ruaridh | Tectonics, Dep. of Geography and Geosciences, Schlossgarten 5 91054 Erlangen | +49 9131 85 25915 ruaridh.smith@fau.de, www.gzn.nat.fau.eu | Modelling Geothermal Systems through Fractured Media |
| **Spannraft**, Lucie | Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen | +49 9131 85-67 620 / - 503, lucie.spannraft@fau.de, www.ltm.tf.fau.eu | Mechanics of Generalised Interfaces and Grain Boundaries |
| **Titlbach**, Anna | Faculty of Mechanical Engineering Kesslerplatz 12 90489 Nürnberg | +49 157 59611854 anna.titlbach@th-nuernberg.de | Computational Bone Remodelling |
| **Wullschläger**, Florian | Computational Chemistry, Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen | +49 9131 85-20 424 / -404, flo.wullschlaeger@fau.de, chemistry.nat.fau.eu/ccc/groups | Atomistic Simulations of 2D Materials |
| **Zhao**, Wuyang | Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen | +49 9131 85-28 511/ -503, wuyang.zhao@fau.de www.ltm.tf.fau.eu | Small-Scale Informed Constitutive Modelling |

*Table 5: Student assistants*

| Name | Supported researchers | Course / field of study | Funded member of FRASCAL (from / to) | Tasks relating to FRASCAL |
|---|---|---|---|---|
| **Adams**, Annina | Christof Bauer P6 | Mechanical Engineering | 25 Apr 21 / 31 Oct 22 | Calculation of displacement field and FE stress measure based on MD simulations: parameter studies |
| **Dasari**, Sai Aakash | Paras Kumar P8 | Mechanical Engineering | 15 Mar 22 / 30 Jun 22 | Support in development of python scripts for automating parameter studies, mesh format conversion and other post-processing tasks |
| **Müller**, Valentin | Julian Konrad P3 | Molecular Science | March 20 / Aug 20; Mar 21 / Feb 22 | Support in structural analyses and data processing; elaboration of molecular scale mechanisms and illustration of mechanistic concepts; execution, documentation and evaluation of numerical studies |
| **Müller-Hillebrand**, Johannes | Julian Konrad P3 | Chemistry | Jan 21 / 15 May 21; Jul 21 / 11 Feb 22 | Support in structural analyses and data processing; elaboration of molecular scale mechanisms and illustration of mechanistic concepts; execution, documentation and evaluation of numerical studies |
| **Prateek**, Prateek | Paras Kumar P8 | Computational Engineering | 15 Aug 22 / 15 Feb 23 | Support in conducting enhanced computational homogenisation-based simulations involving large sized systems in 3D |
| **Rohracker**, Maurice | Paras Kumar P8 | Computational Engineering | Sep 19 / Nov 20; Mar 21 / Apr 22 | Support in the development of RVEGen: a python-based tool for automating the generation of representative volume elements (RVEs) for particulate composites;<br>Support in the development of an in-house finite element code employed for performing the simulations |
| **Seute**, Alexander | Bakul Mathur P13 | Geosciences | Jun 22 / Sep 22; 15 Oct / 14 Dec 22 | Preparation of samples and thin section preparation, analysing samples and support in running simulations |
| **Siah**, Kok Siong | Paras Kumar P8 | Mechanical Engineering | Apr 22 / Jul 22 | Literature review, support in formulation of tangent for nonlinear viscoelastic materials based on Ogden strain energy functional |
| **Topraksal**, Ece | Christian Wick P12 | Advanced Materials and Processes | Apr 21 / Mar 22 | Literature review, COGEF calculations, analysis |
| **Torres Huamani**, David | Wuyang Zhao P6 | Mechanical Engineering | 15 Jun 22 / 15 Sep 22 | Capriccio code development: Matlab to deal.ii |

*Table 6: Mercator Fellows*

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

*Table 7: External Advisory Board*

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

## 1.3 Coordination and administration

*Table 8: Coordination and administration of GRK 2423 FRASCAL*

| | Work Address | Contact Data (Tel / Fax, Email, Web) | Work Area |
|---|---|---|---|
| **Dakkouri-Baldauf**, Andrea, Dr. rer. nat. | Competence Unit for Scientific Computing, CSC, Martensstraße 5a, 91058 Erlangen | +49 9131 85-20782 / -20785, andrea.dakkouri@fau.de, www.frascal.fau.eu | FRASCAL Coordination |
| **Güthlein**, Nicole | Competence Unit for Scientific Computing, CSC, Martensstraße 5a, 91058 Erlangen | +49 9131 85 20780 / -20785, guethlein@math.fau.de, csc.fau.eu | CSC Administration |
| **Herzner**, Ann-Sophie | Competence Unit for Scientific Computing, CSC, Martensstraße 5a, 91058 Erlangen | ann-sophie.herzner@fau.de, www.csc.fau.eu | CSC Administration, student assistant |
| **Pflug**, Lukas, Dr. rer. nat. | Department of Mathematics Chair of Applied Mathematics, Cauerstraße 11, 91058 Erlangen | +49 9131 85 67139 / -67134, lukas.pflug@fau.de, www.csc.fau.eu | CSC Managing Director |

## 1.4 Reporting period

01 January 2022 to 31 December 2022

*Figure 1: Group photo at the 2nd FRASCAL-Retreat in Bad Windsheim on 5 May 2022. (Image: Julia Deserno)*

# 2 Research Programme

## 2.1 Research projects


*Figure 2: Doctoral, associated doctoral and postdoctoral researchers and their projects of the 2nd cohort of FRASCAL.*

Since the second cohort, FRASCAL comprises 12 doctoral projects (P1, P3-P11, P13 and P14), and one overarching postdoctoral project (P12). These range from quantum mechanics (P1) to atomistic and particle-based methods (P1-P4) and continuum mechanics (P8-P11, P13). Several projects (P5-P7, P12, P14) are dedicated to bridging atomistic and particle-based approaches to continuum-based techniques. The postdoctoral project P12 integrates the results and expertise developed in the doctoral projects to realise a concurrent multiscale modelling approach for fracture, ranging from quantum to continuum treatment. The effect of heterogeneities on fracture behaviour 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).

Due to the departure of Prof. Dr. Erik Bitzek in September 2021, P2 was replaced by project P13 as of 1 January 2022. P13 deals with fractures in rocks from the single grain to the geological scale and thus extends FRASCAL's scope to very large length and time scales. In addition, since 1 March 2022, there is another new doctoral project P14 that spans from the atomic to the continuum level and is based on rigorous mathematical approaches, particularly on variational methods.

Table 9 subsumes FRASCAL's projects:

*Table 9: FRASCAL doctoral projects {P1-P14}\P12, postdoctoral project P12, and associated projects (aPA-aPM)*

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

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

## P1: Chemistry at the Crack Tip

Christian L. Ritterhoff and Bernd Meyer

In my PhD project I will build on the flexible boundary “pacman” scheme introduced by Tobias Müller for atomistic calculations of the fracture toughness of real materials. The methodology will be extended to more complex materials, in particular, oxides, perovskites, and minerals relevant in geological processes (see project P13). To be able to perform such demanding calculations, it is mandatory to speed up our atomistic approach for treating the “pacman” cutout.

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

Starting point is the FFTX library of the Quantum Espresso software package. First, I benchmarked different approaches described in the literature.[1,2] I found the 1D+1D+1D decomposition using the FFTW3-library[4] is the most efficient approach on modern multi-core HPC compute nodes.

The goal of the code optimization is to be as fast as possible regardless of the FFT grid size and the architecture of the compute nodes. This led to refactoring most loop structures, data distributions, and communication patterns to make optimal use of combined MPI and OpenMP parallelization.

As shown in Figure 3, the routine receives the data as individual sticks, which are randomly distributed among the processors. After the first 1D-FFT, the sticks are split and redistributed in a communication step. The cylindrical data is then distributed such that each processor is responsible for a complete plane. Subsequently, the two remaining FFTs can be performed without further communication. The data exits the routine in this plane-wise distribution, which is required this way by the rest of the program.

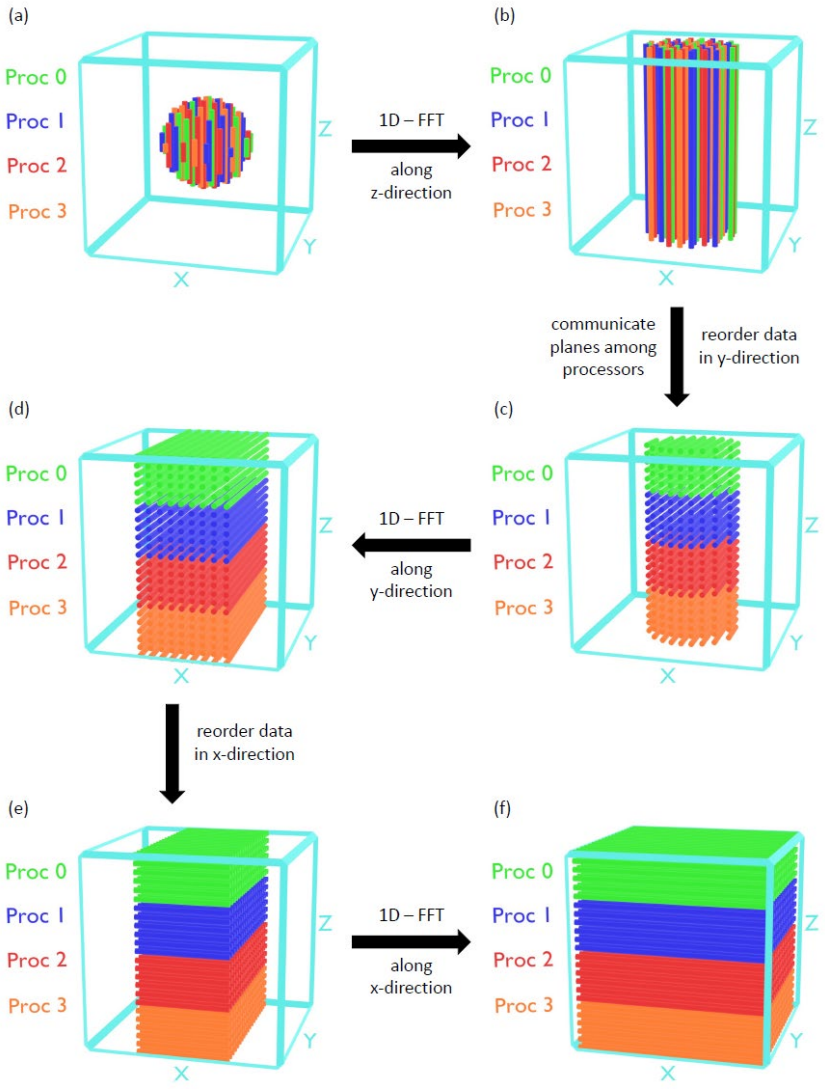



*Figure 3: Graphical representation of the data distribution of the FFT routine.*

Furthermore, each time a task loads a value from main memory into its own internal memory, it automatically loads, in the case of our FFT, 4 values at once. As such, programs running on HPC architectures greatly benefit from write/read-consecutive loop structures, since the processor has to access the memory only every 4th time. I changed from group communication to point-to-point communication to reduce waiting time between tasks with uneven workload. Some parts of the data are already in the correct tasks’ memory in the first place. Thus, point-to-point communication also helps by reducing the communication load to the bare minimum.

Depending on the HPC cluster, the size of the memory bus, which is used for communication, can vary. However, for communication to be as efficient as possible, the communicated size of data must ideally fit perfectly within this memory bus. Thus, to further improve the scalability of the routine, I am combining multiple states into batches. The optimal size for these batches is calculated at the beginning and held constant for the rest of the program execution.

While the communication is an important step in the present scheme, it is a bottleneck since its speed is entirely dependent on the memory bus. Increasing the computational resources does in no way influence the time. Thus, in a last optimization step, I try to further increase the scalability of the routine by overlapping the communication and calculation parts. This is done by separating one processor on each node, which is then only responsible for the communication, while all other processors do the calculations.

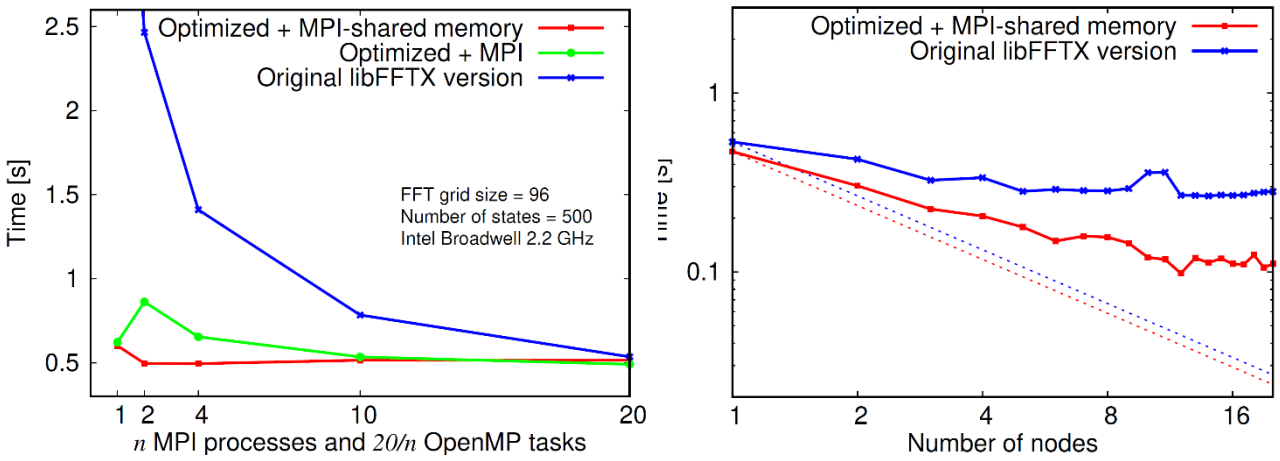



*Figure 4: Performance optimization within the FFTXlib code. Left: Timings of a test set with varying ratio of MPI/OMP processes/tasks. The desired outcome is a straight line parallel to the x-axis. Right: Comparison of old and new code when used on the same test set with multiple nodes. The dotted lines represent ideal scaling.*

As seen in Figure 4, the employed optimizations show promising results. Especially when looking at the single-node timings, one can see the success of the strategy in combining OMP and MPI. Note that the slight peak when using a single MPI task on a node is expected, since the used HPC cluster has 2 NUMA domains per node, making MPI task count of at least 2 per node preferable.

Also, when looking at the multi-node scaling on the right, one can see improvements to the previous version. The old routine stops scaling at around 5 nodes for the chosen test calculation, while the new version continues to scale to a much larger number of nodes.

Instead of continuing to work on this version of the routine inside a test program, it was decided at this point to port the new routines into the CPMD[3] code that was used by Tobias Müller for his “pacman” calculations. Since the data structures of the two quantum chemistry codes, Quantum Espresso and CPMD, are quite different, this took some time and the code needed to be changed quite substantially.

## References

[1] S. Goedecker: Fast Radix 2,3,4, and 5 Kernels for Fast Fourier Transforms on Computers with Overlapping Multiple-Add Instructions (1997) SIAM J. Sci. Comput. 6 1605-1611

[2] A. Canning, L.W. Wang, A. Williamson, and A. Zunger: Parallel Empirical Pseudopotential Electronic Structure Calculations for Million Atom Systems (2000) J. Comput. Phys. 160 29-41

[3] T. Klöffel, G. Mathias, and B. Meyer: Integrating state of the art compute, communication, and autotuning strategies to multiply the performance of ab initio molecular dynamics on massively parallel multi-core supercomputers (2021) Comput. Phys. Commun. 260 107745

[4] M. Frigo and S. G. Johnson: The Design and Implementation of FFTW3 (2005) Proceedings of the IEEE 93 2 216-231

## P2: Ab Initio & Atomistic Modelling of Cracks and Comparisons to Continuum Theories

Tarakeshwar Lakshmipathy and Erik Bitzek

### Objectives and status

Various studies were planned in the context of scale-bridging using atomistic simulations. In the first study, the limitations of using linear elastic fracture mechanics (LEFM) to determine fracture toughness of atomically sharp cracks using critical atomic separation distances were explored. Next, the establishment of a scaling model of fracture toughness as a function of crack tip radius for reinitiation of a sharp crack from a pre-existing blunted crack was planned. A third study involved the benchmarking of various interatomic interactions against DFT for studying blunted cracks in Tungsten. In the fourth study, ramped viscous damping boundary conditions were calibrated to prevent unrealistic reflections of sound waves in atomistic propagating crack simulations.

In the first study, atomistic simulations with nearest neighbour harmonic potentials with varying cut-offs (analogous to networks of springs) were performed. Such potentials have linear elastic responses up to cleavage of bonds and do not show any surface-related phenomena. This makes them suitable for comparisons with LEFM. Cracks were inserted and loaded in the simulations using displacement fields based on LEFM [1]. Although material nonlinearities do not exist with such potentials prior to breaking of bonds, it was found that geometrical nonlinearities are present in the simulations. The geometrical nonlinearities manifest in the form of deviating displacements during relaxation of the cracks at various loads. This leads to deviations from the LEFM prescribed displacement field which in-turn results in deviations of up to 80% in fracture toughness values when compared to analytically determined values from LEFM equations.

The harmonic potentials were also used in the second study to establish the scaling model for fracture reinitiation toughness values as a function of crack tip radius. An earlier work [2] had shown that the Creager-Paris equations based on linear elasticity [3] could predict the fracture reinitiation toughness in cases of macroscopic notches. However, in this work, a factor that accounts for stress amplification at surface steps as well as the aforementioned geometrical nonlinearities is introduced. Furthermore, a lower limit for the maximum crack tip radius for this model was found (~95 nm), above which the original model [3] can be used.

In the third study using Tungsten, the fracture behaviour of blunted cracks in two crack systems was studied using DFT, Embedded Atom Method (EAM) potentials [4,5], and a modified-EAM (MEAM) potential [6]. The empirical potentials (EAM and MEAM) failed to consistently match the results of DFT qualitatively. It was hypothesized that this was due to the empirical potentials not using sufficient data from DFT in their creation, as well as failing to describe surface-related phenomena at blunted crack tips in Tungsten.

The harmonic potentials were again used in the fourth study to calibrate ramped viscous damping boundary conditions in dynamic fracture simulations. The samples consisted of ~3 million atoms, with the size of the damping region being varied between 0% to 30% of the sample. An earlier study [7] had suggested that a damping coefficient value ($\bar{\zeta}$) of twice the Einstein frequency ($\omega_{\mathrm{E}}$) of the material would be optimal for small damping regions and sample sizes. It was found in this study that the optimal value could be an order of magnitude smaller with larger samples and damping regions (see Figure 5). This would allow the sound waves to propagate much further into the damping region, thereby making use of the damping region more effectively. Using low values for the damping coefficient also resulted in no change to the crack speed. Using much higher values (~20 times the Einstein Frequency) on the other hand led to reflection of sound waves from the damping region itself and slower crack speeds.

### Conclusions, main achievements and outlook

The key finding of the first study was that fracture toughness with an incremental loading procedure cannot be re-conciliated with LEFM using only the separation distance of the crack tip atom pair. Even with purely local and linear interactions, fracture is a collective process in atomistics and simulations have to be performed to determine fracture toughness. In the second study, it was found that scaling relations for sharp crack reinitiation from blunted cracks in the atomistic scale must account for phenomena arising from the discrete nature of atoms. The key finding of the third study with Tungsten was that empirical potentials need to consider restructuring of atoms at surfaces in

addition to fracture-relevant bulk properties to accurately simulate the fracture behaviour of blunted cracks. It is currently planned to expand this study with more sophisticated potentials such as Bond-Order Potential (BOP) [8] and an Atomic Cluster Expansion potential [9]. The key finding of the final study was that optimally calibrated boundary conditions maximize the extent to which sound waves propagate into the damping region without reaching the edge of the simulation box, while simultaneously having negligible influence on crack speed and energy release rate.

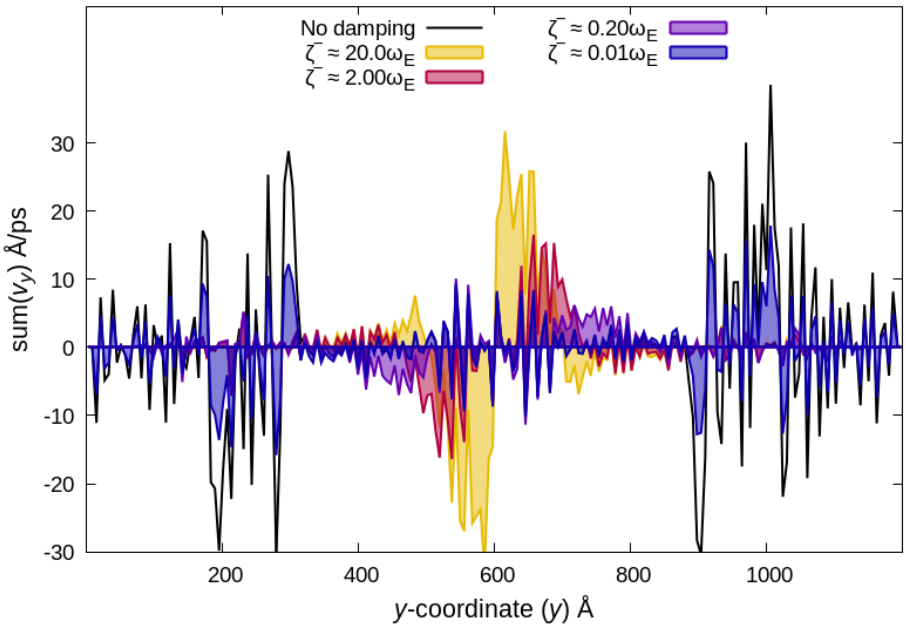



*Figure 5: Sound waves that were initially emitted from the propagating crack tip and are reflected after having travelled towards the simulation box edges. In the case of "No damping" and $\bar{\zeta}$=0.01 $\omega_E$, the waves have been reflected from the box edge. In the other cases, the waves have been reflected from the damping region itself. The sound waves shown in this plot were from simulations with one of the harmonic potentials using a damping region that covered roughly 30% of the sample.*

**References**

[1] G. C. Sih, H. Liebowitz: Mathematical theories of brittle fracture. In: Fracture: An Advanced Treatise (1968), Aca-demic Press, New York 67–190

[2] F. J. Gómez, G. V. Guinea, M. Elices: Failure criteria for linear elastic materials with u-notches (2006) Internation-al Journal of Fracture 141(1) 99–113

[3] M. Creager, P. C. Paris: Elastic field equations for blunt cracks with reference to stress corrosion cracking (1967) International Journal of Fracture Mechanics 3 247–252

[4] G. J. Ackland, R. Thetford: An improved N-body semi-empirical model for body-centred cubic transition metals (1987) Philosophical Magazine A 56(1) 15-30

[5] J. Wang, Y. L. Zhou, M. Li, Q. Hou: A modified W-W interatomic potential based on ab initio calculations (2013) Modelling and Simulation in Materials Science and Engineering 22(1) 015004

[6] P. Hiremath, S. Melin, E. Bitzek, P. A. T. Olsson: Effects of interatomic potential on fracture behaviour in single- and bicrystalline tungsten (2022) Computational Materials Science 207 111283

[7] P. Gumbsch, S. J. Zhou, B. L. Holian: Molecular dynamics investigation of dynamic crack stability (1997) Physi-cal Review B 55 3445

[8] T. Hammerschmidt et al.: BOPfox program for tight-binding and analytic bond-order potential calculations (2019) Computer Physics Communications 235 221–233

[9] R. Drautz: Atomic cluster expansion for accurate and transferable interatomic potentials (2019) Physical Review B 100 249901

## P3: Multi-scale Modelling of Epoxy Resin and Composites

Julian Konrad and Dirk Zahn

In recent decades tail-made materials, comprising polymer and polymer-composites, gained importance due to more extensive requirements along mechanical properties. Technical applications require resistance to friction, impact and elongation as well as a defined degree of elasticity. The corresponding material properties are achieved by a suitable choice of components, which should be easy to process and inexpensive. For example, epoxy resins reinforced with cellulose and aramid fibres and toughened with silica particles are already used in clutch discs. Experimental materials research provides a wide range of materials today, but cutting-edge developments increasingly driven my in-depth understanding of computer-aided modelling and simulation.

To this end, polymer modelling across time and length scales can bridge the gap from molecular considerations to the design of macroscopic components and requires an understanding of a broad spectrum of physical and chemical phenomena. Quantum mechanical (QM) calculations provide the basis for the formation of atomistic polymer networks on the nano-scale with respect to thermodynamics. Monitoring dynamic processes along fracture by means of molecular dynamics (MM) enables the development of coarse-grained models (CG).

We investigated the epoxy system of bisphenol F diglycidyl ether (BFDGE) and 4,6-diethyl-2-methylbenzene-1,3-diamine (DETDA) regarding the crosslinking reaction, as well as bond dissociation, by development of a dissociative Force Field, which facilitates our curing algorithm to reach the experimental crosslinking degree of 99% [1,2]. The resulting, reliable models fulfil bulk, as well as elastic properties, we derived from linear response theory [3]. Furthermore, we studied tensile deformation about inter-molecular reorganization processes along fracture processes and extrapolated occurring stresses to vanishing strain rates, which yielded in accordance with macroscopic specimens [2,3]. We also accomplished the transfer from molecular simulation to constitutive modelling by means of a multi-scale modelling capturing deformation and damage in epoxy resins [4]. Addressing the interplay of composite materials, we studied molecular structuring of epoxy at silica and cellulose interfaces [5] as well as corresponding forces along detaching processes [6].

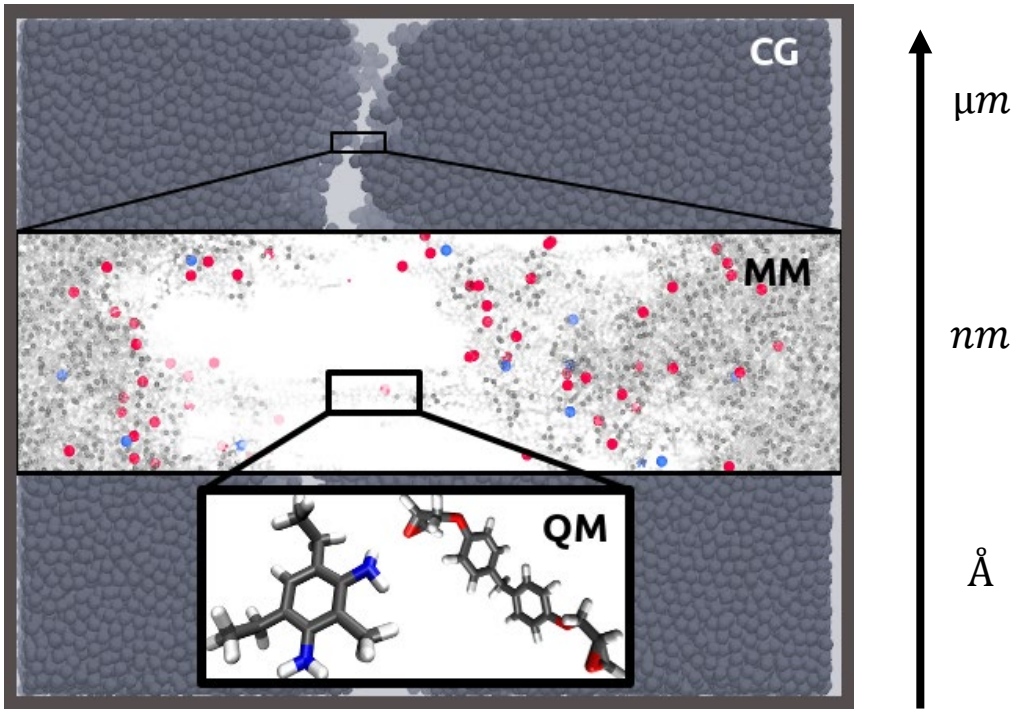



*Figure 6: Investigations covering QM effects as well as valid models on the nm scale (MM) pave the way for investigations on the µm scale (CG).*

In conclusion, there now is a large body of atomic-level insights available to provide the needed inputs for a coarse-grained setup. This setup will hence not rely on ad hoc assumptions, but directly feature the beforehand identified properties from QM and MM methods. In turn, the expected CG model will drastically widen the accessible time- and length scales and enable investigations epoxy-silica and epoxy-cellulose composite materials at mesoscale resolution.

**References**

[1] Molecular simulation of thermosetting polymer hardening: Reactive events enabled by controlled topology transfer. Macromolecules, 2020, 53(22), pp. 9698–9705

[2] A Molecular Simulation Approach to Bond Reorganization in Epoxy Resins: From Curing to Deformation and Fracture. ACS Polym. Au 2021, 1, 3, 165–174

[3] Assessing the mechanical properties of molecular materials from atomic simulation. AIMS Materials Science, 2021, 8(6), pp. 867–880

[4] Multi-Scale Modelling of Plastic Deformation, Damage and Relaxation in Epoxy Resins. Polymers, 2022, 14(16), 3240

[5] Molecular Simulations and Network Analyses of Surface/Interface Effects in Epoxy Resins: How Bonding Adapts to Boundary Conditions. Polymers, 2022, 14(19), 4069

[6] Interaction Forces in reinforced Epoxy Resins: from molecular Scale Understanding towards meso-scale Interfaces. FRASCAL Special Issue in Forces in Mechanics, submitted September 2022

## P4: Fragmentation in Large Scale DEM Simulations

Ahmet Utku Canbolat and Thorsten Pöschel

The project aims to develop large-scale discrete element method (DEM) simulations for the fracture of granular materials. Particle shape is a crucial factor that affects the behaviour of granular systems. Thus, in the first step of the project a novel method was introduced to create multispheres. The multisphere approach is one way to model irregularly shaped grains. In this approach, many small spheres clumped together to represent a grain and therefore the method benefits from the contact models used in the DEM for spheres. In addition to the method developed in the first stage of the project, two new methods were recently added to the toolbox for multisphere creation. One of the new methods is based on Ferellec and McDowell model [1], and the other is based on the novel method called Euclidean Distance Transform proposed recently by V. Angelidakis et al. [2]. With the addition of these methods, we have even faster multisphere generation with higher accuracy for arbitrarily shaped grains.

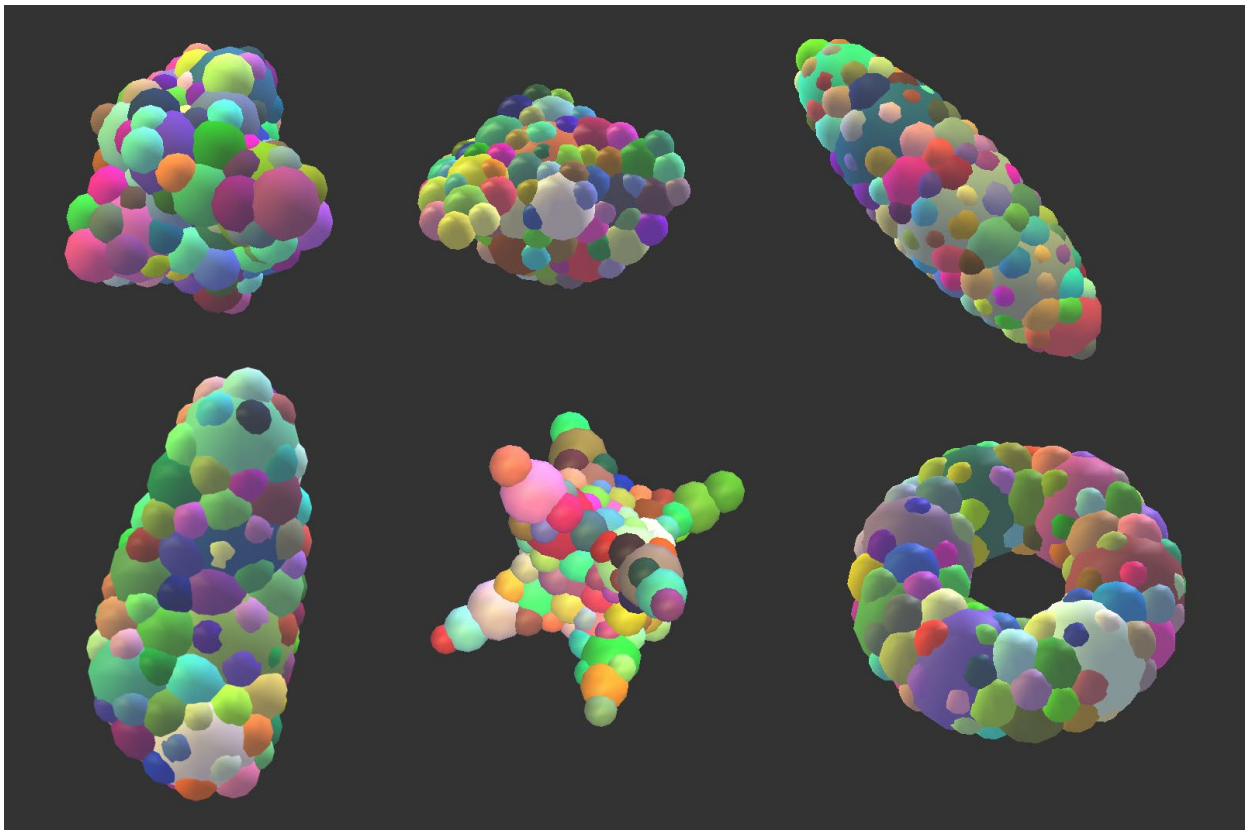


*Figure 7: We can create clumps of spheres for arbitrarily shaped grains from any given stl file.*

The next step of the project focused on the implementation of fracture of grains. To model the fracture, the stress tensor is calculated by considering each particle in contact. The direction of the maximum shear stress defines a plane that splits the grain into two fragments [3]. If the maximum shear stress is larger than a threshold, then we perform the multisphere creation for these smaller grain fragments. Finally, we represent the fragments as clumps again. Multisphere creation and fracture implementation conclude the first part of the project.

The aim of the current part is to implement plastic deformation, heat transfer, and wear based on the previous findings. In a granular system, collisions between particles cause plastic deformation and heat the particles. Because thermal stress can affect fracturing, it is essential to consider the heat transfer between particles due to collision. In the final step, we will implement the wear effect. Wear is the loss of material surface as a consequence of the relative motion of the particles [4]. We will treat wear as a small-scale fracture on grains to model wear.

**References**

[1] Ferellec, J.-F., & McDowell, G. R. (2010). A method to model realistic particle shape and inertia in DEM. In Granular Matter (Vol. 12, Issue 5, pp. 459–467). Springer Science and Business Media LLC. https://doi.org/10.1007/s10035-010-0205-8

[2] Angelidakis, V., Nadimi, S., Otsubo, M., & Utili, S. (2021). CLUMP: A Code Library to generate Universal Multi-sphere Particles. In SoftwareX (Vol. 15, p. 100735). Elsevier BV. https://doi.org/10.1016/j.softx.2021.100735

[3] Iliev, P. S., Wittel, F. K., & Herrmann, H. J. (2019). Evolution of fragment size distributions from the crushing of granular materials. In Physical Review E (Vol. 99, Issue 1). American Physical Society (APS). https://doi.org/10.1103/physreve.99.012904

[4] Williams, J. A. (2005). Wear and wear particles—some fundamentals. Tribology International, 38(10), 863–870. https://doi.org/10.1016/j.triboint.2005.03.007

## aPC: Experimental Study of Mixed Mode I+III Hydraulic Fracturing in Hydrogels Using X-Ray Tomography

Angel Santarossa, Thorsten Pöschel, Achim Sack, Laureano Ortellado, Leopoldo Gómez

Hydraulic fracturing is a process by which a crack is initiated and propagates due to pressure (hydraulic loading) applied by a fluid introduced inside a solid medium. Because of the extremely high pressures and stresses involved in hydraulic fracturing of rock, suitable analogues are used to conduct experiments [1]. Therefore, the usual approach to experimentally study fluid-driven fractures involves using transparent and linear elastic or brittle hydrogels [1,2,3]. These gels allow fluid-driven fracturing at low pressures and low injection rates. Several fracturing phenomena were studied utilizing hydrogels, such as the coalescence of coplanar penny-shaped fractures [2], crack propagation in viscous and tough-dominated cracks [4], or the dynamics of foam-driven fractures [3,6]. However, transparency to visible light is required for the solid material to assure proper visualization of crack formation and propagation, which reduces the range of materials that can be analysed. Furthermore, the usual methods for studying the geometrical properties of the fracture rely on CCD cameras or surface laser scanning [4,5], which only allows for studying cracks in 2D, while fractures are intrinsically 3D.

Natural fractures usually possess complicated geometries. Controlling the fracture geometry is of high interest. On the one hand, most theoretical models rely on well-defined and simple fracture geometries to study the mechanisms behind hydraulic fracturing [5]. On the other hand, to maximize the efficiency of the processes in applications, such as petrol extraction [3,6]. Nonetheless, this is not a simple task. The geometry of a fracture depends highly on the stress distribution, the material properties of the solid sample, and the fluid being injected [5]. Stress heterogeneity and material heterogeneities are the main factors for fracture branching and segmentation, i.e., out-of-plane (crack front) fracture propagation from an initial planar fracture. Most research focuses on planar fractures due to the possibility of studying them from a bi-dimensional perspective [1,2,4,5]. However, natural fractures are usually segmented. Hence, a technique to study mix-mode fractures in 3D is needed, as well as a method for carefully controlling fracture geometry and propagation.

The main objective of this project is to study the leading mechanism controlling the fracture's geometry in a hydraulic fracturing process. In particular, we aim to experimentally mix-mode I+III fluid-driven fractures in hydrogels in 3D. To that aim, we developed a novel experimental setup to produce mix-mode I+III fractures when fluid is injected into a gel at a predefined fluid rate. Mode I and mode III fractures are achieved by selectively applying tensile and shear stress on the hydrogel. The device is designed to be used in an X-ray tomograph, thus allowing for non-invasively studying the geometry of the produced fractures in detail in 3D, even in samples that are opaque to visible light.

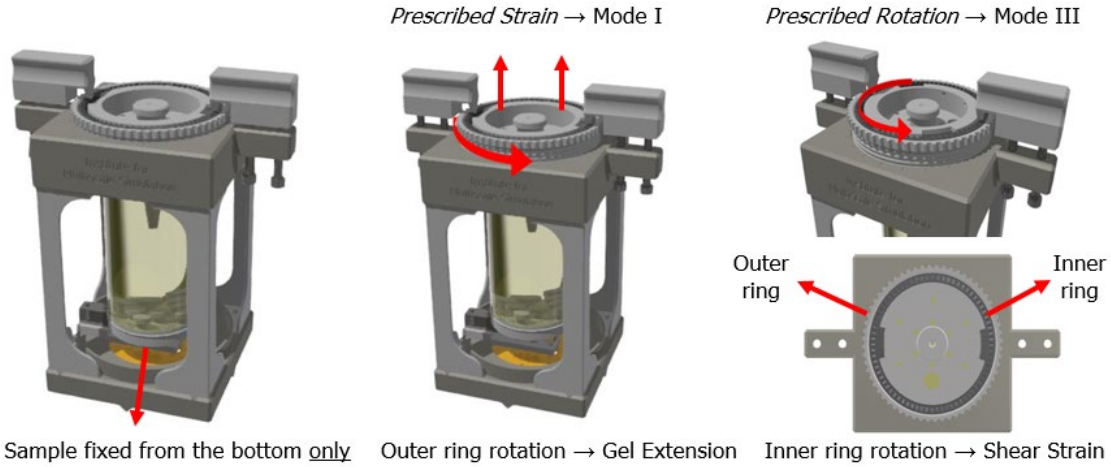



*Figure 8: Sketch of the experimental setup and modes of operations. The experimental setup with hydrogel (right), can be elongated by rotating an outer ring (centre) or sheared by rotating an inner ring a prescribed angle (top left). The figure on the bottom left shows a top view of the device.*

Figure 8 shows a scheme of the experimental setup. The gel is fixed on the bottom of the device. At the bottom, the apparat contains force and torque sensors to measure tension and torque applied to

the gel. On the upper side, the system possesses two rings. The outer one can be screwed or unscrewed to compress or expand the gel. The inner ring can be rotated to apply torque to the hydrogel.

A fracture measurement is performed as follows. First, the gel is elongated by rotating the outer ring, inducing tensile stress on the sample. Afterward, a fluid is injected at a predefined speed, thus producing a planar fracture (mode I). Then, an initial torque value is applied to the solid sample through the inner ring (inducing a mode III fracture), followed by the injection of the fracturing fluid (producing a mixed mode I+III fracture). After this step, a segmentation of the fracture front is observed. Once the measurement is finished, we record an X-ray tomography of the sample. Finally, the 3D volume reconstruction of the fracture is analyzed. The experiment is performed within a thermal bath. The thermal control system was developed in this project. It allows for a stable temperature during a fracturing experiment and the curation of the gel. The fluid is introduced at a controlled rate through an in-house injection system.

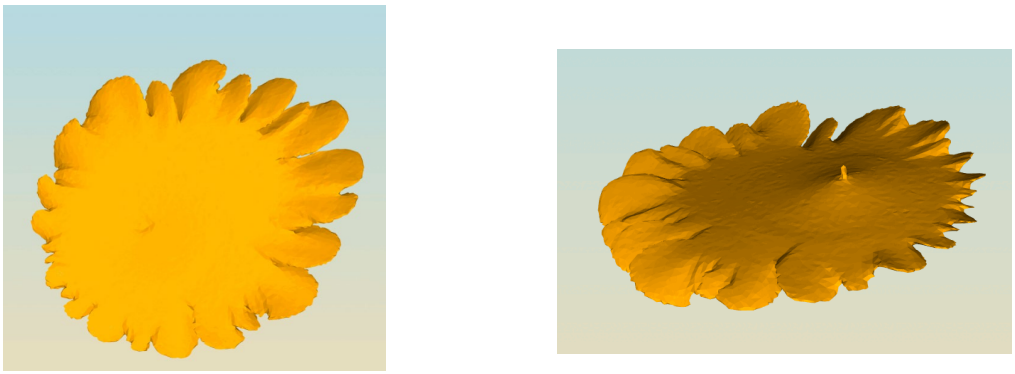


*Figure 9: 3D volume reconstruction of a mixed-mode type I+III hydraulic fracture. The fracturing fluid is air. Top view (left) and side view (right). In the left figure, an initial planar fracture of small diameter can be observed (mode I), followed by a segmentation of the crack front (mode III).*

In summary, we developed a novel experimental device to produce fluid-driven fractures of mixed-mode type I+III (see Figure 9 for an example). Moreover, the system is designed to be used in X-ray tomography, allowing one to study, non-invasively, the produced fracture geometry in 3D.

**References**

[1] N. O'Keeffe, P. Linden: *Hydrogel as a Medium for Fluid-Driven Fracture Study* (2017) Experimental Mechanics **57**, 1483–1493

[2] N. O'Keeffe, Z. Zheng, H. Huppert, P. Linden: *Symmetric coalescence of two hydraulic fractures* (2018) PNAS **115** (41) 10228-10232

[3] C. Lai, B. Rallabandi, A. Perazzo, Z. Zheng, S. Smiddy, H. Stone: *Foam-driven fracture* (2018) PNAS **115** (32) 8082-8086

[4] W. Steinhardt: *The Rules of Roughness: An Experimental Investigation into the Origins of Brittle Fracture Complexity* (2020) Ph.D. Thesis, Harvard

[5] R. Wu: *Some Fundamental Mechanisms of Hydraulic Fracturing* (2006) Ph.D. Thesis, Georgia Institute of Technology

[6] C. Lai: *Fluid-structure interactions for energy and the environment* (2018) Ph.D. Thesis, Princeton University

## P5: Failure in Porous Material

Shucheta Shegufta and Michael Zaiser

The aim of this research project is to study compressive failure in porous materials. To this end, Peridynamics has been chosen as the appropriate method because it can easily handle discontinuities. In the previous years, compressive failure in porous snow structures has been simulated using Peridynamics. However, one of the inherent properties of Peridynamics as a non-local model is a weakening of the material near the surfaces [1]. Since in a porous microstructure, a large amount of surface is present, this weakening is a shortcoming of the method for our purposes.

In order to address this issue, an energetically consistent surface development method has been developed for elastic bond-based materials in Peridynamics [2]. In an elastic bond-based material model, a material point interacts with every other material point within its neighbourhood, specified by a distance called the horizon. The interaction between two material points is called a bond and is independent of all other points within the neighbourhood. Strain energy of a bond depends on the "bond stiffness", which is the constitutive material parameter of elastic bond-based material. Strain energy density of a point is found by integrating over the energy of every single bond within its neighbourhood. This peridynamic strain energy is then compared with strain energy computed by classical continuum mechanics and thus the bond stiffness is found for elastic bond-based material. The assumption here is that every point is in the bulk and therefore has a "complete" neighbourhood. However, this is not the case for material points that are less than a horizon distance away from the surfaces, and therefore at these points the surface is weakened in elastic bond-based material.

The surface correction method reformulates the energy equivalence relation by taking the reduced neighbourhood in the evaluation of the integral into account. The newly reformulated energy equivalence is applied to a material point in the bulk, and a material point in incomplete neighbourhood. By comparing the integrals from these energy equivalent relations in bulk and energy density near surface, a surface correction factor is achieved.

The newly implemented correction scheme not only shows excellent results for benchmark problems (Figure 10), but also for more complex problems like indentation and fracture. The necessity of surface correction becomes evident from the brittle fracture simulation (Figure 11), where without surface correction damage propagates at the top and bottom surfaces and created unrealistic fracture. The surface corrected scheme is able to produce more physically meaningful results where damage initiates at the notch and fracture propagates along the centreline.

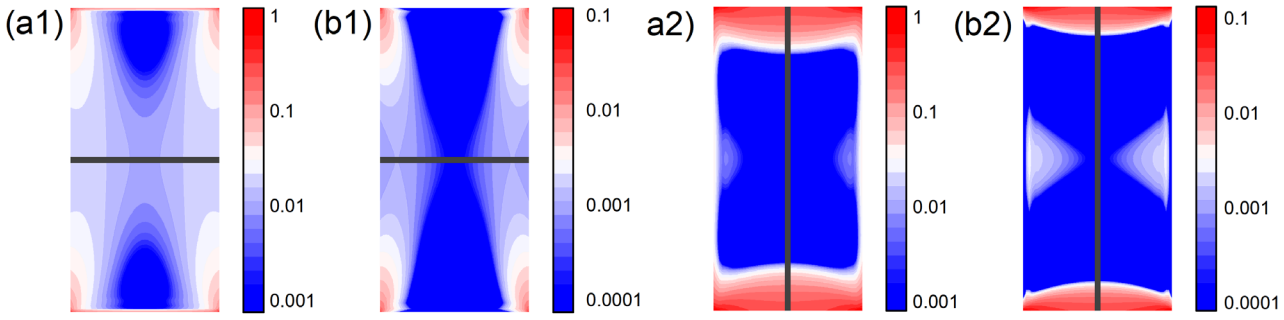



*Figure 10: Relative errors of displacement fields, uni-axial deformation of a free standing sheet of size 50mm × 100mm with constant boundary loads imposed in y (vertical) direction, errors are evaluated relative to the analytical solution; (a) without surface correction: a1) Δuy /uy , (a2) Δux /ux ; (b) with surface correction: (b1) Δuy /uy , (b2) Δux /ux; the black bars represent nodes where for symmetry reasons the analytical displacements are zero such that a relative error is mathematically undefined.*

Moreover, an investigation of the influence of disorder on failure of porous material is currently under way. For this, artificially generated two-dimensional random porous structures with various degrees of disorder have been created. Preliminary simulations have been conducted and an automated workflow is being established to deal with a large quantity of data. Figure 12 shows some of the microstructures created and their fracture patterns for a tensile test.

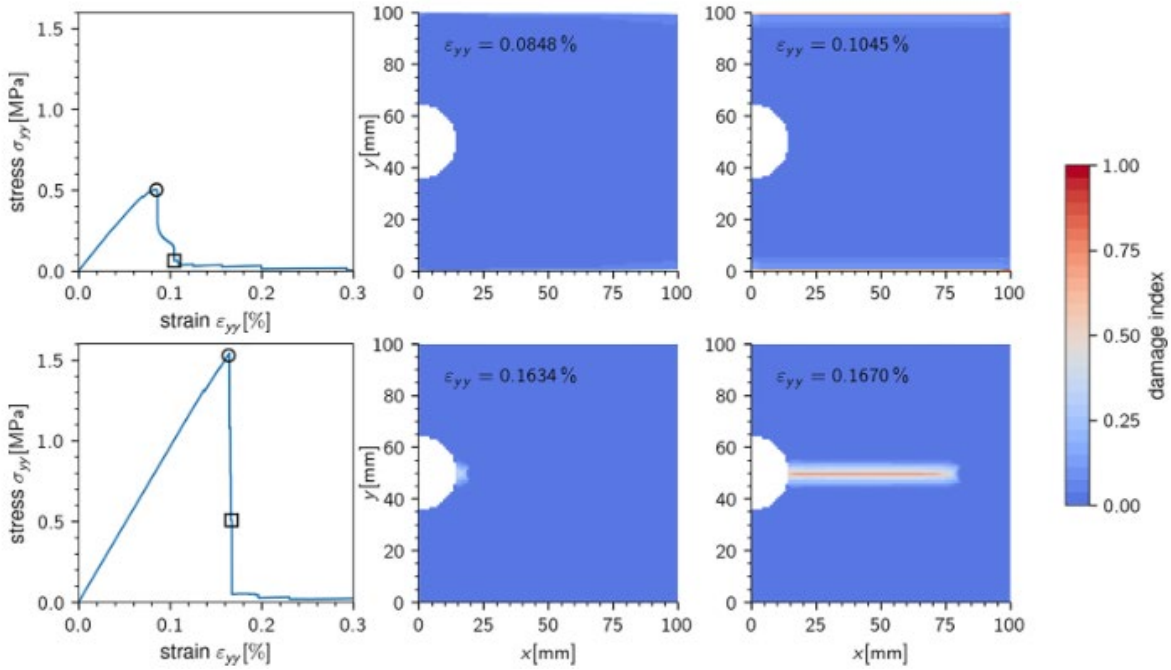



*Figure 11: Stress-strain curves and damage patterns in a simulated fracture test of a notched specimen with tensile displacements imposed in y direction on the top and bottom surfaces, left panels: stress-strain curves, centre panels: damage pattern on the descending branch of the stress-strain curve (square symbol in left panel); top: PD simulation without surface correction, bottom: PD simulation with surface correction.*

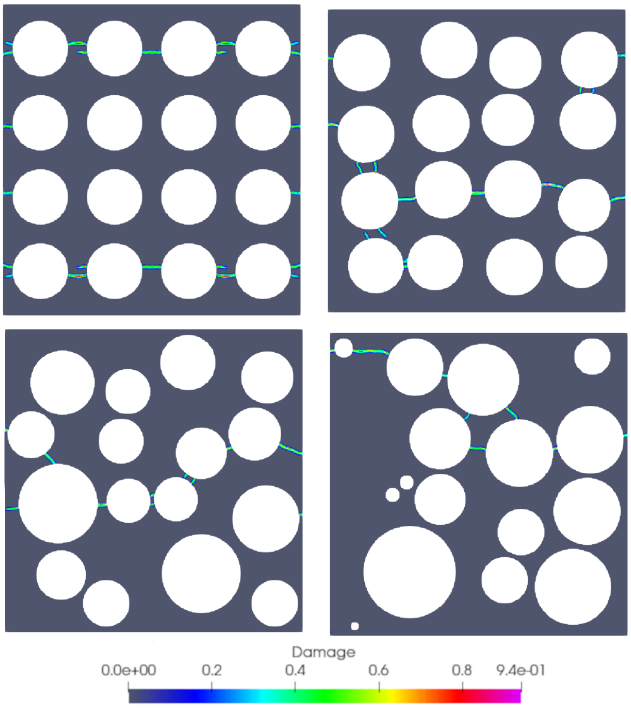



*Figure 12: Damage patterns in various microstructures subjected to tensile displacements imposed in vertical direction. All microstructures are of size 100mm x 100 mm with 45% porosity, 16 pores and disorder parameter of 0, 3, 6 and 12 (Clockwise from top left).*

## References

[1] Q.V. Le, F. Bobaru, Surface corrections for peridynamic models in elasticity and fracture. Comput Mech 61, 499–518, 2018. doi: https://doi.org/10.1007/s00466-017-1469-1

[2] J. Ritter, S. Shegufta, P. Steinmann, M. Zaiser, An energetically consistent surface correction method for bond-based peridynamics, FRASCAL Special Issue in Forces in Mechanics, vol. 9, 2022, 100132, ISSN 2666-3597, doi: https://doi.org/10.1016/j.finmec.2022.100132.

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

Stefan Hiemer and Michael Zaiser

### Objectives and status

This project's focus is to study subcritical failure in disordered systems with machine learning to identify governing variables and patterns preceding failure. The computational methods are molecular dynamics (MD) of glasses, a novel stochastic creep random fuse network model (RFM) and finite element method (FEM) based on creep data from a previous work of this chair [1]. The network model and the FEM data try to describe failure dynamics on the mesoscale and serve as a comparison for experiments. As creep simulations are impossible to realize with MD due to time constraints, we try to identify precursors of plasticity.

As the first goal, we aim to predict the time to failure of the RFM and FEM creep data with a machine learning (ML) method called random forests. This technique does not require a special functional form and allows to weigh the importance of individual features. We tried to identify the change of predictability with regard to physical parameters of the model (temperature, disorder, etc.) and input features for the ML model. In the case of the RFM, temperature, disorder, size and applied load were investigated with respect to a change in performance of the ML model. Predictions become more successful with increasing network size, temperature and order whereas increasing the load decreases the prediction performance. Sample-by-sample variation is reduced when increasing the network size, higher order leads to narrow lifetime distributions due to smaller structural fluctuations and higher loads decrease the number of events thus reducing information. Higher temperatures induce additional failure compared to quasistatic fracture (which is roughly speaking equivalent to zero-temperature limit fracture) at different sites of the network thus emitting more information and on the other hand decreases the structural fluctuations represented by the yield/failure strength of individual network edges. Features found to be most important for predictions in the case of FEM are the damage localized in a shear band and the total damage whereas for RFM we find the equivalent strain to be most important contrary to literature which suggest avalanche rate and strain rate features. These findings have been published in Forces in Mechanics [2]. The current ML method has no functional bias as it basically consists of a series of step functions which makes it versatile but prone to overfitting and limited by its discontinuous nature. To gain further theoretical insight, we have formulated a creep fibre bundle model based on the same relationship to calculate the event rate based on the stress/forces, temperature, the local energy barriers/yield strengths. Some preliminary results are the exact lifetime distributions, mean (Figure 13 left) and variance Figure 13 right) for a fibre bundles with identical thresholds. For heterogenous thresholds the functional relationship has also been found to be a nested integral over a high dimensional path integral and therefore is hard to verify due to the combinatorial complexity of the number of possible fracture paths.

For MD we created 2D silica glass, applied uniaxial tension and identify the site of the first bond break. 2D silica is suited as a test case as it allows for off-the-shelf image recognition approaches to be used and it decreases computational and memory cost. A standard image recognition approach via a convolutional neural network and a new local approach based on symmetry functions and a support vector classifier (SVC). For the CNN, snapshots of the initial configuration are converted to images and the CNN is made to predict the coordinate of the broken bond (point in the middle between the two atoms breaking the bond). The CNN is made by interpretable Gradient-weighted Class Activation Mapping (Grad-CAM) which colours pixels according to their importance for the classification. The local encodes the neighbourhood of an atom via a set of rotation and translation invariant symmetry functions and the prediction is made for each atom whether it is involved in the first breaking of a bond. We apply an affine transformation to the system according to the loading to incorporate the orientation of the atomic neighbourhood with respect to the load. This way all symmetries (rotation invariance, translation invariance, orientation dependence with respect to the load) are incorporated. The rupture strain is predicted with reasonable accuracy (coefficient of determination $R^2$~0.7) and the rupture location within the standard deviation of predictions made for result-invariant transformations of the image as the CNN itself does not know/incorporate this invariance. The local approach identifies a set of particles which contains ~ 97 % of the particles involved in the first bond breaking while classifies ~ 96 % correctly as particles with no bond breaking. The results presented here have been published this year [3].

**Conclusions, achievements, and outlook**

The next steps in this project are to finish the last details like the asymptotic avalanche distribution for the theoretical fibre bundle model, submit it for publication and then move towards the PhD thesis.

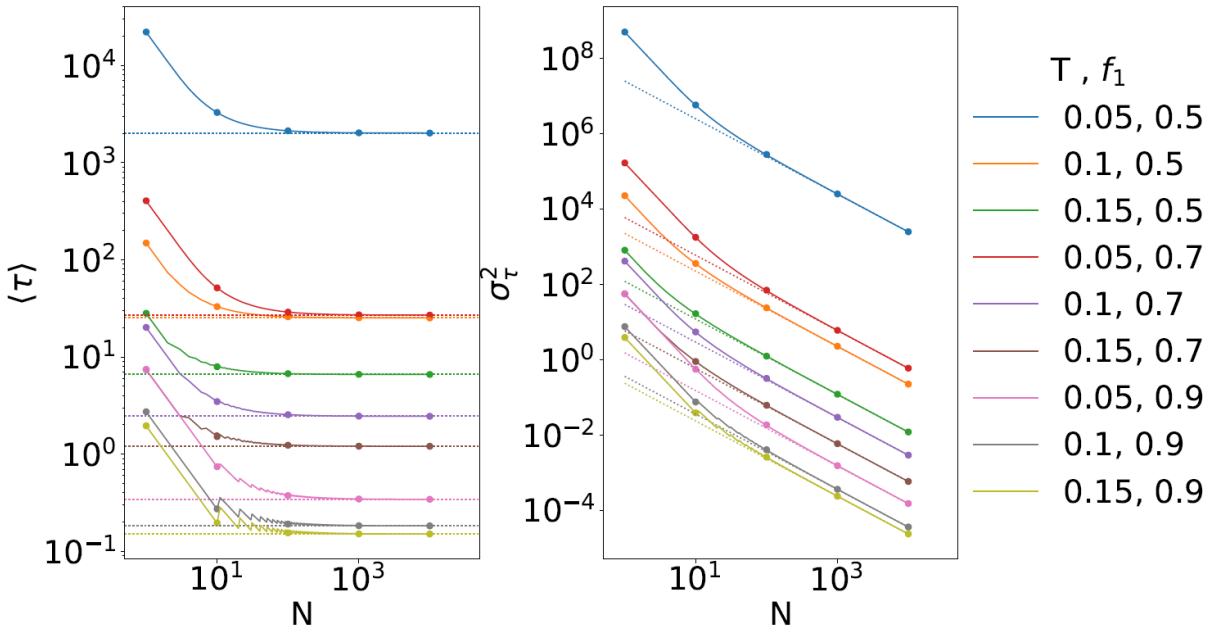



*Figure 13: Comparison for the average (left) and variance (right) of the lifetimes of simulation results (dots) versus exact (full lines) and asymptotic (dotted lines) theoretical predictions of the failure lifetime $\tau$ plotted against the number of fibres in the bundle $N$ for different temperatures $T$ and applied initial force per fiber $f_1$.*

## P6: Preliminary Studies Regarding FE-MD Fracture Simulations of Polymer NCs

Felix Weber, Christian R. Wick, Ana-Sunčana Smith and Sebastian Pfaller

### Equilibration of non-periodic MD samples of amorphous polymers

As one of our long-term goals, we aim to utilize the Capriccio method [1] for multiscale fracture simulations of polymer nanocomposites. In the Capriccio method, which concurrently couples a molecular dynamics (MD) region to a continuum domain discretized by finite elements (FE), the MD region is subjected to non-periodic, so-called stochastic boundary conditions (SBC), which were recently extended by an additional padding region (the *fur*) to avoid surface effects [2], see Figure 14. The MD domain is obtained from a larger *master system* prepared under classical periodic boundary conditions (PBC) by cutting out a smaller subsystem. Due to the induced perturbation of the system behaviour, the FE-MD setup must be relaxed until an equilibrium state is obtained. In a study regarding the relaxation behaviour of an FE-MD coupled MD domain utilizing non-periodic boundary conditions [3], we showed the insensitivity of the relaxation behaviour of the MD systems to the specific coupling parameters of the method chosen to implement the boundary conditions. Figure 15 shows the deviation of mass density of the MD samples for the parameter set considered as optimal compared to simulations under PBC. Here, the grey curves represent the results from the observation region of the five coupled systems, the red one is the resulting average curve. The associated particle domains have been obtained from the PBC master system at five different time points of its preparation.

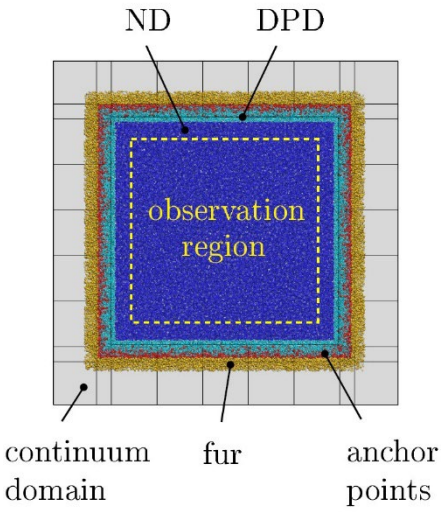



*Figure 14: Setup of the FE-MD simulations (cross-section through a central plane), from [3].*

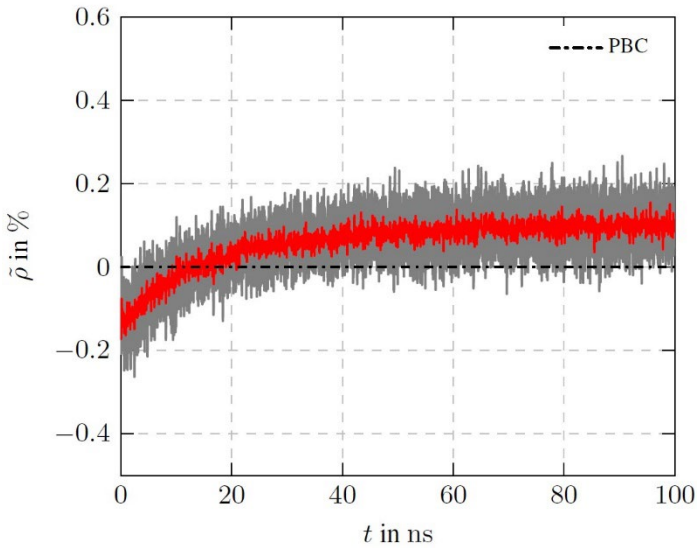



*Figure 15: Normalized difference of density in the observation region and global density obtained under periodic boundary conditions $\tilde{\rho}$ over time t, from [3].*

### Modelling size effects in polymer nanocomposites with a quantitative interphase model

In [4], we verified and validated an interphase model for nano-silica-reinforced polystyrene proposed in a previous publication [5]. Especially, we investigated the capability of this model to reproduce the dependence of the mechanical behaviour of nanocomposites on the filler size and content reported in the literature.

The preceding study presented in [5] yielded the material properties within the interphase which evolves between the pure bulk polymer and the filler particles. To this end, the goal data for an inverse parameter identification was obtained from so-called FE-MD “pseudo-experiments”, subjecting samples containing two nanoparticles to a uniaxial tensile load (Figure 16). The corresponding MD simulations used a coarse-grained description of bulk and filler particles. Please note that we extensively investigated the material properties of the coarse-grained silicon dioxide in a parallel study [6]. The FE-MD simulations yielded the reaction forces on the Dirichlet boundaries of the FE domain and the strain of the interparticle axis. Afterwards, pure FE surrogate models were set up and subjected to the same load case. In this surrogate representation, the interphase was split up into four shells of equal thickness and the material properties of each interphase layer were obtained by an optimization scheme utilizing the FE-MD goal data. Finally, using exponentially saturating

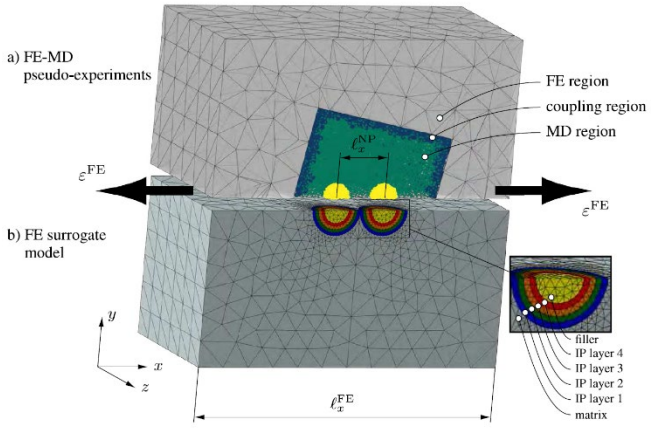



*Figure 16: a) Setup of the FE-MD pseudo-experiments and b) of the FE surrogate model. In the surrogate representation, the interphase is split into four layers, whereby the material properties are constant over each of the layers, from [4].*

of FE nodes does not influence the results. The same applies to varying the number of interphase layers. For the validation of the interphase model, three initial interparticle distances which were not used in the model calibration were considered.

Finally, we thoroughly scrutinized if the interphase model is capable of reproducing the dependence of the mechanical behaviour on the filler size and the filler content. On the one hand, we used two different filler volume ratios, whereby we chose six different nanoparticle radii within a range from 1 to 50 nm in each case. On the other hand, three different distances between the particle surfaces were considered, resulting in overlapping, slightly touching, and separated interphases. Indeed, we observed the expected stiffening effect when decreasing the filler size, cf. Figure 17, as well as when increasing the filler volume ratio.

functions for the interphase properties resulted in an almost perfect reproduction of the FE-MD pseudo-experiments.

We first verified the interphase model in a numerical sense, whereby we chose the same two representative initial distances between the nanoparticle centres which were also used for the calibration of the interphase model. On the one hand, we determined the influence of the FE mesh quality. We could prove that the number

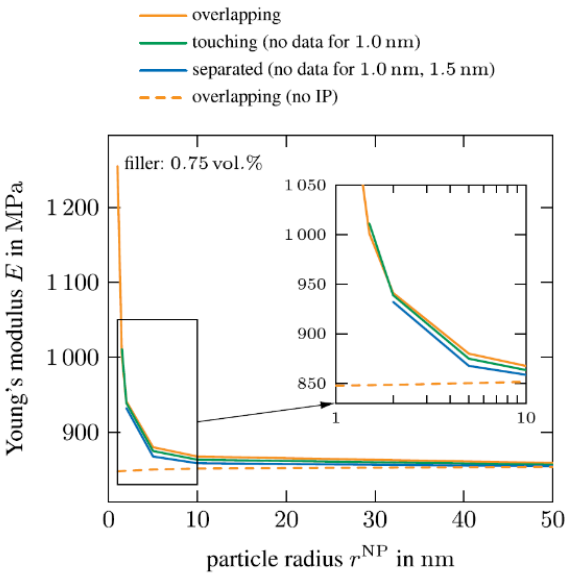



*Figure 17: Young's modulus E over nanoparticle radius $r^{NP}$ obtained in the uniaxial tension simulations of the FE surrogate representation with filler volume fraction 0.75 vol.%. Setups with overlapping, slightly touching, and separated interphases are compared, together with the "overlapping" case without consideration of the interphase, from [4].*

**References**

[1] S. Pfaller, M. Rahimi, G, Possart, P. Steinmann, F. Müller-Plathe, M.C. Böhm: *An Arlequin-based method to couple molecular dynamics and finite element simulations of amorphous polymers and nanocomposites* (2013) Computer Methods in Applied Mechanics and Engineering 260 109-129

[2] Y. Jain, M. Ries, S. Pfaller, F. Müller-Plathe: *Addressing surface effects at the particle-continuum interface in a molecular dynamics and finite elements coupled multiscale simulation technique* (2022) Journal of Chemical Theory and Computation 18 2375-2387

[3] F. Weber, M. Ries, C. Bauer, C. R. Wick, S. Pfaller: *On equilibrating non-periodic molecular dynamics samples for coupled particle-continuum simulations of amorphous polymers* FRASCAL Special Issue in Forces in Mechanics, vol. 10, 100159, 2023

[4] M. Ries, F. Weber, G. Possart, P. Steinmann, S. Pfaller: *A quantitative interphase model for polymer nanocomposites: Verification, validation, and consequences regarding size effects* (2022) Composites Part A: Applied Science and Manufacturing 161 107094

[5] M. Ries, G. Possart, P. Steinmann, S. Pfaller: *A coupled MD-FE methodology to characterize mechanical interphases in polymeric nanocomposites* (2021) International Journal of Mechanical Sciences 204 106564

[6] M. Ries, C. Bauer, F. Weber, P. Steinmann, S. Pfaller: *Characterization of the material behavior and identification of effective elastic moduli based on molecular dynamics simulations of coarse-grained silica* (2022) Mathematics and Mechanics of Solids p. 108128652211080

## aPG: Analysing the Mechanical Behaviour of Polymer Nanocomposites with a Fast Coarse-Grained Molecular Dynamics Model

Maximilian Ries, Jakob Seibert, Vincent Dötschel, Paul Steinmann, Sebastian Pfaller

The addition of nano-sized filler to polymers significantly enhances their mechanical performance. This reinforcement is mainly attributed to the formation of an interphase layer surrounding the nanoparticles, where the polymer's properties are altered due to the vicinity of the fillers. From an engineering point of view, these molecular mechanisms and their impact on the macroscopic material behaviour are not fully understood. Therefore, we rely on coarse-grained molecular dynamics since classical continuum mechanical approaches cannot capture the effects on the molecular scale. However, molecular dynamics is computationally very expensive, limiting possible investigations.

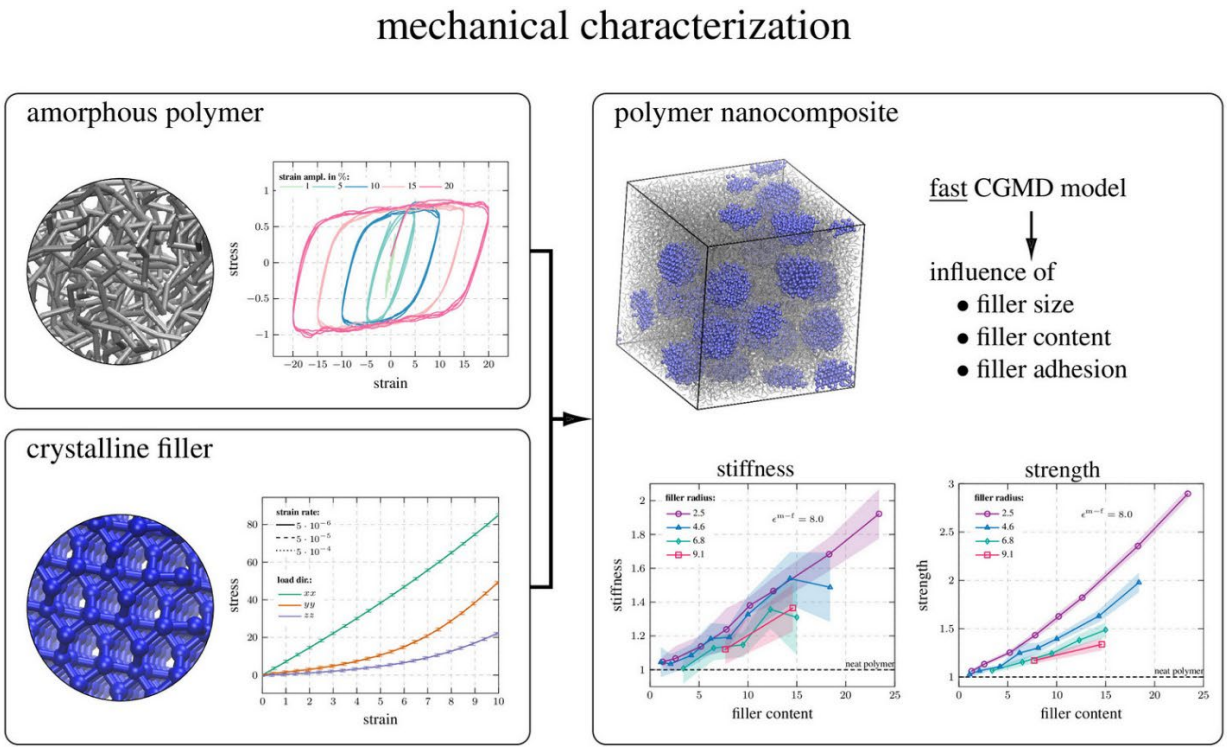



*Figure 18: Generic model to study the mechanical performance of polymer nanocomposites: characterization of neat matrix and filler and subsequent investigation of composite [1].*

Therefore, we introduce a fast coarse-grained molecular dynamics model of a generic thermoplastic re-enforced with spherical filler particles and thoroughly characterize the material behaviour of neat polymer, neat filler, and composite, as depicted in Figure 18.

In [1], we employ a strategy to characterize the mechanical behaviour based on molecular dynamics simulations, which already provided promising results in earlier studies on neat silica [2] and neat polystyrene [3]. The thorough mechanical characterization of the generic model reveals elasto-viscoplasticity and anisotropic elasticity for amorphous polymer and crystalline filler, respectively.

For the resulting nanocomposite, we are able to detect the matrix-filler interphase region through the entanglement density and the radius of gyration, depicted in Figure 19 left and mid, respectively. Overall, the generic composite features the typical characteristics of polymer nanocomposites: Stiffness and strength increase with increasing filler content and decreasing filler radius (size effect). Due to the simplicity of the new MD model, individual influences can be examined in more detail. For instance, Figure 19 (right) shows that the tensile strength depends not only on the filler content but also significantly on the filler-matrix adhesion. Consequently, the introduced generic model is suitable for future investigations to improve our understanding of polymer nanocomposites.

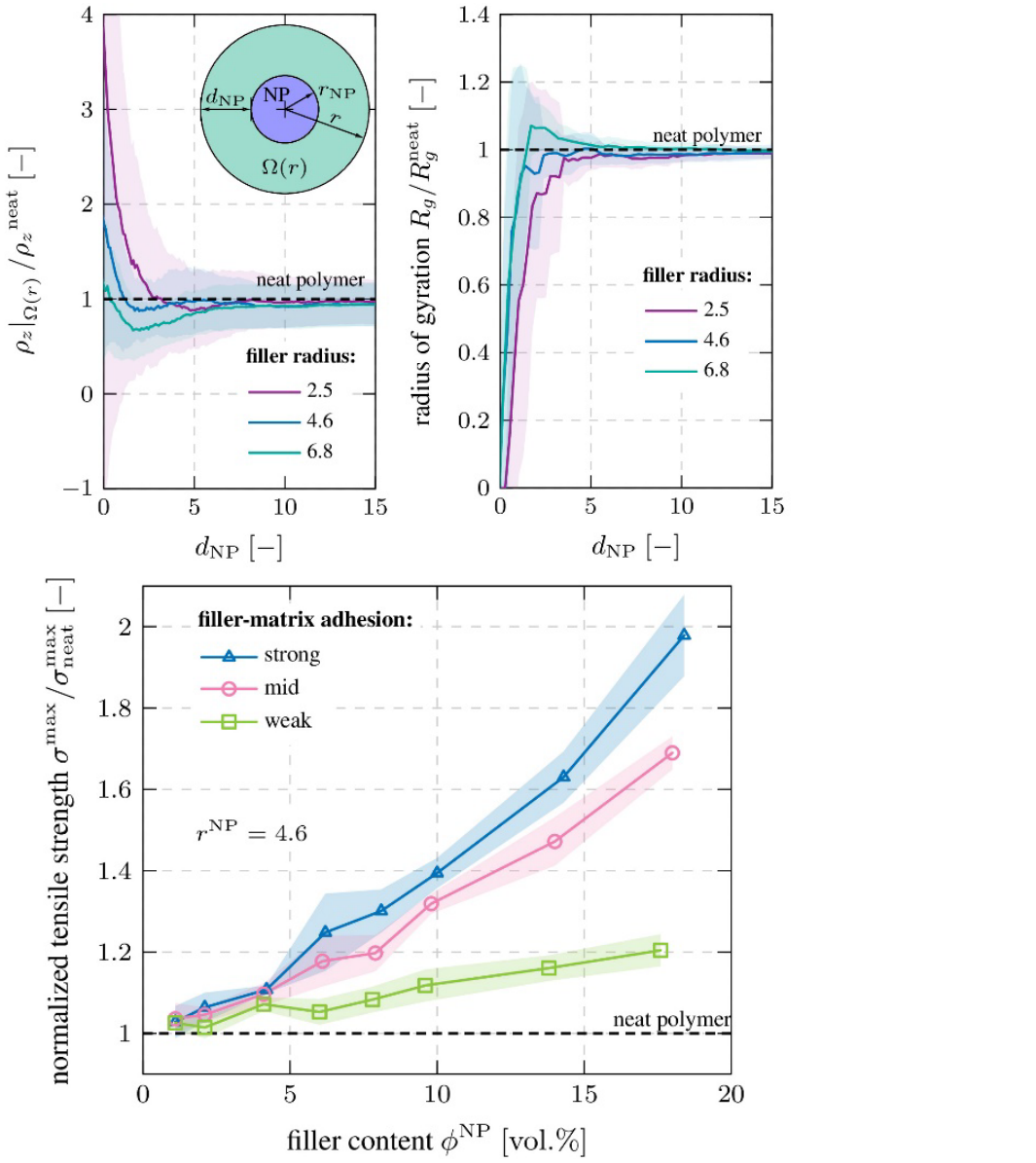



*Figure 19: Interphase region surrounding the filler particles revealed by entanglement density (left), and radius of gyration (mid); impact of filler-matrix adhesion on tensile strength (right).*

**References:**

[1] M. Ries, J. Seibert, P. Steinmann, & S. Pfaller, "Applying a generic and fast coarse-grained molecular dynamics model to extensively study the mechanical behavior of polymer nanocomposites," Express Polymer Letters, vol. 16, (12), pp. 1304–1321, 2022.

[2] M. Ries, C. Bauer, F. Weber, P. Steinmann, & S. Pfaller, Characterization of the material behavior and identification of effective elastic moduli based on molecular dynamics simulations of coarse-grained silica," Mathematics and Mechanics of Solids, p. 108 128 652 211 080, 2022.

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

## aPH: Coupled Particle-Continuum Simulations of Amorphous Polymers with Hybrid Boundary Conditions at Large Strains

Wuyang Zhao, Paul Steinmann and Sebastian Pfaller

The Capriccio method [1] has been designed for coupled atomistic-continuum simulations for amorphous polymers, where the atomistic domain is treated by MD simulations while the continuum domain is discretized by the Finite Element (FE) method. This method has been i) extended to inelasticity that allows for simulations at much larger deformation [2] and ii) improved to address the interface effects between the MD and FE domains by introducing the fur beads [3]. The Capriccio method is appropriate for fracture simulations of polymers since the FE domain can provide more realistic boundary conditions for the MD domain and hence enables non-affine deformations. The application of the Capriccio method to fracture simulations of amorphous polymers has been first attempted in [3], where a pre-crack has been introduced by deleting the corresponding atoms and elements. In addition, hybrid boundary conditions (HBC) are introduced for the MD domain to implement Mode-I loading, where periodic boundary conditions (PBC) are used in one direction while non-PBC are employed in the other two directions. However, due to limited available deformation region, fracture has not been observed in [3]. To study the fracture process of amorphous polymers, we improved the available strains in the coupled method [5] and summarized important results in this report.

At first, we extended the viscoelastic-viscoplastic constitutive model [4] to strains of 100% with small modifications. Furthermore, we incorporated the fur concepts introduced in [3] into the coupling scheme and studied the fur effects in the coupled system with HBC. As shown in Figure 20, the systems with fur have larger deviations between the internal MD domain and the reference pure MD and pure FE systems in terms of stresses after the yield point, independent of the fur length. This indicates that the mechanism of chain sliding dominates at larger strains and thus the atom positions cannot be interpolated by the deformation of the FE domain.

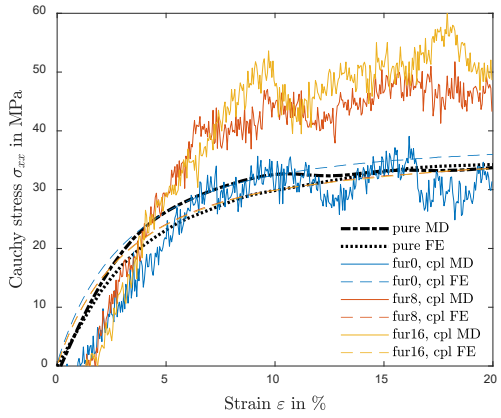



*Figure 20: Parameter study: Stress-strain curves of the internal MD and the FE domain in the coupled systems with various fur length compared to the reference pure MD and pure FE simulations in uniaxial tension with the strain rate of 1%/ns.*

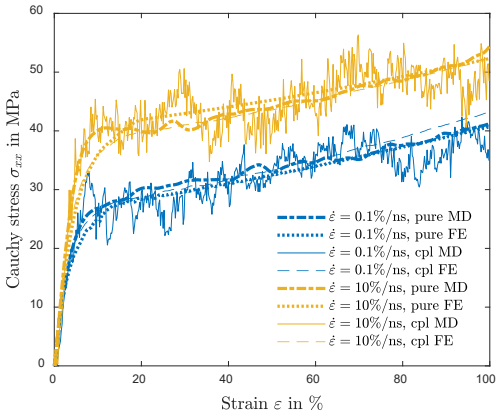



*Figure 21: Validation: Stress-strain curves of the internal MD and the FE domain in the coupled system without fur compared to the reference pure MD and pure FE simulations in uniaxial tension up to a strain of 100% with different strain rates.*

Thus, we use the systems without fur for simulations at large strains. With appropriate parameters, we validated the coupled system by comparing their stress-strain curves to the reference pure FE and MD simulations in uniaxial tension up to a strain of 100% with the strain rates of 0.1%/ns and 10%/ns. Figure 21 presents the averaged stresses of the inner MD observation region and the FE domain in the coupled system as well as the results of the reference pure MD and FE systems.

Moreover, we consider the deformation state of the coupled system at large deformations. Figure 22 shows the screenshot of the coupled system at a strain of 100% with the strain rate of 10%/ns, where the bulge at finite strains observed in [2] has been eliminated. With this updated coupling method, fracture behaviour has been observed in [5] and further studies in this regard are work in progress.

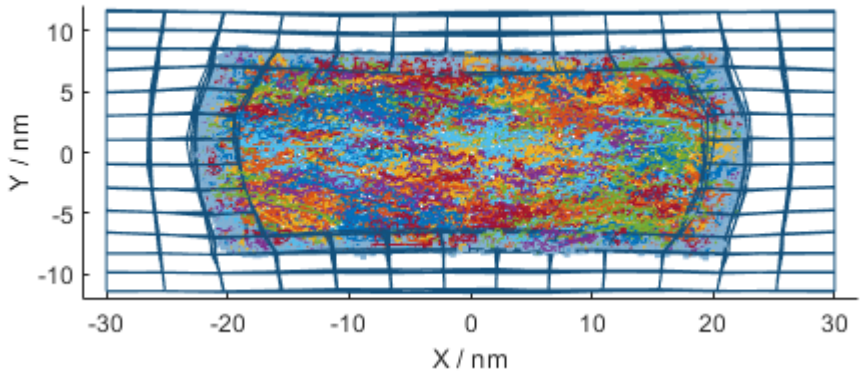



*Figure 22: Snapshot of the deformed MD-FE coupled system without fur at the strain of 100%/ns with the strain rate of 10%/ns. The colours in the MD domain represent different polymer chains.*

## References

[1] S. Pfaller, M. Rahimi, G. Possart, P. Steinmann, F. Müller-Plathe, and M.C. Böhm. "An Arlequin-based method to couple molecular dynamics and finite element simulations of amorphous polymers and nanocomposites". Comput. Methods Appl. Mech. Eng. 260 (2013), pp. 109 – 129.

[2] W. Zhao, P. Steinmann, and S. Pfaller. A particle-continuum coupling method for multiscale simulations of viscoelastic-viscoplastic amorphous glassy polymers. International Journal for Numerical Methods in Engineering (2021).

[3] Y. Jain, M. Ries, S. Pfaller, and F. Müller-Plathe. Addressing surface effects at the particle-continuum interface in a molecular dynamics and finite elements coupled multiscale simulation technique. Journal of Chemical Theory and Computation 18.4 (2022), pp. 2375-2387.

[4] W. Zhao and S. Pfaller. A concurrent MD-FE coupling method towards simulations of fracture of thermoplastic polymers. Ed. by E. F. Onate, D. Peric, C. M., and E. de Souza Neto. 2022.

[5] W. Zhao, Y. Jain, P. Steinmann, F. Müller-Plathe, and S. Pfaller. Multiscale simulations for fracture of glassy polymers coupling atomistic and continuum scales. In preparation.

## P7: Tuning Adhesion Properties of Hierarchical Materials

Christian Greff and Paolo Moretti

The research during the first cohort of this project used network-based models to investigate the failure and detachment of hierarchically structured materials using statistical analysis and graph theory. Real world examples of such systems would be, for example, the gecko pad[1] and dry adhesives developed to mimic it[2]. The heterogeneities in brittle materials are incorporated into the model by assigning randomly distributed failure thresholds to the edges of the network, with a scaling parameter t defining the ratio between the adhesion connections at the lower interface to the cohesion connections within the network. The focus lies here on the influence of material structure, which is formed in the simulated systems through initially deleted edges in the network, in the following referred to as gaps.

In the first year of the second cohort, we extended our research from 3D deterministic hierarchical structures that need perfect order to systems termed shuffled hierarchical. The shuffled part of the name stems from them being networks that are constructed by randomly changing the positions of gaps compared to a deterministic hierarchical network, visualized for the 2D case in Figure 23. Former simulations had shown that for such 2D systems, these structures of shuffled gaps lead to a behaviour that closely matches that of the corresponding deterministic hierarchical system.

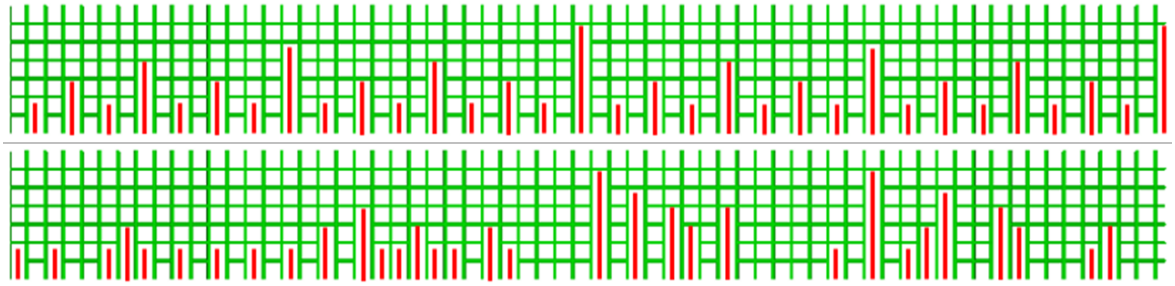


*Figure 23: Structure of 2D deterministic (top) and shuffled (bottom) hierarchical systems with gaps marked in red.*

This observation held true for the higher dimensional case of 3D, with spectral analysis showing that 3D shuffled and deterministic hierarchical systems have very similar eigenvalues and therefore deformation modes, both being softer than random reference systems as shown in Figure 24. The breaking pattern of deterministic hierarchical systems, with the system-spanning critical crack being located towards the bottom side of the system, was likewise replicated by the shuffled hierarchical systems. This shows that shuffled hierarchical systems can achieve equivalent behaviour to the deterministic hierarchical ones while placing less stringent requirements on construction.

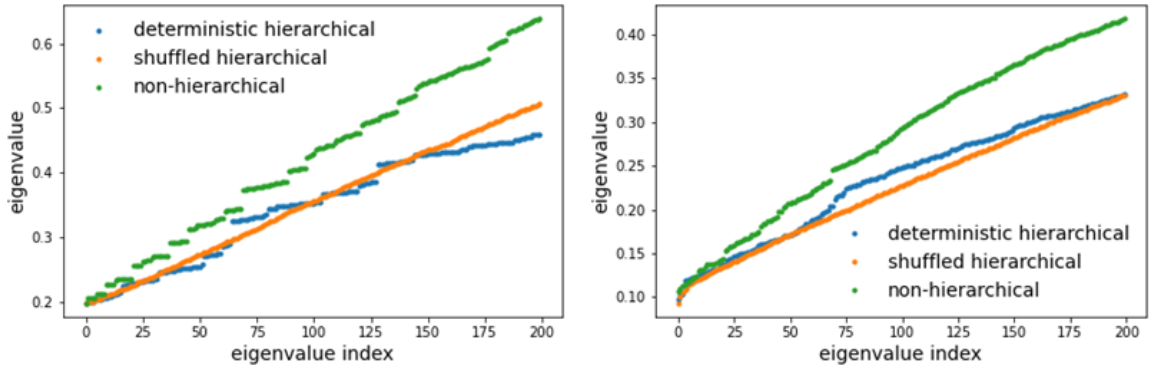



*Figure 24: First 200 eigenvalues of the reduced Laplacian of networks with different gap structures in pristine condition (left) and at peak load of the system (right).*

These simulations were performed as fuse models, which achieve higher computational efficiency at the cost of simplifying the behaviour of forces and displacements from tensorial to scalar. To show the reliability of this method, a model was applied to a set of the same network structures, where the edges of the structure were instead treated as Timoshenko beams. Consequently, stress then accurately behaves as a tensor in the simulation. The breaking pattern within those networks matches closely to those of the fuse simulations, as presented in Figure 25. The fuse networks show a slight overestimation of broken edges in z-direction for the lowest and upper layers but capture the relevant

behaviour well. With this, the trust in the fuse models as being a sensible approximation for describing the behaviour of such network systems increases. Using their much faster computation, they can therefore allow for more realizations of networks to be simulated and therefore achieve a better statistical sampling of shuffled hierarchical structures.

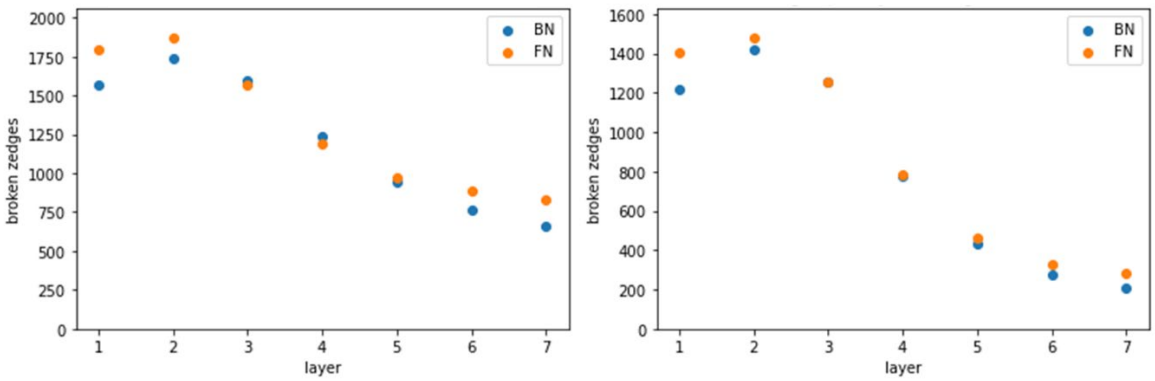



*Figure 25: Number of broken z-edges per layer that are part of the critical, system-spanning crack for fuse (FN) and beam (BN) networks for a system with high (left) and intermediate (right) disorder of local strength.*

Furthermore, first simulations were performed to extend the scope of this project towards modelling of systems composed of multiple different materials, to enable the investigation of phase-based structures in composites. For this, 2D systems composed of a harder and a softer phase arranged in a hierarchical manner were chosen as a trial system. Investigations into their behaviour are currently ongoing.

## References

[1] Autumn, K., Gravish, N. (2008). Gecko adhesion: evolutionary nanotechnology, Phil. Trans. R. Soc. A 366, 1575-1590.

[2] Li, Xiaosong, et al. (2019) Recent developments in gecko-inspired dry adhesive surfaces from fabrication to application, Surface Topography: Metrology and Properties 7.2

## P8: A Comparative Assessment of Different Adaptive Spatial Refinement Strategies in Phase-Field Fracture Models for Brittle Fracture

Maurice Rohracker, Paras Kumar and Julia Mergheim

For the smeared approximation of a discrete crack (compare Figure 26) phase-field fracture simulations (cf. eq. (1) based on [1]) of brittle materials require suitable finite element meshes to get an accurate resolution of the phase-field function in regions where crack propagation is expected. For the single edge notched shear (SENS) problem the smeared approximation is depicted in Figure 27. In order to get the crack path for the phase-field fracture simulations the following problem must be solved: Find $\mathbf{u} \in \mathcal{B} \rightarrow \mathbb{R}^{dim}, \mathrm{z} \in \mathcal{B} \rightarrow [0,\,1]$, with $\mathrm{z} = 1 \;\Rightarrow$ intact and $\mathrm{z} = 0 \;\Rightarrow$ broken, s. t.

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

The straightforward option is to pre-refine the mesh in regions of the expected crack paths, i.e., in the lower left quadrant of the specimen as done in Figure 28, which results in $20695$ elements and in a total simulation time of $2850\ s$ for the SENS test.

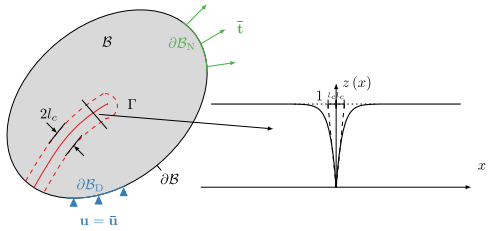



*Figure 26: Smeared model of the phase-field fracture model.*

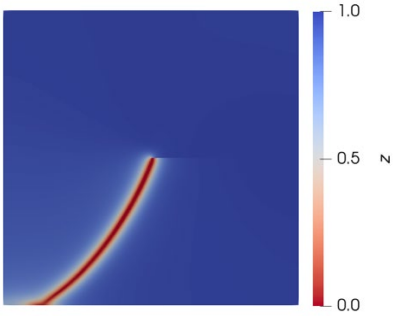



*Figure 27: Phase-field contour of the SENS test.*

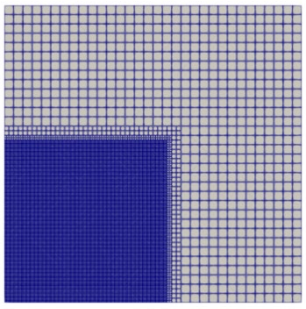


*Figure 28: Pre-refined mesh in the lower left quadrant.*

This is however very computationally intensive due to the high number of elements, which can even increase further for three-dimensional problems. Alternatively, adaptive spatial refinement (ASR) of the finite element mesh is utilized based on appropriate error indicators to obtain the required accuracy in the areas of crack propagation. The approach for ASR is depicted in Figure 29, firstly the minimization problem is solved to get the solutions $\boldsymbol{u}$ and $z$ on the current mesh $m$ and written to an output file. Then ASR is applied as a pure post-processing step, which involves computing the error indicator, coarsening and refining the elements, and transferring the solution as well as the History values to the new mesh $m+1$ by an interpolation scheme. The criterion used for coarsening and refinement is based on different error indicators: the most common one for phase-field fracture simulations is the threshold-based approach, in which elements are refined depending on the value of the phase-field function. Alternatively, the Kelly error indicator can be used as a criterion for spatial

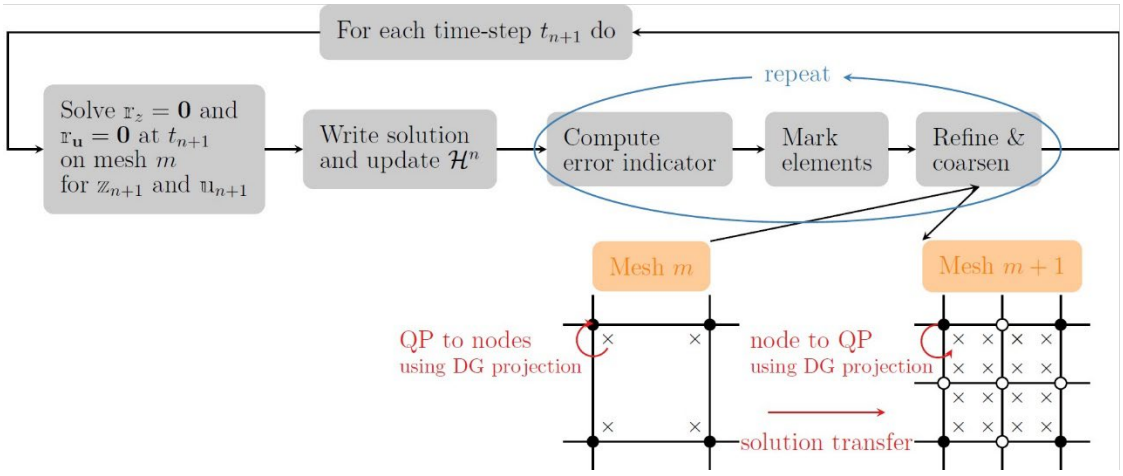



*Figure 29: Flowchart of the general approach of ASR in the FE method.*

adaptivity. It considers the jumps in the gradients of the phase-field function between the elements. We additionally introduced in our recent paper (cf. [2]) a newly derived error indicator based on configurational forces, that depend on the Eshelby stress tensor $\boldsymbol{\Sigma}$. For mode I loading in linear elastic fracture mechanics, the configurational forces have a close connection to the $\mathcal{J}$-Integral and the critical fracture energy $\mathrm{G_c}$, respectively. Therefore, a suitable norm of the configurational forces is introduced as an error indicator here. Due to the phase-field fracture formulation, different contributions of the Eshelby stress tensor can be used to compute the error indicator. These are the pure fracture Eshelby stress tensor, its pure elastic part, and the summation of both, the total Eshelby stress tensor.

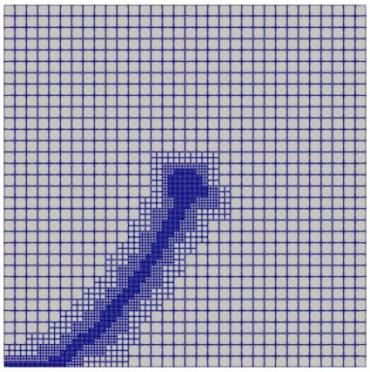


*Figure 30a: Mesh for ASR using error based on $\boldsymbol{\Sigma}^{frac}$.*

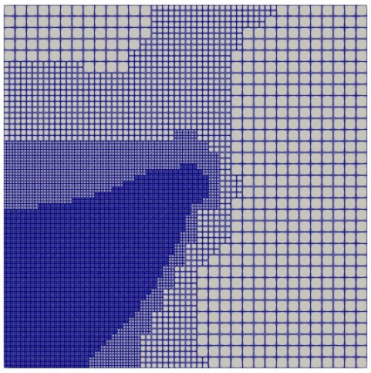


*Figure 30b: Mesh for ASR using error based on $\boldsymbol{\Sigma}^{el}$.*

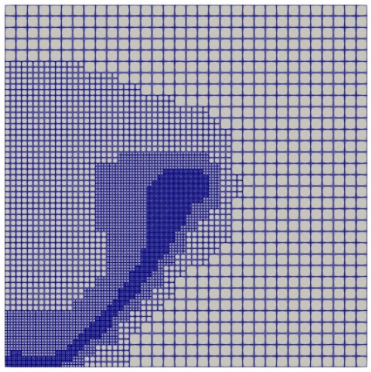


*Figure 30c: Mesh for ASR using error based on $\boldsymbol{\Sigma}$.*

The resulting meshes for a refinement fraction of 5% are sketched in Figure 30a – c. For the pure fracture part, refinement is only done on the crack path. The thickness of the refinement region depends on the used refinement fraction. In contrast, using the pure elastic Eshelby stress tensor results in refinement also away from the crack path, which is again closer to the pre-refined mesh and therefore the most accurate approach. For the total Eshelby stress tensor, the results of the two previous contributions superpose, and refinement is less pronounced away from the crack path. It still offers very accurate simulation results as well as good speedups. For suitable refinement fractions, speedups of around 4 were achieved. The later contribution with the best compromise between accuracy and speedup is then used to compare the three different error indicators for appropriate refinement fractions and a phase-field threshold. In our recent publication (Rohracker et al. [2]) this comparison of the three different error indicators is performed in terms of accuracy (error measure of the load-displacement curve) and efficiency (speedup) for the numerical example of crack propagation in the SENS test. For suitable parameters, they show very good accuracy and efficiency compared to the simulation on a pre-refined mesh, as the Kelly error indicator and the configurational force-based error indicator using the total Eshelby stress tensor are comparable in terms of accuracy and speedup. Only the phase-field threshold-based error indicator could outperform the two other strategies by means of the speedup due to its simple and inexpensive evaluation.

**References**

[1] C. Miehe, F. Welschinger, and M. Hofacker. “Thermodynamically consistent phase-field models of fracture: Variational principles and multi-field FE implementations”. *International Journal for Numerical Methods in Engineering* 83.10 (2010), pp. 1273-1311.

[2] M. Rohracker, P. Kumar, and J. Mergheim. “A comparative assessment of different adaptive spatial refinement strategies in phase-field fracture models for brittle fracture”. *FRASCAL Special Issue in Forces in Mechanics, vol. 10, 100157, 2023.*

## aPJ: Generalized Interfaces Enabling Macroscopic Modelling of Soft and Brittle Adhesives and their Failure

Lucie Spannraft, Gunnar Possart, Paul Steinmann and Julia Mergheim

The application of soft and brittle adhesives in industrial production has been steadily increasing for decades. For instance, soft adhesives are used in convenience products, e.g. to glue thin elastomeric sheets, or for sealing applications in engineering. Structural adhesives, such as brittle epoxies, are employed for bonding numerous materials in lightweight construction, vehicle and aircraft production.

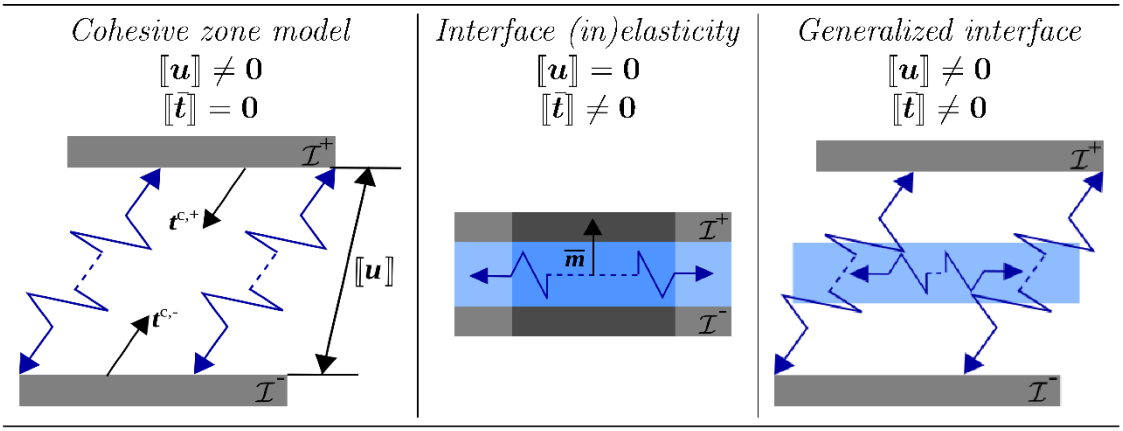



*Figure 31: Categorization of interface models with regard to the displacement jump [[**u**]] and the tractions jump [[$\bar{\boldsymbol{t}}$]]:=**σ**·$\bar{\boldsymbol{m}}$ with the bulk Cauchy stress **σ** and the interface normal vector $\bar{\boldsymbol{m}}$, cf. [1].*

Such adhesive layers, commonly of small thickness, have previously been modelled as zero-thickness elements for efficiency using interface elasticity or cohesive zone models (CZM). CZM allow for displacement jumps, but not for jumps in the tractions across the interfaces. Thus, those models cannot capture the physical response of an adhesive being stretched in in-plane direction. In contrast, interface elasticity allows for a membrane response by considering energetic and dissipative structures in the interface. However, they do not account for displacement jumps, compare Figure 31. Since brittle and soft adhesives undergo combinations of tension, shear and in-plane loading in various applications, we developed generalized interface models, cf. [1, 2], to properly capture the adhesives' macroscopic behaviours. On the one hand, our models account for a displacement jump and for anisotropic cohesive failure. On the other hand, a jump in the tractions across the interface can arise and induce membrane stiffness and failure under in-plane stretch.

Brittle adhesives are already fully damaged at small strains. However, soft adhesive joints can undergo large deformations prior to failure. For the thermodynamically consistent interface model, the anisotropic cohesive law, i.e. dependent on the spatial interface normal, induces additional shear-like stresses for nonlinear kinematics within the interface to satisfy the balance of angular momentum, see Figure 32 (a).

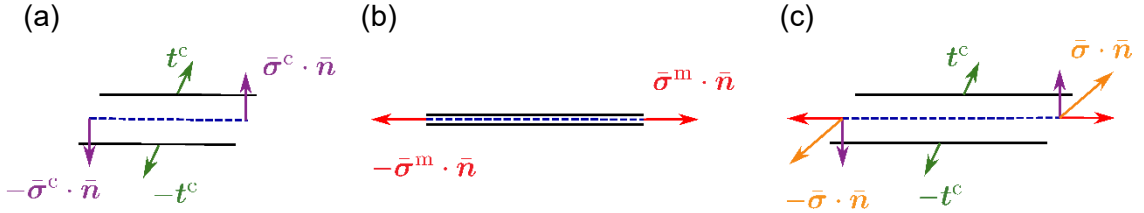



*Figure 32: Two-dimensional graphical representation of interfacial tractions for (a) a coherent elastic, (b) an anisotropic cohesive, and (c) a generalized interface with the cohesive tractions $\bar{\boldsymbol{t}}^c$, the normal to the interface boundary $\bar{\boldsymbol{n}}$, the interface Cauchy stresses $\bar{\boldsymbol{\sigma}} = \bar{\boldsymbol{\sigma}}^m + \bar{\boldsymbol{\sigma}}^c$ with a membrane and a cohesive contribution, cf. [2].*

We couple the different damage modes normal, tangential and in-plane to capture the effects of their interaction, such as reduced reaction forces, stresses and changed deformations. Figure 33 depicts

the deformation and the effective normal cohesive damage in (a) buckling and (b) peel simulations with pre-stretched (a) soft and (b) brittle adhesive interfaces. Thereby, Case 1 of not coupling the damage modes and Case 2 of coupling the damage modes are juxtaposed to show the performance and versatility of our models. Furthermore, Figure 34 exemplarily illustrates effects on the stresses and the resulting forces for the brittle interface, such as the adhesive interface accounting for damage coupling having a smaller stiffness and withstanding less load.

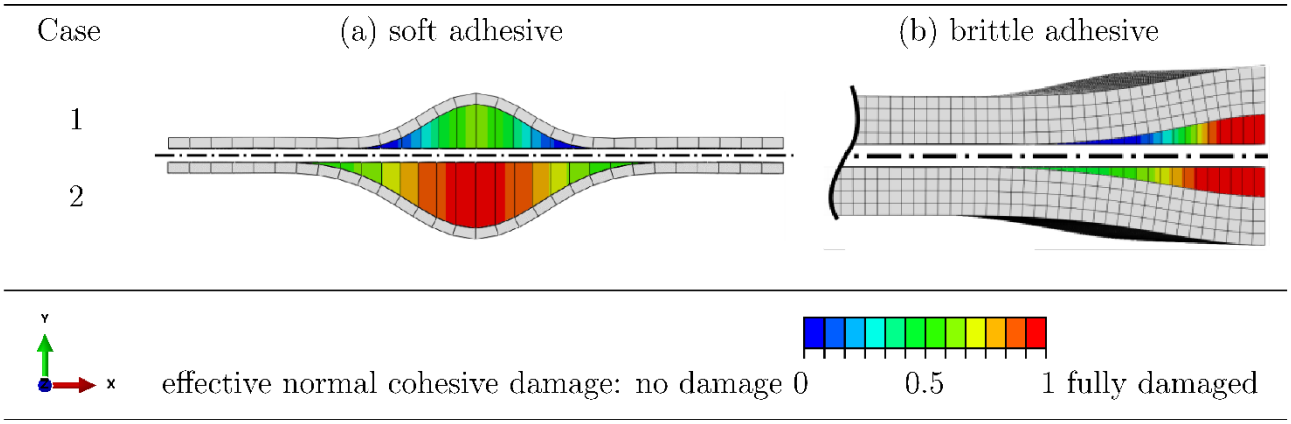



*Figure 33: Deformation and effective normal cohesive damage in a cross-section: Upper half of simulation with Case 1 (uncoupled damage modes) and lower half of simulation with Case 2 (coupled damage modes). (a) Buckling of pre-stretched (300% strain) sandwich-structure with soft adhesive, cf. [2]. (b) Peel test of pre-stretched (5% strain) structural bond, cf. [1]*

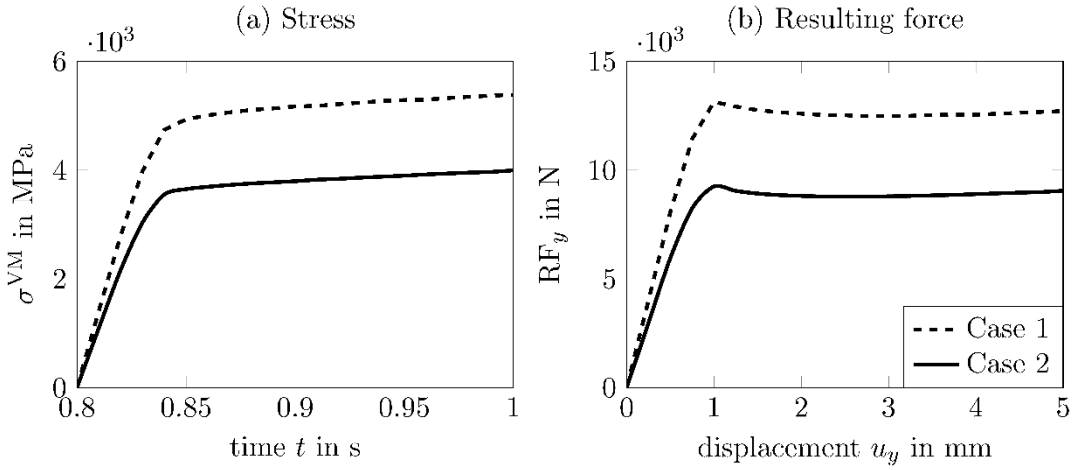



*Figure 34: Stresses and resulting forces in the upper substrate of dimensions of 150mm · 20mm · 2mm with the pre-stretched brittle interface of Cases 1 and 2. (a) Von Mises stresses $\sigma^{VM}$ in MPa plotted at one integration point over time t during the peel test. (b) Resulting forces $RF_y$ in N, summed over the upper right edge of the top substrate, plotted over the displacement $u_y$ in mm. Cf. [1].*

## References

[1] L. Spannraft, G. Possart, P. Steinmann, J. Mergheim, “Generalized interfaces enabling macroscopic modelling of structural adhesives and their failure,” FRASCAL Special Issue in Forces in Mechanics, vol. 9, 100137, 2022.

[2] L. Spannraft, P. Steinmann, J. Mergheim, “A generalized anisotropic damage interface model for finite strains,” submitted, 2022.

## P9: Different Convergence Concepts for the Newmark Algorithm

Dhananjay Phansalkar, Michael Ortiz[1], Kerstin Weinberg[2], Sigrid Leyendecker
[1] Division of Engineering and Applied Sciences, California Institute of Technology, California, USA
[2] Lehrstuhl für Festkörpermechanik, Universität Siegen, 57076 Siegen, Germany

The general focus of this work is the prediction of the crack propagation in brittle material under dynamic loading. Over the years, there are broadly two approaches being developed to understand the fracture in a complex geometry. They are either sharp crack approaches like an extended finite element method (XFEM) [1] or smeared crack approaches like phase-field models [1]. We are interested in the phase-field models for fracture due to their potential to track complex crack paths without any additional ad-hoc algorithms. These phase-field models have an intrinsic length scale parameter $\epsilon$. In our previous work, we developed a variational based approach to compute an optimised spatially varying $\epsilon$ along with a corresponding mesh refinement strategy for quasi-static scenarios [2]. We then extended our approach to the case of dynamic phasefield model leading to following action with time $t \in [0,T]$ and the domain $\Omega$

$$S(\mathbf{u},\dot{\mathbf{u}},\nabla\mathbf{u},c,\nabla c,\epsilon) = \int_0^T \int_\Omega \left[\frac{1}{2}\rho\dot{\mathbf{u}}\cdot\dot{\mathbf{u}} - [1-c]^2\psi(\boldsymbol{\varepsilon}) - \mathcal{G}_c\left[\frac{c^2+\eta}{2\epsilon} + \frac{\epsilon}{2}|\nabla c|^2\right] - \beta\epsilon\right] d\mathbf{x}\, dt \quad (1)$$

$$\psi(\boldsymbol{\varepsilon}) = \frac{1}{2}\boldsymbol{\varepsilon}(\mathbf{u}) : [\mathbb{C}\boldsymbol{\varepsilon}(\mathbf{u})] = \frac{1}{2}\lambda[\mathrm{tr}(\boldsymbol{\varepsilon})]^2 + \mu[\boldsymbol{\varepsilon}:\boldsymbol{\varepsilon}].$$

where $\mathbf{u}(\mathbf{x},t)$ is the displacement field, $\dot{\mathbf{u}}$ is the temporal derivative of $\mathbf{u}$ called velocity, $\boldsymbol{\varepsilon}$ is strain tensor, and $c(\mathbf{x})$ is the phase field. Furthermore, $\epsilon(\mathbf{x})$ is a spatially varying regularisation parameter, and $\rho$, $\mathcal{G}_c$, $\lambda$ and $\mu$ are material parameters, while $\eta$ and $\beta$ are model and penalty parameters. Minimising the functional (1) yields coupled PDEs. Using the notion of minimum energy, we performed a numerical convergence investigation in a quasi-static system [2]. However, in the dynamic scenario, this is not as straightforward; thus, we first analyse a simple ODE problem to investigate different convergence concepts in a numerical framework. Consider a single spring and mass system, as shown in Figure 35, with no additional friction or gravitational acceleration. The behaviour of a general spring-mass system can be modelled by the following action

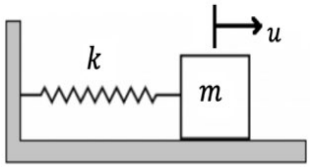


*Figure 35: Configuration of spring-mass system.*

$$S(\mathbf{u},\dot{\mathbf{u}}) = \int_0^T L\,(\mathbf{u},\dot{\mathbf{u}})dt = \int_0^T \left[\frac{1}{2}\dot{\mathbf{u}}\cdot\mathbf{M}\cdot\dot{\mathbf{u}} - \frac{1}{2}\mathbf{u}\cdot\mathbf{K}\cdot\mathbf{u}\right] dt. \quad (2)$$

Here $\mathbf{u}(t)$ is the displacement and $\dot{\mathbf{u}}$ is the velocity of the mass, while $\mathbf{M}$ and $\mathbf{K}$ are the mass and stiffness matrices, respectively. The equation of motion for such a spring-mass system is derived by stationarity of the action (2) leading to the following Euler-Lagrange equation.

$$\mathbf{M}\cdot\ddot{\mathbf{u}} + \mathbf{K}\cdot\mathbf{u} = \mathbf{0} \qquad \text{in} \quad (0,T] \quad (3)$$

This second order ODE is discretised using the Newmark method with parameters $\alpha = 0.25$ and $\gamma = 0.5$. The mass and the stiffness used for the simulation of the system depicted in Figure 35 is $m = 0.5, k = 1.0$ with initial condition $u(0) = 0.2, \dot{u}(0) = v(0) = 0.7$. The simulation is carried out untill $T = 0.1$ with time steps $\Delta t \in \{0.1, 0.01, 0.001, 0.0001\}$. According to the literature [3], with the chosen parameters, the Newmark method has a convergence rate of order 2 for displacements and velocities. This can be validated by comparing the Newmark solution to the analytical result. The analytical solution for such a single spring-mass system is provided by

$$u_{\mathrm{a}}(t) = u(0)\cos(f\cdot t) + \frac{v(0)}{f}\sin(f\cdot t) \qquad v_{\mathrm{a}}(t) = -u(0)\cdot f\sin(f\cdot t) + \frac{v(0)}{\cos}(f\cdot t) \quad (4)$$

where $f = \sqrt{k/m}$. The analytical solution (4) are utilised to calculate the error in displacement, velocity, and action given by

$$e_u = \max_{t\in[0,T]}|u(t) - u_{\mathrm{a}}(t)| \qquad e_v = \max_{t\in[0,T]}|v(t) - v_{\mathrm{a}}(t)| \qquad e_s = |S - S_{\mathrm{a}}|. \quad (5)$$

Where $S_{\mathrm{a}}$ is the action computed from the analytical solution.

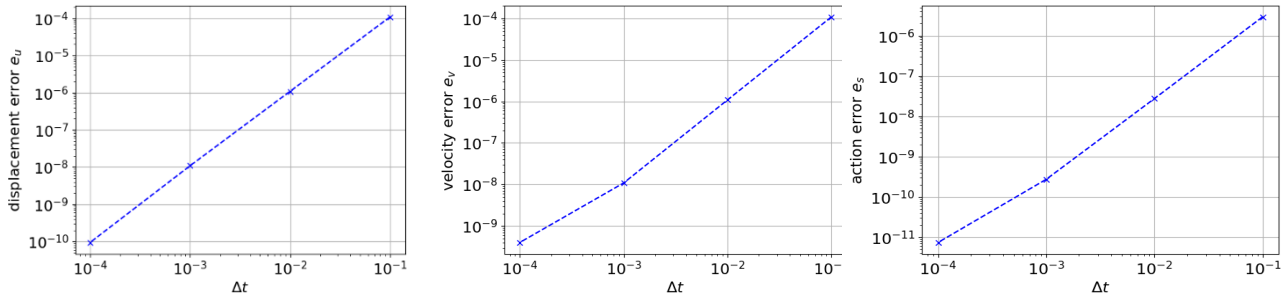



*Figure 36: From left to right: Convergence behaviour of displacement, velocity and action.*

Figure 36, shows the different errors (5) and illustrates the convergence behaviour for displacement, velocity, and action. It exhibits quadratic convergence for all three quantities. Because analytical solutions are not always available, we also conduct the convergence analysis based on the approach described in [4]. To accomplish this, we replace the acceleration in equation (3) with Newmark's discrete acceleration, yielding

$$\mathbf{M} \cdot \frac{\mathbf{u}_{n+1} - \tilde{\mathbf{u}}_{n+1}}{\Delta t^2 \alpha} + \mathbf{K} \cdot \mathbf{u}_{n+1} = \mathbf{0} \tag{6}$$

where $\mathbf{u}_{n+1}$ is the unknown displacement, and $\tilde{\mathbf{u}}_{n+1}$ is the known predictor for the displacement. The solution of the problem (6) is equivalent to a static problem resulting from minimising a potential $E$ with respect to $\mathbf{u}_{n+1}$, where $E$ is defined by

$$E(\mathbf{u}_{n+1}, \mathbf{u}_n, \mathbf{v}_n) = \frac{\Delta t^2 \alpha}{2} \frac{\mathbf{u}_{n+1} - \tilde{\mathbf{u}}_{n+1}}{\Delta t^2 \alpha} \cdot \mathbf{M} \cdot \frac{\mathbf{u}_{n+1} - \tilde{\mathbf{u}}_{n+1}}{\Delta t^2 \alpha} + \frac{1}{2} \mathbf{u}_{n+1} \cdot \mathbf{K} \cdot \mathbf{u}_{n+1} \tag{7}$$

We examine convergence using the potential $E$ in (7) and the action $S$ in (2). Fitting $E$ and $S$ with a power law reveals quadratic convergence in each variable individually, as depicted in Figure 37 and Figure 38, respectively. The next step is to extend this framework of convergence studies to the phase-field modelling of dynamic fracture.

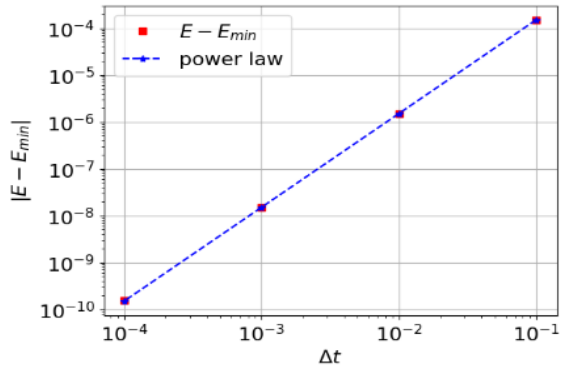



*Figure 37: Convergence behaviour of quasi-static potential.*

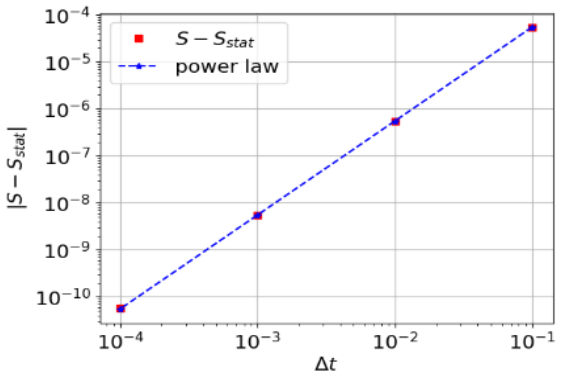



*Figure 38: Convergence behaviour of action.*

## References

[1] A. Egger, U. Pillai, K. Agathos, E. Kakouris, E. Chatzi, I.A. Aschroft and S.P. Triantafyllou. *Discrete and Phase Field Methods for Linear Elastic Fracture Mechanics: A Comparative Study and State-of-the-Art Review*. Applied Sciences, 9:2436, 2019.

[2] D. Phansalkar, K. Weinberg, M. Ortiz and S. Leyendecker. *A Spatially Adaptive Phase-Field Model of Fracture*. Computer Methods in Applied Mechanics and Engineering, 395:114880, 2022.

[3] C. Kane, J.E. Marsden, M. Ortiz and M. West. *Variational Integrators and the Newmark Algorithm for Conservative and Dissipative Mechanical Systems*. International Journal for Numerical Methods in Engineering, 49:1295-1325, 2000.

[4] R. Radovitzky and M. Ortiz. *Error estimation and adaptive meshing in strongly nonlinear dynamic problems*. Computer Methods in Applied Mechanics and Engineering, 172:203-240, 1999.

## P9: Application of the Spatially Adaptive Phase-Field Model to the Splitting Test

Deepak Jadhav, Dhananjay Phansalkar, Michael Ortiz[1], Kerstin Weinberg[2], Sigrid Leyendecker

[1] Division of Engineering and Applied Sciences, California Institute of Technology, California, USA
[2] Lehrstuhl für Festkörpermechanik, Universität Siegen, 57076 Siegen, Germany

In fracture mechanics, there are two primary computational modelling strategies: discrete and diffusive crack approaches. Generally, the discrete crack strategies are complex to implement and computationally expensive. On the other hand, the diffusive crack approach is easy to implement by using standard finite element libraries. The diffusive crack approach has been broadly studied and reported in publications for different material models and complex applications [4, 5]. It is based on the regularization length parameter $\epsilon$ under the condition that $h << \epsilon$, where $h$ is the mesh size. Hence, to resolve the small length parameter $\epsilon$, very fine meshes are needed which may cause high computational costs.

This issue was addressed by interpreting $\epsilon$ as a field variable [1] modifying the energy function used in the standard phase field model [2]. We extend the spatially adaptive phase field model [1] by employing the strain energy split [3] to guarantee only tensile strain energy drives crack propagation. This results in an energy functional given as

$$E(\boldsymbol{u}, c, \epsilon) = \int_\Omega [1-c]^2 \psi^+(\boldsymbol{\varepsilon}) + \psi^-(\boldsymbol{\varepsilon}) + \mathcal{G}_c \left[ \frac{c^2+\eta}{2\epsilon} + \frac{\epsilon}{2} |\nabla c|^2 \right] + \beta \epsilon \, \mathrm{d}\boldsymbol{x} \tag{1}$$

where $\boldsymbol{u}(\boldsymbol{x})$ is the displacement and $c(\boldsymbol{x})$ the phase-field; $\boldsymbol{\varepsilon} = \mathrm{sym}(\nabla \boldsymbol{u}(\boldsymbol{x}))$ represents the strain tensor, $\epsilon(\mathbf{x})$ is the regularisation length variable, $\beta$ and $\eta$ are penalty and model parameter respectively, and the strain energy $\psi(\epsilon)$ is split into tensile $\psi^+(\epsilon)$ and compressive $\psi^-(\epsilon)$ parts according to [3]. Minimizing the above-mentioned energy functional with respect to $\boldsymbol{u}(\boldsymbol{x})$, c($\boldsymbol{x}$) and $\epsilon(\boldsymbol{x})$ leads to the following Euler-Lagrange equations,

$$\mathrm{DIV}[[1-c]^2 \boldsymbol{\sigma}^+ + \boldsymbol{\sigma}^-] = \mathbf{0} \quad \text{in} \quad \Omega \tag{2}$$

$$\frac{c\mathcal{G}_c}{\epsilon} - 2\,[1-c]\,\psi^+(\boldsymbol{\varepsilon}) - \mathcal{G}_c \nabla \cdot [\epsilon \nabla c] = 0 \quad \text{in} \quad \Omega \tag{3}$$

$$\epsilon = \sqrt{\frac{c^2+\eta}{|\nabla c|^2 + \frac{2\beta}{\mathcal{G}_c}}} \quad \text{in} \quad \Omega \tag{4}$$

In these equations, tensile and compressive stresses are expressed by $\boldsymbol{\sigma}$+ and $\boldsymbol{\sigma}$− respectively. These equations are then solved in combination with the boundary conditions $\boldsymbol{u} = \boldsymbol{u_0}$ on $\partial\Omega_d$, $c = c_0$ on $\partial\Omega_p$, and $\nabla c \cdot \boldsymbol{n}$=0 on $\partial\Omega \setminus \partial\Omega_p$ with the outward normal of the mesh $\boldsymbol{n}$.

Previously, the spatially adaptive phase-field model was employed to study single-edge notch tension specimen [1]. We have extended this model to investigate fracture in a splitting test specimen. The specimen is a rectangular plate with an initial notch, as shown in Figure 39. It is composed of two regions, region 1 and region 2, which have a critical energy release rate $G_c$ = 2.70 MPa mm and $G_c$ = 0.54 MPa mm, respectively. However, we have employed the same Lamé parameters $\mu$ = $80.7692 \cdot 10^3$ MPa, $\lambda$ = $121.1538 \cdot 10^3$ MPa for both the regions. The boundary conditions are as illustrated in Figure 39. Due to the fact that the fracture energy varies between the two regions, the parameters $\eta$ and $\beta$ are calculated separately for each zone in accordance with [1]. The parameters used in the simulation are $\eta_1$ = 0.6875, $\beta_1$ = 29.0039, $\eta_2$ = 0.6875, and $\beta_2$ = 145.0195. The simulation is performed by applying a monotonically increasing displacement in increments of $\Delta u = 1 \cdot 10^{-5}$ mm to the splitting test specimen. Figure 40 compares the computed force vs. displacement curves for the spatially varying length variable $\epsilon(\boldsymbol{x})$ to those of a given constant $\epsilon$ = 0.08 with an initial mesh size $h$ = 0.04 and $h$ = 0.005. It demonstrates that the adaptive phase-field model is capable of producing a superior outcome or a result equivalent to a fine mesh while starting with a very coarse mesh. Figure 41 depicts the distribution of the $\epsilon(\boldsymbol{x})$ field and mesh refinement at the crack tip in the

spatially adaptive phase-field model. In the future, we will include temporal adaptation into the spatially adaptive phase field model and employ it to investigate the dynamic brittle fracture in greater depth.

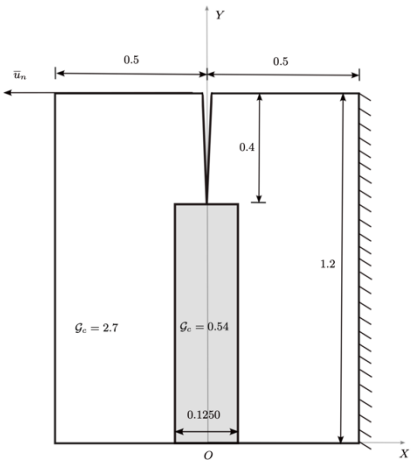



*Figure 39: Geometry and boundary conditions for the splitting test.*

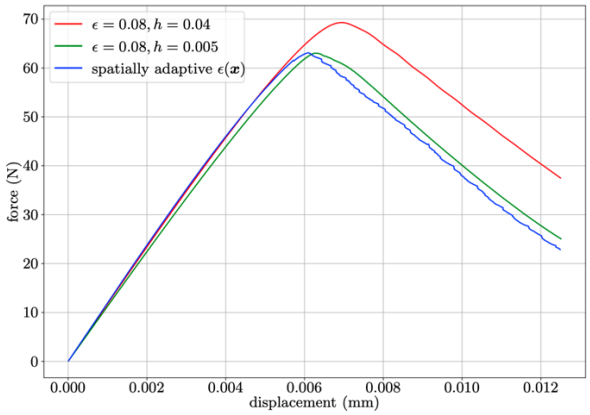



*Figure 40: Force vs. displacement plot for the splitting test.*

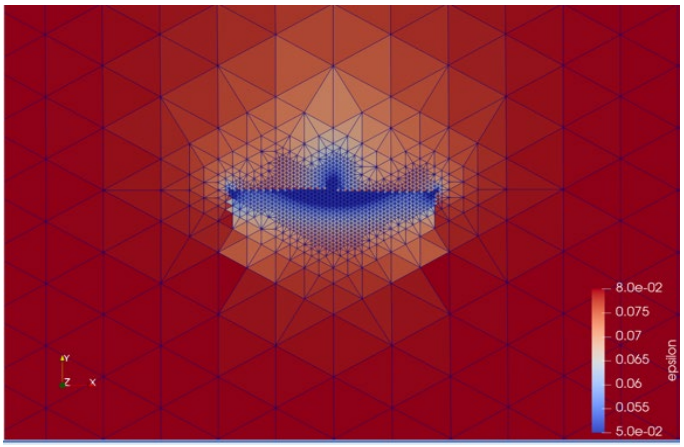



*Figure 41: Mesh refinement at un = 0.00002 and contour plot for the length variable ϵ(x) near the crack tip; blue and red regions represent small and large values of ϵ, respectively.*

## References

[1] D. Phansalkar, K. Weinberg, M. Ortiz, Michael and S. Leyendecker, “A spatially adaptive phase-field model of fracture,” Computer Methods in Applied Mechanics and Engineering, 395, 114880, 2022. https://doi.org/10.1016/j.cma.2022.114880

[2] A. Giacomini, “Approximation of Quasi-Static Evolution of Brittle Fractures,” Calculus of Variations and Partial Differential Equations, 22:129–172, 2005. https://doi.org/10.1007/s00526-004-0269-6

[3] H. Amor, J.-J. Marigo, C. Maurini, “Regularized formulation of the variational brittle fracture with unilateral contact: Numerical experiments,” Journal of the Mechanics and Physics of Solids, 57,1209–1229, 2009. https://doi.org/10.1016/j.jmps.2009.04.011

[4] C. Miehe, F. Welschinger and M. Hofacker, “Thermodynamically consistent phase-field models of fracture: Variational principles and multi-field FE implementations,” INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING, 83:1273–1311, 2010. https://doi.org/10.1002/nme.2861

[5] M. Ambati, T. Gerasimov, Laura De Lorenzis, “A review on phase-field models of brittle fracture and a new fast hybrid formulation,” Computational Mechanics, 55:383–405, 2014. https://doi.org/10.1007/s00466-014-1109-y

## P10: Nonlocal Degrading Interfaces in Continuum-Kinematics-Inspired Peridynamics

Marie Laurien, Ali Javili and Paul Steinmann

Peridynamics (PD) is a nonlocal continuum formulation that aims at bridging the gap between classical continuum mechanics and molecular dynamics. In PD, a length-scale is introduced into a continuum framework, defining the distance over which continuum points interact. The nonlocal interaction forces are determined by an integral over the neighbourhood of a point. In this manner, the peridynamic perspective captures nonlocal effects without the requirement of a molecular resolution. As an extension of the basic version of PD [1], continuum-kinematics-inspired peridynamics (CPD) [2] considers interactions between pairs, triplets and quadruplets of points.

In this nonlocal setting, damage can easily be incorporated by activating the breakage of a bond between two points once a critical bond stretch is exceeded. Since material interfaces might be weak and prone to damage, the goal of this work is to employ CPD to develop a model for nonlocal interfaces that allows for interfacial opening and damage. Based on our recent method presented in [3], our modelling approach relies on an interfacial region of finite thickness, where the subdomains overlap. Within this nonlocal interface, the peridynamic points are pairwise connected through interface bonding forces, cf. Figure 42. The bonding forces are governed by a force-opening law (FOL), which allows for assigning a characteristic opening and damage behaviour to the interface. To this end, a bilinear (cf. Figure 43), a polynomial, an exponential and a linear-exponential FOL are utilized. Moreover, the modelling of irreversible interfacial damage under cyclic loading is achieved through suitable unloading-reloading conditions. In order to be able to compare different FOLs, a damage variable is introduced that is based on the dissipated energy, since existing opening-, force- or energy-based damage measures are not applicable to all types of FOLs.

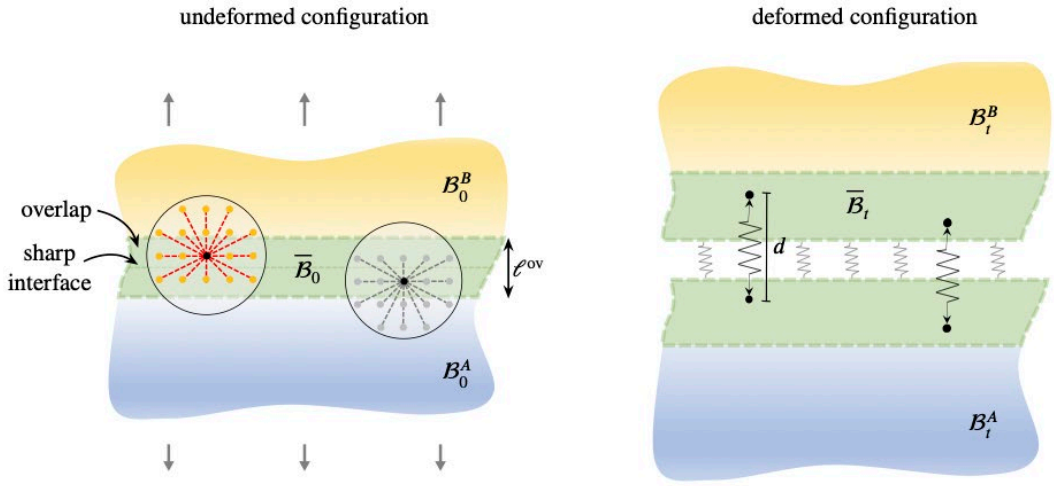



*Figure 42: Illustration of the nonlocal interface approach.*

In several parameter studies, the influence of the interfacial stiffness as well as the horizon size and the overlap size were investigated, especially to assess the effect of nonlocality on the material response. Figure 44 shows the effect of the size of the nonlocal interface on the interfacial damage of a sheared bilayer.

A major motivation of using PD is the investigation of nonlocal effects, which might not be negligible when analysing materials on small scales, such as nanocomposites. We therefore applied our interface model to a matrix-inclusion composite and assessed the effect of a nonlocal interface on the effective properties in several parameter studies [4]. Our results show that a higher degree of nonlocality is reflected in an increase of material stiffness and a growing influence of the interface, which highlights the importance of a nonlocal perspective when modelling composites on small scales.

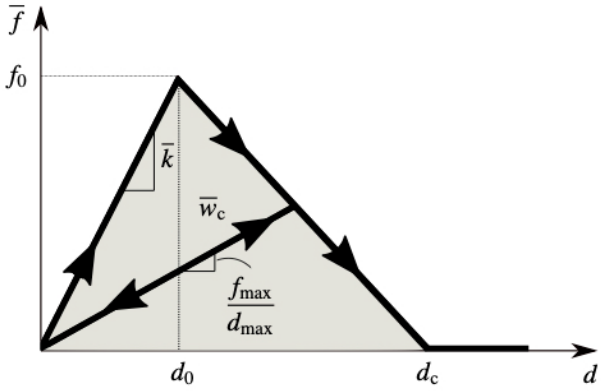



*Figure 43: Bilinear force-opening law.*

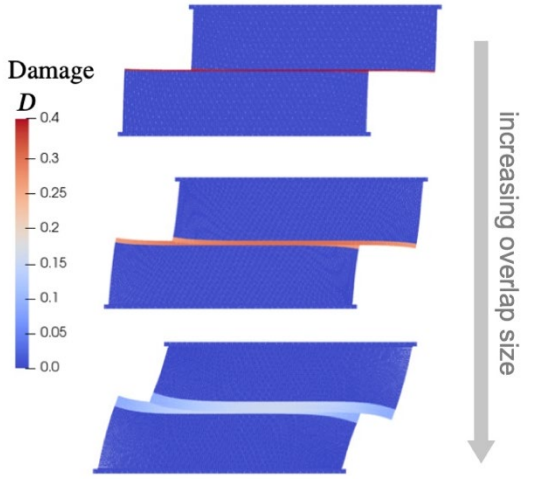



*Figure 44: Variation of the overlap size in a sheared bilayer.*

## References

[1] S. A. Silling, “Reformulation of elasticity theory for discontinuities and long-range forces,” Journal of the Mechanics and Physics of Solids, vol. 48 (1), pp. 175-209, 2000.

[2] A. Javili, A. T. McBride and P. Steinmann, “Continuum-kinematics-inspired peridynamics. Mechanical problems,” Journal of the Mechanics and Physics of Solids, 131, pp. 125-146, 2019.

[3] M. Laurien, A. Javili and P. Steinmann, “A nonlocal interface approach to peridynamics exemplified by continuum-kinematics-inspired peridynamics,” International Journal for Numerical Methods in Engineering, vol. 123 (5), pp. 3464-3484, 2022.

[4] M. Laurien, A. Javili and P. Steinmann, “Peridynamic modeling of nonlocal degrading interfaces in composites,” FRASCAL Special Issue in Forces in Mechanics, vol. 10, 100124, 2022.

## aPL: A Micromorphic Approach for Bone Density Adaption

Anna Titlbach, Paul Steinmann, Michael Stingl and Areti Papastavrou

This project builds on the work of Ina Schmidt (P10), who established the modelling and simulation of adaption processes in human bones under load considered on longer time scales. Age dependence, nutrient availability and the distinction between cortical and cancellous bone were identified as key factors of these processes in the prediction of density development, growth or degeneration in human bone; the modelling was refined accordingly [1,2,3]. In addition, an approach to simulating fracture healing has already been developed [4].

The present work addresses the issue of fracture healing with the aim of incorporating the flexoelectric effect into the modelling. This effect has been experimentally demonstrated in bone material [5] and generally occurs when a stress gradient builds up in a material due to inhomogeneous loading. It becomes particularly relevant at microcracks of bone, since high stress gradients act here when the bone is in motion. Due to these gradients, an electric field builds up around the crack tip. This effect is called flexoelectricity. The electric field then acts as a trigger for the osteoblasts to initiate the crack healing process.

With this background, the first step agreed upon for this year was to embed the classical bone remodelling approach in a micromorphic environment. This is necessary because, particularly in the classical theory of bone remodelling, bone is modelled at the macroscopic scale as continuous matter with a local approach; thus, the microstructure of bone is not taken into account. However, this becomes relevant when the material is considered at small scales, which becomes necessary when mechanisms at a fracture tip are studied.

Based on [6], a successful implementation of the micromorphic approach was carried out, the model was validated, and a large number of studies with different geometries, parameter sets, and loading types were performed to properly describe fundamental effects. Finally, the new approach was applied to a femur. Figure 45 shows how the density in a femoral head evolves under load after a certain simulation time when the classical and the micromorphic approaches are used, respectively.

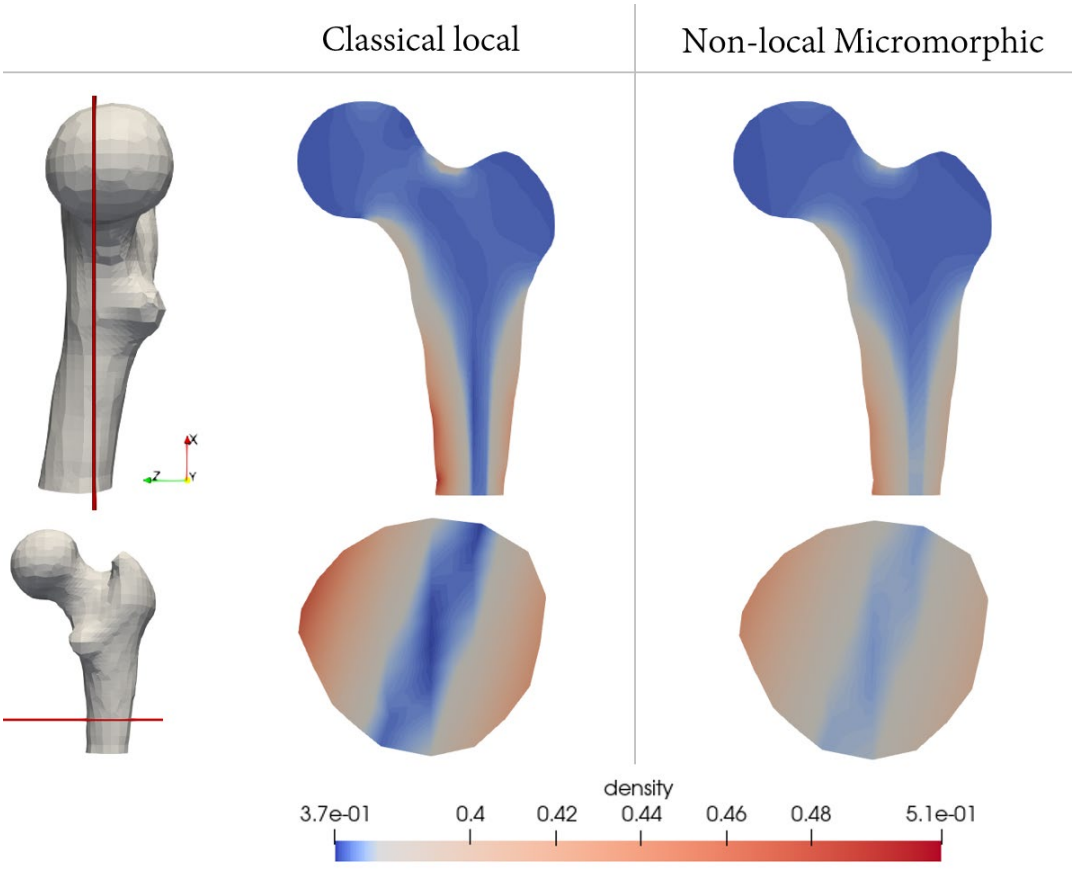



*Figure 45: Comparison of the classical local and the micromorphic approach based on the density distribution in a femoral head.*

Due to the perpendicular load transferred from the hip to the hip joint, the femur experiences a compressive load on the inner side and a tensile load on the outer side of the bone, as also described in the schematic in Figure 46. It can be seen that the micromorphic approach in this scenario produces a more homogeneous density distribution than the classical approach. This also manifests itself in a higher stiffness of the bone. Within the micromorphic approach, the interaction between the continuum points can be influenced. The size of the microcontinuum and the coupling between micro- and macro-deformation can be used to control how strong this interaction is.

For the examination of microcracks in bone, we use a cantilever beam representing a bone specimen from the femoral neck region. Since the femoral head is subjected to a bending load, as explained earlier, this represents a reasonable approximation of the loading conditions, see Figure 46.

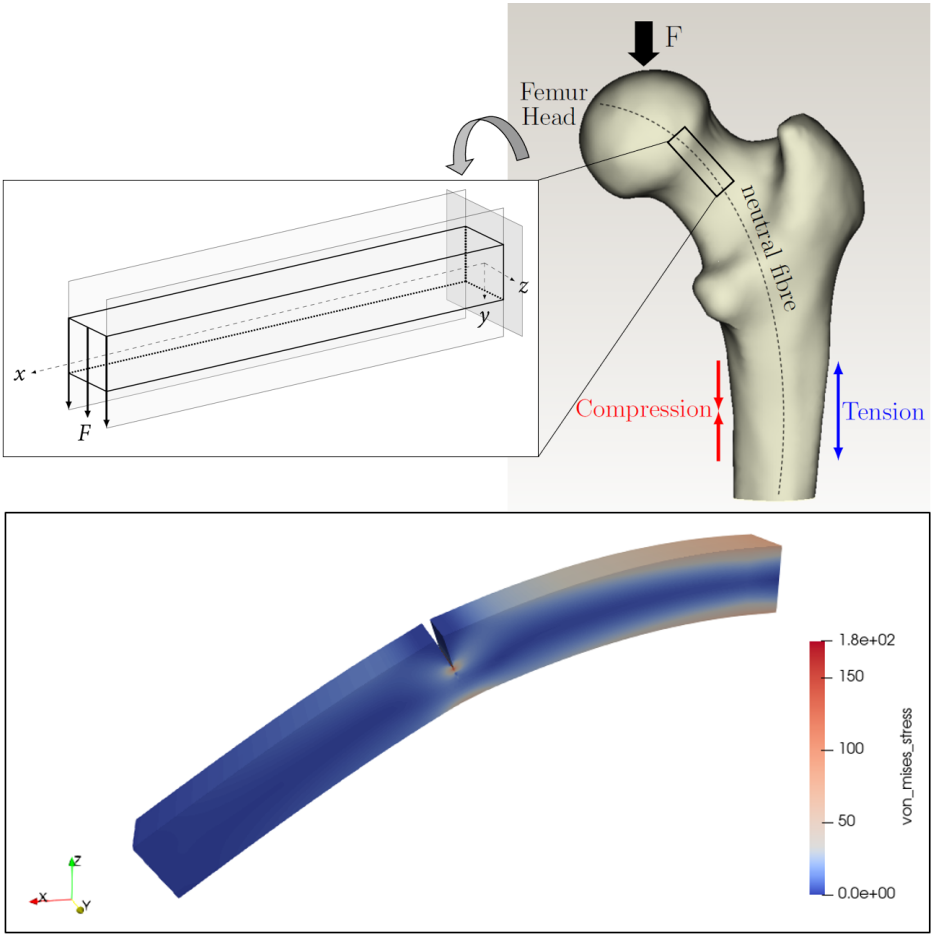



*Figure 46: Modelling of a cantilever beam as a bone specimen in the region of the femoral neck to study the mechanisms at a crack tip.*

When a bone specimen is modelled as an ordinary cantilever beam, bone density increases only at the top and bottom of the beam; the neutral fibre experiences almost no density gain. In the case of a beam with a crack, as shown in Figure 46, particularly high stresses occur at the crack tip, resulting in a significant increase in density. At this point, the increased stress gradients are also expected to initiate the flexoelectric effect. For this reason, a flexoelectric contribution will also be included in the modelling in order to obtain a better understanding of the healing processes in human bone.

**References**

1. Papastavrou A et al., Journal of Biomechanics, 103:109701 (2020)
2. Papastavrou A et al., CMBBE, 23:432–444 (2020)
3. Schmidt I et al., CMBBE, 24:1274-1212 (2021)
4. Schmidt I et al., CMBBE; 25:1040-1050 (2022)
5. Vasquez-Sancho F et al., Advanced Materials, 30:1705316 (2018)
6. McBride AT et al., Comp. Methods in Applied Mechanics and Engineering; 371:113320 (2020)

## P11: Stochastic Optimization with High Dimensional Uncertainties with Application to Fracture Control

Lennart Igel, Julia Mergheim and Michael Stingl

### Motivation

In the past approaches to fracture optimisation, which were based on discontinuous crack models, e.g. Cohesive Zone Models, only certain sets of crack paths could be considered, the choices usually being restricted in different ways or required additional heuristics in the modelling, e.g. no crack branching and initiation during the propagation being possible or the crack propagation being restricted to prescribed crack paths [1]. Such restrictions, which arise due to the treatment of the crack as a discontinuity in the domain, are overcome in the so-called Phase Field Model, first proposed by Bourdin and Francfort in [3] as a regularized version of the energy minimization in the Griffith model, introducing a smooth variable parametrizing the crack set. Diffusing the crack discontinuity over the domain in this way allows for modelling of more complex types of cracks without any further prior heuristics or restrictions during the simulation [2]. This allows for more flexibility in the choice of fracture types and opens up a wide range of problem classes to which a general fracture optimization framework based on Phase Field simulations could be applied.

However, some uncertainties either inherent to crack evolution or due to properties of the model remain. Fracture evolution can show unstable behaviour with regard to design changes, e.g. snapping between configurations, which manifest themselves in discontinuities of the objective functional and cause the problem to become ill-posed [4]. This complicates the application of conventional optimisation procedures, as they rely on gradient information, which might not exist at these points of discontinuity, however. For these cases the problem needs some regularization, e.g. stochastic methods can be used to approximate a stochastic gradient by smoothing it over a surrounding area in which the function is differentiable [5].

### Objectives

To lay the basic groundwork, the first major objective was to develop an optimisation framework with which crack paths described by Phase Fields can be optimised in a mathematically rigorous way with regard to design, e.g. material properties. To tackle this issue, I first considered how different regularisations and numerical parameters affect the crack propagation under the Phase Field model and how the interplay between different parameters influences the solution. In the next step I then determined a set of suitable design parameters, as well as derived the sensitivities of the objective functional with regard to said parameters and employing these sensitivities I have already implemented a design optimization scheme using a standard gradient descent method.

This framework will form the basis for the second major objective, a conditional stochastic gradient method I plan to develop in the future. This conditional stochastic method is constructed similar to a general stochastic optimization method. However, instead of approximating the gradient in each step by performing an integration with a derivative kernel over the sampled space, which becomes very expensive especially for high-dimensional design spaces, the idea is to use as much of the available deterministic sensitivities as possible. By using some condition on when the gradient does not exist or becomes unreliable, e.g. when near a bifurcation point, this approach would be much less expensive especially in high dimension. Additionally, we are working on a method, to use only a lower dimensional integration when a discontinuity is actually encountered, that would remove costly high dimensional integrals in general.

Thus, a criterion is needed to determine when the derivative of the objective functional does not exist or becomes unreliable, e.g. when passing bifurcation or unstable states during the fracture evolution. To determine a suitable criterion, I started by considering a simple tracking for the condition number of the system matrix of the state equation solved during the crack evolution. This should indicate whether a solution is unique and if not unique then indicate the stability of the solution with regard to the minimization of local energy.

However, the behaviour of eigenvalues during a fracture evolution in the Phase-Field Model can be somewhat nebulous and difficult to understand. Hence, to form a clearer understanding, I set up simple discrete spring models, which form easy to understand one-dimensional analogues, and compare them with the continuous phase field setting in two dimensions. For these simple spring models,

the stable and unstable states can be analytically determined and the eigenvalue evolution easily compared between the two for similarities in behaviour to and thus to gain a better understanding of how the system in the continuous case behaves.

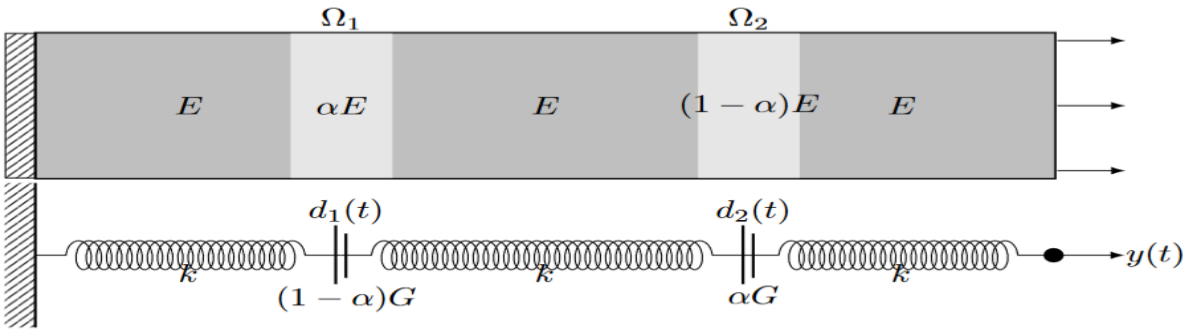



*Figure 47: Setup for the spring models and the two-dimensional analogue. The spring model has two interfaces, whose strength is governed by design parameter alpha in (0,1) and a load is applied to the right side of it while being fixed on the left. The two-dimensional analogue is a long rectangular plate, which has two subdomains symmetric to the centre, on which the material strength is weaker, the strength again being governed by alpha, and strain is applied on the right side, while being fixed on the left.*

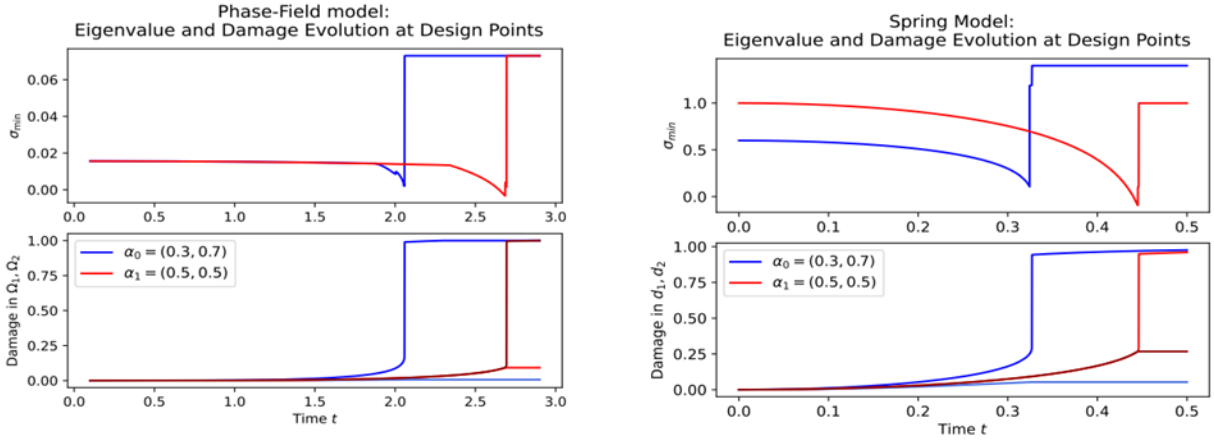



*Figure 48: Plot of the evolution of the eigenvalues and damage in the subdomains/interfaces over time for both models for two selected designs. Note that for both models the eigenvalues decrease in size while approaching critical breakage and then jump back to the initial starting size once one section of the plate/interface is fully broken.*

## References

[1] S. Singh, M. Stingl, L. Pflug: *Material optimization to enhance delamination resistance of composite structures using viscous regularization* (2021) Computer Methods in Applied Mechanics and Engineering 382 113881

[2] J. Y. Wu, V. P. Nguyen, C. T. Nguyen, D. Sutula, S. Sinaie, S. P. Bordas: *Phase-field modeling of fracture* (2020) Advances in applied mechanics 53 1-183

[3] B. Bourdin, G. A. Francfort, J. J. Marigo: *The variational approach to fracture* (2008) Journal of elasticity 91 5-148

[4] T. Gerasimov, U. Römer, J. Vondřejc, H.G. Matthies, L. De Lorenzis: *Stochastic phase-field modeling of brittle fracture: computing multiple crack patterns and their probabilities* (2020) Computer Methods in Applied Mechanics and Engineering 372 113353

[5] S. Singh, J. Mergheim, M. Stingl, L. Pflug: Robust design optimization for enhancing delamination resistance of composites (2022), International Journal for Numerical Methods in Engineering

## P12: Modelling Bond Breaking Processes from Small to Large Epoxy Networks by QM and Hybrid QM/MM Strategies

Christian R. Wick, Sampanna Pahi and Ana-Sunčana Smith

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

This year, we established the onset of spin contamination within the framework of unrestricted Kohn-Sham density functional theory as ultimate criterion to identify bond rupture in molecular compounds. This was based on both one- and two-dimensional Constraint Geometries simulate external force calculations (COGEF) with small model compounds, as well as molecular dynamics based in silico tensile tests on large cured DGEBA/DDS epoxy networks.

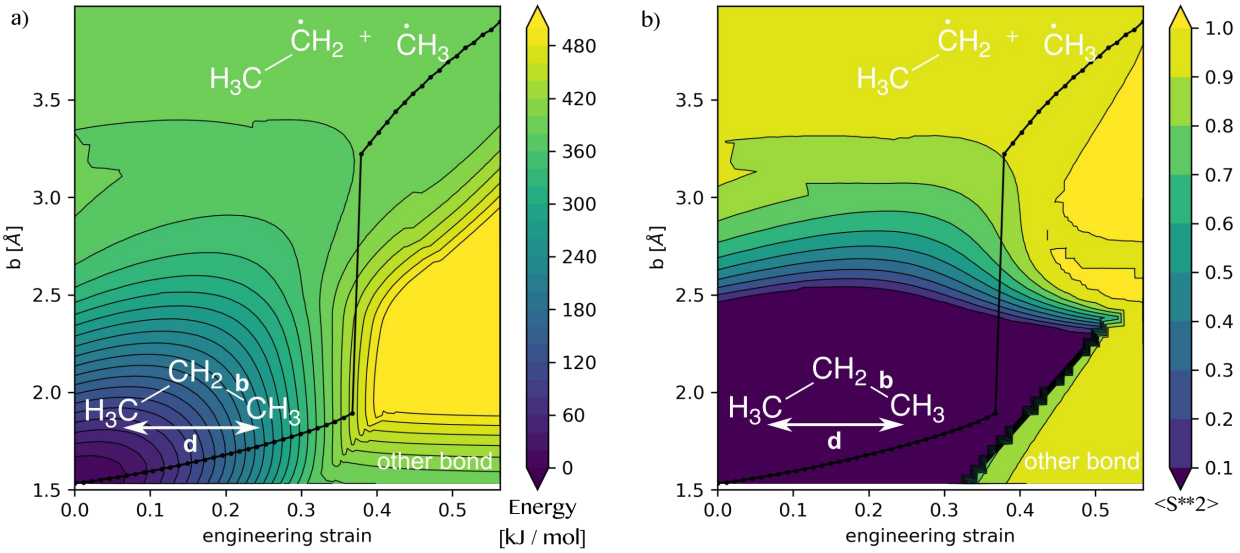



*Figure 49: 2D-Cogef profiles obtained for propane. The outermost carbon atoms were used as COGEF coordinate d. One of the outer carbon-carbon bonds (b) was increased at all points along the COGEF coordinate. The energy is plotted in a) while the square of expectation value of the spin operator is plotted in b). The 1D-COGEF curve is indicated as black line.*

Our COGEF calculations where conducted with our cogef.py tool [1]. While the predicted scission products obtained with the one-dimensional COGEF approximation were validated against experimental expectations [2], we performed a more detailed evaluation of the method at various levels of theory. Using model compounds to investigate the influence of an external force on covalent and non-covalent backbones, and mechanophores, we revealed the strong method and conformation dependence of the 1D-COGEF approach, which questioned its real predictive character [3,4]. Nevertheless, a 2D approach elucidates the complex nature of the molecular response to stretching. As indicated in Figure 49 for the example of propane, the 1D COGEF profile follows the “unbroken states” until ~ 3.7% of strain and the jumps to the broken state. This is accompanied by breaking the spin symmetry of the converged unrestricted wavefunction to obtain a diradical state as indicated by the plot of the square of the expectation value of the spin operator. We, therefore, use this drastic increase of the expectation value of the spin squared operator as a direct quantum mechanical indicator that the bond is broken at the molecular mechanics level. This is the necessary criterion as delineated in our previous reports to be utilized in our large-scale QM/MM approach to model epoxy fracture via MD simulations.

Our envisaged QM/MM hybrid scheme is exemplified in Figure 50a) using *in silico* MD based tensile tests of DGEBA/DDS. A more detailed summary of the procedure can be found in [5]. In short, we conduct a tensile test with molecular mechanics-based description of DGEBA/DDS using our own block chemistry derived force field [6,7]. Harmonic bonding terms were replaced by Morse potentials to allow the onset of bond breaking. At frequent intervals, the simulation is stopped, and the bond length of all backbone bonds is checked to identify bonds exceeding a previously set criterion 1. Consequently, our program chemBreak.py creates a suitable QM/MM subsystem for all selected bonds (which fulfil criterion 1), to conduct ONIOM type QM/MM single point calculations on-the-fly.

Those QM/MM calculations are used to check for criterion 2, the presence of a diradical state in the ONIOM subsystems via computing <S**2> by means of stability analysis at the QM level. If this test is successful, the bond will be selected as broken and the open valences can be quenched with hydrogen atoms to simulate the expected radical chain reactions following such a force induced bond rupture. A representative stress-strain plot is shown in Figure 50b), which utilized an empirically estimated value for criterion 1 based on 1D-COGEF calculations on model compounds reflecting the entire backbone bonding of our epoxy resin. Currently, we are optimizing criterion 1 by running intensive brute-force calculations investigating all backbone bonds along predefined intervals during in silico tensile tests with smaller systems. This will allow us to identify the optimal criteria 1 to initiate a QM/MM calculation to identify the broken bonds reducing the number of unnecessary tests (false positives) and minimizing the risk to miss a bond which was already broken but not identified as such in our simulations.

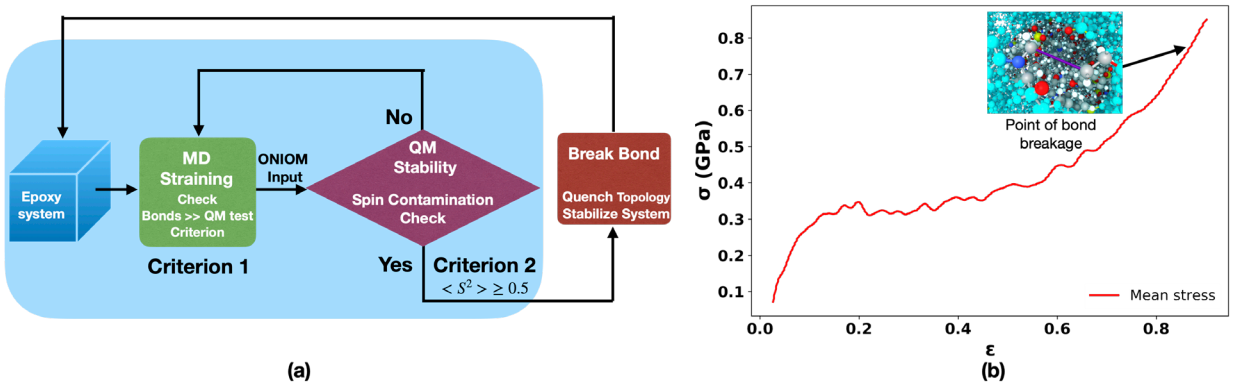



*Figure 50: a) Adaptive concurrent modelling of Bond Rupture events during in silico tensile tests. b) Example stress-strain plot of an in silico tensile test with our model epoxy resin (127000 atoms) at a strain rate of $2 \times 10^{-8} Å/fs$ following the scheme presented in a). First bond rupture was detected at a strain of 97 %.*

## References

[1] C.R. Wick, E. Topraksal, D.M. Smith, A.-S. Smith, cogef.py: Tools to run COnstraint Geometries simulate External Force calculations, (2022). https://doi.org/10.5281/ZENODO.7079733.

[2] I.M. Klein, C.C. Husic, D.P. Kovács, N.J. Choquette, M.J. Robb, Validation of the CoGEF Method as a Predictive Tool for Polymer Mechanochemistry, J. Am. Chem. Soc. 142 (2020) 16364–16381. https://doi.org/10.1021/jacs.0c06868.

[3] C.R. Wick, E. Topraksal, D.M. Smith, A.-S. Smith, Evaluating the predictive character of the method of Constrained Geometries Simulate External Force with Density Functional Theory., FRASCAL Special Issue in Forces in Mechanics, vol. 9, 100143, 2022. https://doi.org/10.1016/j.finmec.2022.100143.

[4] C.R. Wick, E. Topraksal, D.M. Smith, A.-S. Smith, Evaluating the predictive character of the method of Constrained Geometries Simulate External Force with Density Functional Theory., Zenodo - Dataset. (2022). https://doi.org/10.5281/ZENODO.6948605.

[5] S. Pahi, Modelling mechanochemical bond scission of Epoxy resins under stress, Master Thesis. (2022).

[6] M. Livraghi, S. Pahi, P. Nowakowski, D.M. Smith, C.R. Wick, A.-S. Smith, Block chemistry for accurate modeling of epoxy resins, Chemistry, 2022. https://doi.org/10.26434/chemrxiv-2022-d5cwr.

[7] M. Livraghi, S. Pahi, P. Nowakowski, D.M. Smith, C.R. Wick, A.-S. Smith, Block chemistry for accurate modeling of epoxy resins, (2021). https://doi.org/10.5281/ZENODO.5795936.

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

Bakul Mathur and Daniel Koehn

The primary objective of this research is to develop a multiscale approach to study fragmentation of grains and development of deformation bands in geological rock formations. Deformation bands are formed as a response to localized compression, shear and/or dilation stresses in porous rocks sandstones and sediments [1]. The study can be divided into three phases: (1) single grain fragmentation, (2) multiple grain fragmentation, (3) large scale deformation. The research is currently in the transitioning phase from the single grain fragmentation stage to multiple grain stage.

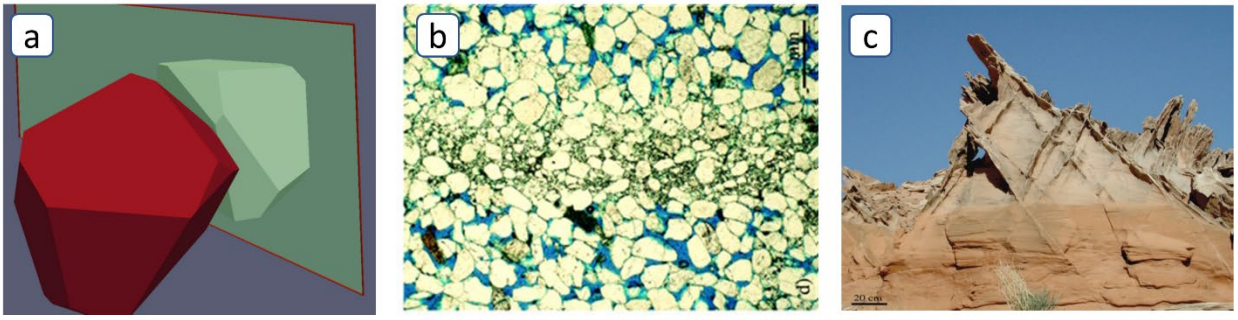



*Figure 51: Project phases (a) single grain fragmentation, (b) Photomicrograph of a single cataclastic deformation band [1], and (c) an example of large-scale deformation band system in Entrada Sandstone, Utah [2].*

Grain failure in rocks can be caused by many reasons, such as compressive loading, shear displacement, thermal, hydraulic or chemical effects [3]. For a realistic model, polyhedral shaped grains are considered in this project. The single grain fragmentation is realised with the Mohr-Coulomb approach, which is a classical failure criterion for brittle particle systems [4]. The failure criterion is combined with the Weibull statistical distribution that captures the grain size effect [5]. The simulations are carried out with an open-source discrete numerical modelling framework YADE [6]. It has been observed that the energy required for grain failure increases with a decrease in particle size during the fragmentation process [5]. The following section summarises the combined Mohr-Coulomb-Weibull failure criterion as described by Gladky and Kuna [5].

The Mohr-Coulomb failure criterion in terms of the minimum principal stress ($\sigma_3$), maximum principal stress ($\sigma_1$) and the shear stress ($\sigma_T$) applied at the grain can be summarized as followed:

$$\text{Failure}\begin{cases}\text{compression: } (\sigma_1 < 0) \text{ and } (\sigma_3 < 0) \text{ and } (\sigma_3 < -\sigma_{CD}), \text{ or} \\ \text{tension: } (\sigma_1 > 0) \text{and } (\sigma_3 > 0) \text{ and } (\sigma_1 > \sigma_{CZ}), \text{ or} \\ \text{shear: } (|\sigma_T| > |\sigma_{CZ}|)\end{cases} \tag{1}$$

where $\sigma_{CD}$ is the maximal uniaxial compressive strength and $\sigma_{CZ}$ is the maximal uniaxial tensile strength of the given material. The minimum and maximum principal stresses are calculated by an eigenvalue analysis of the average constant stress tensor given by

$$\sigma_{ij} = \frac{1}{V}\sum_{c=1}^{n_c} l^{(c)} \otimes f^{(c)} \tag{2}$$

where $l^{(c)}$ is the contact position vector, $f^{(c)}$ is the contact force, V is the particle volume, and $n_c$ is the number of active contacts. The size effect can be taken into account with the Weibull probability distribution.

$$P = 1 - \exp\left(-\frac{V}{V_0}\left(\frac{\sigma_{eff}}{\sigma_0}\right)^m\right) \tag{3}$$

where P denotes the failure probability, m represents the Weibull modulus which is generally taken as 3 for brittle geological materials [5], $V_0$ is a representative reference volume, at which the Weakest-Link-Theory is valid, $\sigma_{eff}$ denotes the effective stress which differs for different failure modes: it is $\sigma_{CD}$ for compression, $\sigma_{CZ}$ for tension and $\sigma_{CZ}$ for shear failure case. The failure plane is set to go through the mass centroid of the particle and it coincides with the plane of maximum shear stress with the orientation ($n_{split}$) calculated with the help of unit vectors corresponding to the maximum ($l_{max}$) and minimum ($l_{min}$) components of the principal stress axes.

$$n_{split} = (I_{max} + I_{min})/2 \quad (4)$$

The implementation of the above described numerical scheme in YADE was also validated by Gladky and Kuna [5] showing a qualitative agreement with the experimentally observed particle size distribution.

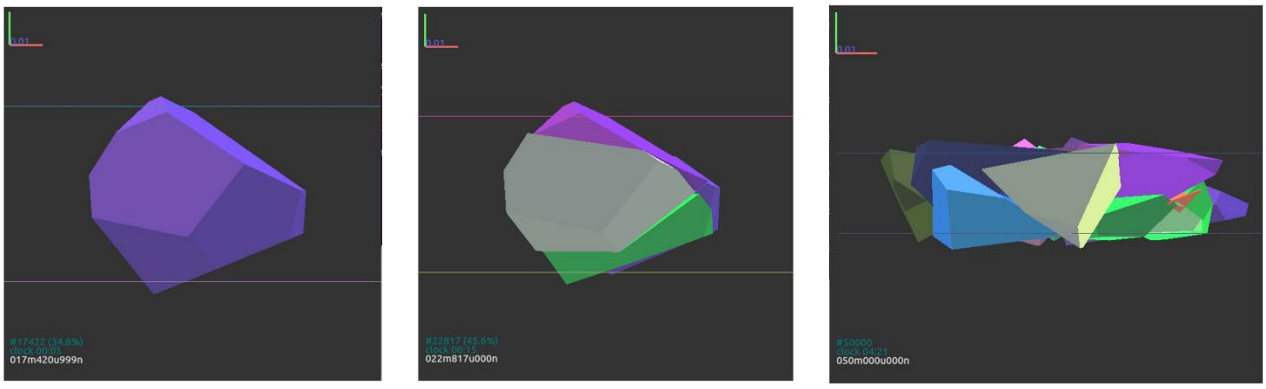


*Figure 52: Progressive fragmentation of polyhedral grain model with Mohr-Coulomb-Weibull approach. Simulation carried out with the open source application YADE [6].*

The second phase of the project deals with a multiple grain model simulated with discrete element method (DEM) combined with the Mohr-Coulomb-Weibull concept. The DEM method consists of the equations of motion and linear elastic contact model [6]. The up-scaling parameters such as rock permeability and density after fragmentation will be determined in the second phase of the project. In the third phase of the project, a reservoir scale continuum model will be simulated with the help of Finite Element Method (FEM).

**References**

[1] H. Fossen, R. A. Schultz, Z. K. Shipton and K. Mair, “Deformation bands in sandstone: a review”, Journal of the Geological Society, London, vol. 164, pp. 1-15, 2007.

[2] H. Fossen, A. Bale, “Deformation bands and their influence on fluid flow”, AAPG Bulletin, vol. 91, no. 12, pp. 1685-1700.

[3] Yupeng Jiang, Hans J. Herrmann, Fernando Alonso-Marroquin, "A boundary-spheropolygon element method for modelling sub-particle stress and particle breakage", Computers and Geotechnics, Volume 113, pp. 103087, 2019.

[4] J. F: Labuz, F. Zeng, R. Makhnenko, Y. Li, “Brittle failure of rock: a review and general linear criterion”, Journal of Structural Geology, vol. 112, pp. 7-28, ISN 0191-8141, 2018.

[5] A. Gladky, M. Kuna, “DEM simulation of polyhedral particle cracking using a combined Mohr–Coulomb–Weibull failure criterion”, Granular Matter, vol. 19, pp. 41, doi. 19. 41. 10.1007/s10035-017-0731-8, 2017.

[6] V. Šmilauer et al., Yade Documentation 3rd ed, The Yade Project, doi. 10.5281/zenodo.5705394, 2021.

## aPM Modelling Geothermal Systems in Faulted and Fractured Media

### Homogenising fracture networks from outcrop and investigating scale relationships

Ruaridh Smith and Daniel Koehn

### General Motivation and Aims

Geothermal energy is becoming a much sought-after renewable energy resource, especially as governments and corporations are transitioning away from traditional sources such as oil and gas. Germany is no different and finding alternatives to gas in heating homes and businesses is at the forefront (e.g., Weber *et al.,* 2020). Current projects within Germany focus on the geothermal potential in Bavaria and utilising the high heat flows within both high and low permeable (K) reservoirs (Schulz *et al.,* 2013). In Northern Bavaria (Franconia) there are two target reservoirs; Muschelkalk (Triassic) and Malm (Jurassic) which are both low permeable carbonates (e.g., Freitag *et al.,* 2022) In these types of reservoirs, fractures form the primary mechanism for fluid flow and therefore understanding the interactions of the fractures within the network is vital for geothermal production.

Subsurface data (borehole and seismic), which can be used to determine and model fracture properties, are limited in Northern Bavaria. Outcrop analogues (surface quarries) can be especially useful for detecting and measuring fracture properties within geological formations which can be target reservoirs also found at depth. Outcrop data can then be integrated into larger models through upscaling workflows.

The primary aims of this research is to better develop workflow to upscale outcrop data to aid in geothermal simulations of the reservoirs in the Bamberg region. This workflow includes calculating permeability tensors (2D to 3D) which will drive the simulations. A secondary aim from this project is investigating scale relationships from outcrop data and how fracture permeability varies with scale.

### Methodology and Data Collection

Fracture data has been collected from the Jurassic Malm Formation within two quarries (Kirchleus and Oberachtel). Data collection comprised of fracture measurements (azimuth and dip angle; aperture) and imaging (photogrammetry and LiDAR). 2D geometric fracture analysis from the photogrammetry can provide additional fracture network properties, such as fracture density/intensity, connectivity and variations in fracture orientations. Furthermore, using this data, 2D fracture networks can be meshed (GMSH) for simulations. Using REDBACK (part of the MOOSE Framework) fluid flow simulations can be undertaken to calculate the average fluid velocities within the 2D fracture network. These values can then be used to determine the overall 2D permeability tensor for the network.

The tensor workflow forms the main methodology for the scale relationship study. 2D fractured sections from Oberachtel quarry were analysed at different scales (e.g., 1mx1m; 5mx5m; 10mx10m). The permeability tensor for each scale is calculated to compare the difference in the permeability. It is expected that at certain scale the tensors will begin to match.

### Permeability Tensors

The results from the permeability tensors (Figure 53) calculated from the fracture networks in Kirchleus Quarry show a variation in orientation and magnitude of permeability. The variation can be attributed to a nearby fault (Kulmbach Fault) which is influencing the fracture networks. Site 1 (Figure 53) shows a strong orientation parallel to the orientation of the main fault. This influence subsides

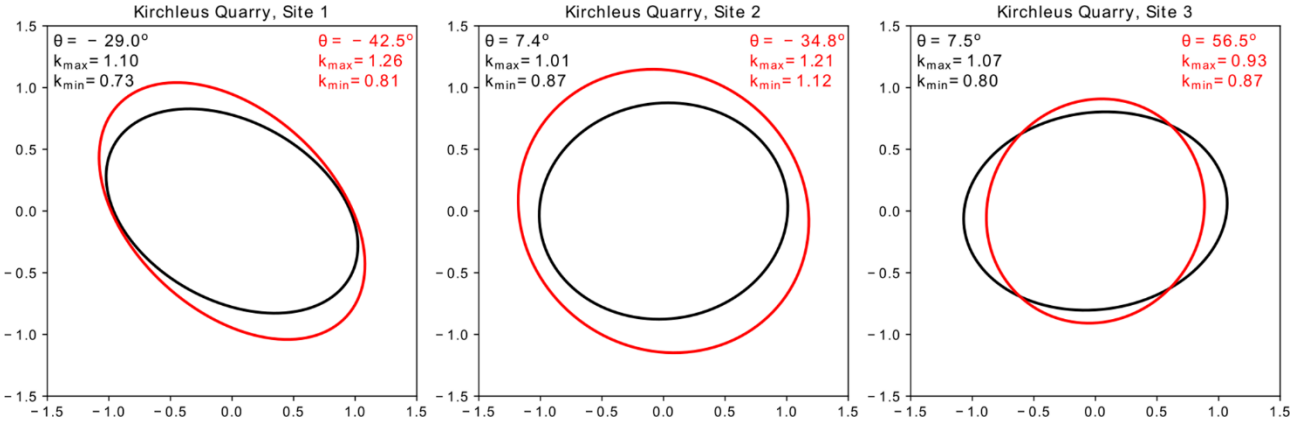



*Figure 53: Calculated permeability ellipses from the tensor workflow using data from Kirchleus Quarry (Smith et al., 2022).*

away from the fault zone in Sites 2 and 3. The Kulmbach Fault is a seismic scale fault and as such can be identified from subsurface data. Understanding the influence these large-scale faults have on the fractures networks as observed in Kirchleus.

An additional study of the permeability tensors shows that varying individual fracture aperture based on field observations can influence the tensor at larger scales and therefore accurately estimated aperture will be important in future studies.

Additional information on methodology, results and discussion can be found in Smith *et al.* (2022).

**Scale Relationship Investigation**

A supplementary investigation is currently being undertaken on the new data from the quarries to understand variations in the tensors at different scales. Using 2D fractured cliff sections from Oberachtel Quarry (NE Nürnberg), tensors are calculated using different sized sampling windows (2.5m x 2.5m; 5m x 5m; 10m x 10m; 25m x 25m). The aim is to investigate how the tensor varies across the scales and at what scale does the tensor become constant (little to zero variation), i.e., the network becomes constant. As part of the workflow, addition aperture modelling is also being applied to the fracture modelling and therefore the several sections of the code are being updated to allow for this. An example of the tensor variation can be observed in Figure 54 where we can see how the tensor orientation changes from the small scale to the larger scale.

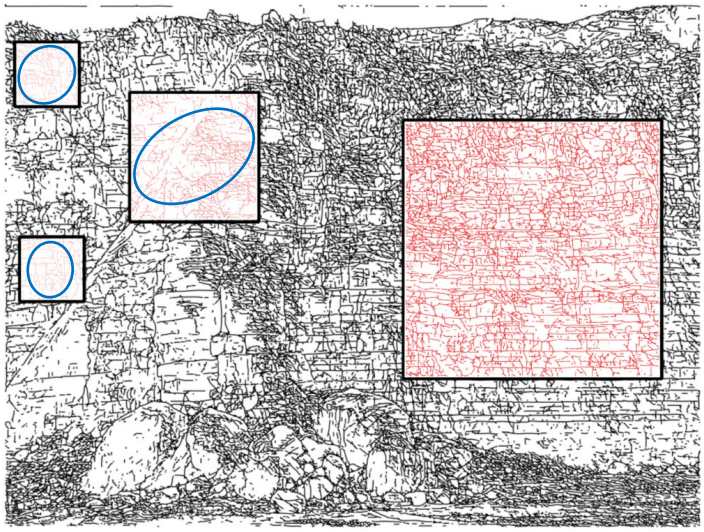


*Figure 54: Variation in permeability tensor across different scales from a 2D quarry section.*

**Future Work and Collaborations**

The planned work for 2023 includes developing a method to calculate 3D permeability tensors. This will be undertaken through generating stochastic fracture models and integrating multiple 2D slices together to calculate “pseudo” 3D tensors. Once this process is working we plan to test on multiple quarry sites.

During summer 2023, a further field season will be undertaken to gather more data from quarries, outcrops and caves. Drone and LiDAR photogrammetry will be used to capture 3D fracture data from quarries and caves, including generating 3D models of open quarries. Integrating the data from multiple sites will aid in modelling a larger scale model for geothermal simulations.

There is a developing project planned for the upcoming year with FRASCAL P4 and aPC where fractures and natural fracturing mechanisms will be investigated using X-ray tomography.

**References**

[1] Freitag, S., Klaver, J., Malai, I. S., Klitzsch, N., Urai, J. L., Stollhofen, H., ... & Schmatz, J. (2022). Petrophysical characterization, BIB-SEM imaging, and permeability models of tight carbonates from the Upper Jurassic (Malm ß), SE Germany. *Geothermal Energy*, *10*(1), 1-45.

[2] Schulz et al. (2013). Geothermieatlas zur Darstellung möglicher Nutzungskonkurrenzen zwischen CCS und Tiefer Geothermie. Endbericht, LIAG, Hannover.

[3] Smith, R. Y., Lesueur, M., Kelka, U., Poulet, T., & Koehn, D. (2022). Using fractured outcrops to calculate permeability tensors: implications for geothermal fluid flow and the influence of seismic-scale faults. *Geological Magazine*, 1-17.

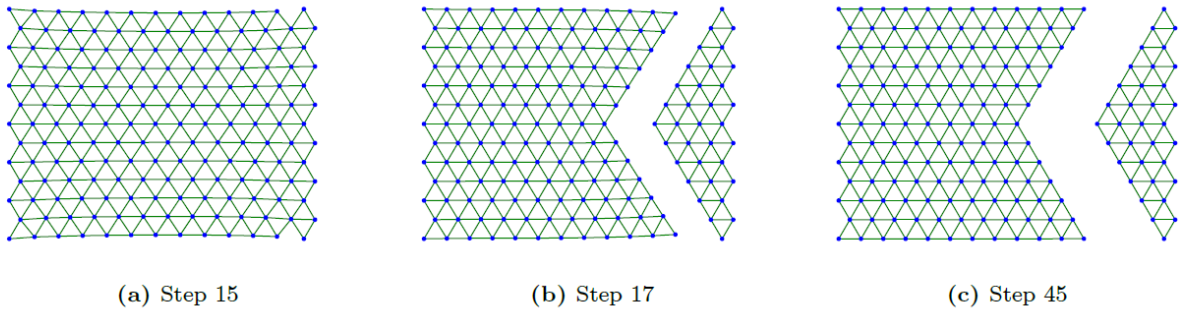
[4] Weber, J., Born, H., Pester, S., & Moeck, I. (2020). Geothermal Energy Use in Germany, Country Update 2015–2019. In *Proceedings of the World Geothermal Congress*.

## P14: Atomistic-to-Continuum Passage for Crack Growth

Joscha Seutter and Manuel Friedrich

One major challenge in materials science is to identify critical loads for failure of brittle materials and to determine the geometry and the time evolution of crack paths in the fractured regime. Ever since the groundbreaking work of Francfort and Marigo [5], a natural mathematical framework for theoretical studies is given by so-called free discontinuity problems, where displacements and crack paths are determined from an energy minimization principle. To justify these models on the continuum level one aims for rigorous results that relate the free discontinuity problem to minimization problems on the atomistic level. This is usually done by means of Gamma-convergence, which is a variational convergence that ensures convergence of minimizers of a series of energy-functionals to the minimizer of the limit energy [3]. However, for the dynamic case, i.e., the investigation of crack evolution in time, an understanding of the connection between atomistic and continuum systems is completely missing.

Our goal is therefore to establish existence of an atomistic continuous–time evolution and relate it rigorously to continuum quasi-static evolutions [1] by means of evolutionary Gamma-convergence for rate-independent systems. To get accustomed with the problem, I spent the first couple of weeks reading carefully the two papers [1] and [3], which we want to combine in some sense. For the first step, namely the existence of an atomistic quasi-static evolution, we then tried to carefully adapt the procedure from [1] to the atomistic setting. One delicate issue was finding a suitable irreversibility condition for "broken interactions" on the atomistic level. In fact, we incorporated the maximal opening memory variable, which was used in [4] for the passage from cohesive-to-brittle quasi-static crack evolutions, in the simple nearest-neighbour model that was used in [2]. However, we ran into some difficulties trying to prove that the global stability condition of such a model is preserved in the time-continuous limit. We noticed that one fundamental problem lies in the definition of the “brokenness”-criterion for a spring in the atomistic mass-spring model. Instead of assuming that one spring switches abruptly from the elastic to the broken state we introduced a small transition area, where the memory variable already comes into play, but the elastic energy of the spring still plays a role. Thus, we were able to overcome this technical issue by a slight change of the model, that we believe is also physically quite reasonable.



(a) Step 15 (b) Step 17 (c) Step 45

*Figure 55: Evolution for horizontal stretching.*

Another issue was the missing continuity of the memory variable with respect to the time-step variable. Due to the lacking uniform convergence of the deformation, the memory variable is only semi-continuous and therefore the passage to global stability in the limit cannot be achieved. Nonetheless, another change of the model, namely adding a viscosity term to the considered energy, overcame this problem and lead to a mathematically sound description of an atomistic crack dynamics. Furthermore, the arisen issues don’t apply to the atomistic-to-continuum case but are rather inherent of the atomistic setting and would vanish if one passes to the continuum-limit simultaneously. We hence were able to prove an existence result for atomistic quasi-static crack growth, by passing to the limit in a time-discrete minimizing movement scheme. Interestingly, this leads to a delay-differential equation depending on the complete history of the deformation at previous times. We furthermore conducted numerical experiments for the prediction of quasi-static crack evolution in particle systems.

Here, we implemented the incremental minimizing movement scheme that we also used for the existence proof. Although our model potentially captures a wide variety of possible atomic interactions and lattice structures, we focused on simulations for a triangular lattice in 2D and nearest-neighbours as well as next-to-nearest neighbours interactions. The numerical computations were performed via an interior point optimizer accessed through the JuMP modelling language [8]. Figure 55 shows one exemplary simulation, where we investigated the behaviour of the model for horizontal stretching and observed that the crack line is formed along crystallographic lines but still can be kinked, which is in accordance with analytical results from [2]. We also considered a model variant, where the L2-dissipation is replaced by a dissipation that corresponds to a model in the Kelvin-Voigt's rheology and compared these two numerically. For more details see [6], where we also briefly commented on a possible enhancement of the model to three-body interaction potentials.

As a next step we want to investigate the atomistic-to-continuum limit of such two-dimensional mass-spring models and derive the corresponding continuum models by means of evolutionary Gamma-convergence. The plan is to adapt the arguments of the Gamma-convergence result from [3] for an energy that includes the maximum memory variable that we used before. For simplicity, we are now only considering the antiplane case, i.e., scalar valued deformations. The main difficulty lies in the transfer of the irreversibility condition to the limiting energy. More precisely, one has to ensure the global stability of a unilateral minimality condition on the energy. We hope to make use of the results from [7], where the authors addressed these issues in a very general setting and adapt and apply their techniques to our problem.

**References**

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

[2] M. Friedrich, B. Schmidt: *An atomistic-to-continuum analysis of crystal cleavage in a two-dimensional model problem* (2014) J. Nonlin. Sci. **24** 145-183

[3] M. Friedrich, B. Schmidt: *On a discrete-to-continuum convergence result for a two-dimensional brittle material in the small displacement regime* (2015) Netw. Heterog. Media **10** 321-342

[4] A. Giacomini: *Size effects on quasi-static growth of cracks* (2005) SIAM J. Math. Anal. **36** 1887-1928

[5] G. A. Francfort, J. J. Marigo: *Revisiting brittle fracture as an energy minimization problem* (1998) J. Mech. Phys. Solids **46** 1319-1342

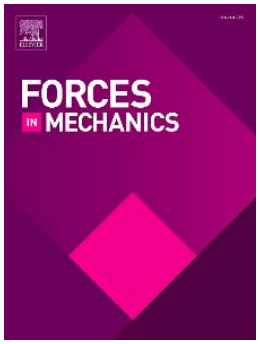
[6] Rufat Badal, Manuel Friedrich, Joscha Seutter: *Existence of quasi-static crack growth in atomistic systems* FRASCAL Special Issue in Forces in Mechanics, vol. 9, p. 100138, 2022.

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

[8] I. Dunning, J. Huchette, M. Lubin: *JuMP: A Modeling Language for Mathematical Optimization*. SIAM Review 59(2) (2017), 295-320.

## 2.2 Publications

### 2.2.1 Articles in peer-review journals, peer-reviewed contributions to conferences or anthology volumes, and book publications




In 2022, FRASCAL was organising a special issue on “Fracture across Scales” in the Elsevier journal “Forces in Mechanics” (https://www.sciencedirect.com/journal/forces-in-mechanics). The editors-in-chief of “Forces in Mechanics” ensure scientific quality assurance at the highest level. The special issue consists of around a dozen peer-reviewed contributions (highlighted in pink in the publication lists below) that will highlight the most important research success of the FRASCAL projects. As of December 2022, eleven manuscripts have already been accepted, most of which are already published with open access. Some further submissions are currently under review. The special issue is scheduled to appear in early 2023.

FRASCAL’s participants in the list of publications are highlighted as follows:

| | |
|---|---|
| **Doctoral Researcher (DR)** | **associated Doctoral Researcher (aDR)** |
| **Postdoctoral Researcher (PDR** | **associated Postdoctoral Researcher aPDR** |
| Principal Advisor (PA) | Co-Principal Advisor (PA) |
| *Mercator Fellow (MF)* | |

(in alphabetical order)

| | |
|---|---|
| 1 | R. Badal, M. Friedrich and **J. Seutter**, “Existence of quasi-static crack evolution for atomistic systems,“ FRASCAL Special Issue in Forces in Mechanics, vol. 9, 100138, 2022. https://doi.org/10.1016/j.finmec.2022.100138 |
| 2 | **C. Bauer**, **M. Ries** and S. Pfaller, “Accelerating molecular dynamics simulations by a hybrid molecular dynamics-continuum mechanical approach,” Soft Materials, vol. 20 (4), pp. 428-443, 2022. https://doi.org/10.1080/1539445X.2022.2061513 |
| 3 | **N. Esfandiary**, M. Zaiser and P. Moretti, “Statistical aspects of interface adhesion and detachment of hierarchically patterned structures,“ Journal of Statistical Mechanics: Theory and Experiment, vol. 2022 (2), p. 023301, 2022. https://doi.org/10.1088/1742-5468/ac52a4 |
| 4 | F. Font-Clos, M. Zanchi, **S. Hiemer**, S. Bonfanti, R. Guerra, M. Zaiser and S. Zapperi, “Predicting the failure of two-dimensional silica glasses,“ Nature communications, vol. 13 (1), p. 1–11, 2022. https://doi.org/10.1038/s41467-022-30530-1 |
| 5 | **S. Hiemer**, H. Fan and M. Zaiser, “Relating plasticity to dislocation properties by data analysis: scaling vs. machine learning approaches,“ Mater Theory, vol. 7 (1), 2023 https://doi.org/10.1186/s41313-022-00050-y |
| 6 | **S. Hiemer**, P. Moretti, S. Zapperi and M. Zaiser, “Predicting creep failure by machine learning - which features matter?,“ FRASCAL Special Issue in Forces in Mechanics , vol. 9, 100141, 2022. https://doi.org/10.1016/j.finmec.2022.100141 |
| 7 | Y. Jain, **M. Ries**, S. Pfaller and F. Müller-Plathe, “Addressing Surface Effects at the Particle-Continuum Interface in a Molecular Dynamics and Finite Elements Coupled 45Multiscale Simulation Technique,“ Journal of Chemical Theory and Computation, vol. 1846 (4), p. 2375–2387, 2022. https://doi.org/10.1021/acs.jctc.1c00940 |
| 8 | **J. Konrad**, P. Moretti and D. Zahn, “Molecular Simulations and Network Analyses of Surface/Interface Effects in Epoxy Resins: How bonding adapts to boundary conditions,“ Polymers, vol. 14(19), 4069; 2022. https://doi.org/10.3390/polym14194069 |
| 9 | **J. Konrad**, S. Pfaller and D. Zahn, “Multi-Scale Modelling of Plastic Deformation, Damage and Relaxation in Epoxy Resins,“ Polymers, vol. 14 (16), p. 3240, August 2022. https://doi.org/10.3390/polym14163240 |
| 10 | **P. Kumar**, P. Steinmann and J. Mergheim, “A graded interphase enhanced phase-field approach for modeling fracture in polymer composites,” FRASCAL Special Issue in Forces in Mechanics, vol. 9, 100135, 2022. https://doi.org/10.1016/j.finmec.2022.100135 |

| | |
|---|---|
| 11 | **M. Laurien**, A. Javili and P. Steinmann, "A nonlocal interface approach to peridynamics exemplified by continuum-kinematics-inspired peridynamics," International Journal for Numerical Methods in Engineering, vol. 123 (15), pp. 3464-3484, 2022. https://doi.org/10.1002/nme.6975 |
| 12 | **M. Laurien**, A. Javili and P. Steinmann, "Peridynamic modeling of nonlocal degrading interfaces in composites," FRASCAL Special Issue in Forces in Mechanics, vol.10, 100124, 2023 https://doi.org/10.1016/j.finmec.2022.100124 |
| 13 | **T. Lakshmipathy**, P. Steinmann and E. Bitzek, "LEFM is agnostic to geometrical nonlinearities arising at atomistic crack tips," FRASCAL Special Issue in Forces in Mechanics, vol. 9, 100127, 2022. https://doi.org/10.1016/j.finmec.2022.100127 |
| 14 | **D. Phansalkar**, **D. B. Jadhav**, K. Weinberg, *M. Ortiz*, S. Leyendecker, "Extension of the spatially adaptive phase-field model to various forms of fracture," FRASCAL Special Issue in Forces in Mechanics, vol. 10, 100161, 2023 https://doi.org/10.1016/j.finmec.2022.100161 |
| 15 | **D. Phansalkar**, K. Weinberg, *M. Ortiz* and S. Leyendecker, "A spatially adaptive phase-field model of fracture," Computer Methods in Applied Mechanics and Engineering, vol. 395, p. 114880, 2022. https://doi.org/10.1016/j.cma.2022.114880 |
| 16 | M. Qu, J. Fang, C. Mu, Y. Li, S. Huang, L. Han, **S. Hiemer**, W. Xu and Y. Qin, "A novel study on the sandwich-structure strain sensor using ethylene-vinyl acetate-based hot-melt adhesive mesh web: Fabrication, properties, and modelling," Journal of Applied Polymer Science, vol. n/a, No. n/a p. e53209, 2022. https://doi.org/10.1002/app.53209 |
| 17 | **M. Ries**, **C. Bauer**, **F. Weber**, P. Steinmann and S. Pfaller, "Characterization of the material behavior and identification of effective elastic moduli based on molecular dynamics simulations of coarse-grained silica," Mathematics and Mechanics of Solids, p. 108128652211080, 2022. https://doi.org/10.1177/10812865221108099 |
| 18 | **M. Ries**, J. Seibert, P. Steinmann and S. Pfaller, "Applying a generic and fast coarse-grained molecular dynamics model to extensively study the mechanical behavior of polymer nanocomposites," Express Polymer Letters, vol.16, No.12 1304–1321, 2022. https://doi.org/10.3144/expresspolymlett.2022.94 |
| 19 | **M. Ries**, **F. Weber**, G. Possart, P. Steinmann and S. Pfaller, "A quantitative interphase model for polymer nanocomposites: Verification, validation, and consequences regarding size effects," Composites Part A: Applied Science and Manufacturing, vol. 161, p. 107094, 2022. https://doi.org/10.1016/j.compositesa.2022.107094 |
| 20 | **M. Rohracker**, **P. Kumar**, J. Mergheim: "A comparative assessment of different adaptive spatial refinement strategies in phase-field fracture models for brittle fracture", FRASCAL Special Issue in Forces in Mechanics, vol. 10, 100157, 2023. https://doi.org/10.1016/j.finmec.2022.100157 |
| 21 | **J. Ritter**, **S. Shegufta**, P. Steinmann and M. Zaiser, "An energetically consistent surface correction method for bond-based peridynamics," FRASCAL Special Issue in Forces in Mechanics, vol. 9, 100132, 2022. https://doi.org/10.1016/j.finmec.2022.1001322 |
| 22 | **I. Schmidt**, J. Albert, M. Ritthaler, A. Papastavrou and P. Steinmann, "Bone fracture healing within a continuum bone remodelling framework," Computer Methods in Biomechanics and Biomedical Engineering, vol. 25 (9), pp. 1040–1050, 2022. https://doi.org/10.1080/10255842.2021.1998465 |
| 23 | **R. Y. Smith**, M. Lesueur, U. Kelka, T. Poulet and D. Koehn, "Using fractured outcrops to calculate permeability tensors: implications for geothermal fluid flow and the influence of seismic-scale faults," Geological Magazine, pp. 1–17, 2022. https://doi.org/10.1017/S0016756822000309 |
| 24 | **S. Singh**, L. Pflug, J. Mergheim and M. Stingl, "Robust design optimization for enhancing delamination resistance of composites (2022)," International Journal for Numerical Methods in Engineering , vol. n/a, no. n/a. https://doi.org/10.1002/nme.7168 |
| 25 | **L. Spannraft**, G. Possart, P. Steinmann, J. Mergheim: "Generalized interfaces enabling macroscopic modeling of structural adhesives and their failure," FRASCAL Special Issue in Forces in Mechanics, vol. 9, 100137, 2022. https://doi.org/10.1016/j.finmec.2022.100137 |
| 26 | S. Trishin, **T. Müller**, D. Rolf, C. Lotze, P. Rietsch, S. Eigler, B. Meyer and K. J. Franke, "Resolution of Intramolecular Dipoles and a Push-Back Effect of Individual Molecules on a Metal Surface," The Journal of Physical Chemistry C, vol. 126, p. 7667–7673, 2022. https://doi.org/10.1021/acs.jpcc.2c00334 |

| | |
|---|---|
| 27 | **F. Weber**, **M. Ries**, **C. Bauer**, **C. R. Wick**, S. Pfaller, “On equilibrating non-periodic molecular dynamics samples for coupled particle-continuum simulations of amorphous polymers,“ FRASCAL Special Issue in Forces in Mechanics, vol. 10, 100159, 2023. https://doi.org/10.1016/j.finmec.2022.100159 |
| 28 | **C. R. Wick**, E. Topraksal, D. M. Smith and A.-S. Smith, “Predicting mechanochemical reactivity with the method of Constrained Geometries Simulate External Force,“ FRASCAL Special Issue in Forces in Mechanics, vol. 9, 100143, 2022. https://doi.org/10.1016/j.finmec.2022.100143 |
| 29 | P. Wolf, **C. R. Wick**, J. Mehler, D. Blaumeiser, S. Schötz, T. Bauer, J. Libuda, D. Smith, A.-S. Smith and M. Haumann, “Improving the Performance of Supported Ionic Liquid Phase Catalysts for the Ultra-Low-Temperature Water Gas Shift Reaction Using Organic Salt Additives,“ ACS catalysis, vol. 12 (9), p. 5661–5672, 2022. https://doi.org/10.1021/acscatal.1c05979 |

Forces in Mechanics 9 (2022) 100138

Contents lists available at ScienceDirect

Forces in Mechanics

journal homepage: www.sciencedirect.com/journal/forces-in-mechanics

# Existence of quasi-static crack evolution for atomistic systems

Rufat Badal [a], Manuel Friedrich [a, b], Joscha Seutter [a, c, *]

[a] Department of Mathematics, Friedrich-Alexander Universität Erlangen-Nürnberg, Cauerstr. 11, Erlangen D-91058, Germany
[b] Mathematics Münster, University of Münster, Einsteinstr. 62, Münster D-48149, Germany
[c] Competence Unit for Scientific Computing (CSC), Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), Germany

ARTICLE INFO

*Keywords:*
Atomistic systems
Delay differential equations
Minimizing movements
Quasi-static crack growth
Irreversibility condition

ABSTRACT

We consider atomistic systems consisting of interacting particles arranged in atomic lattices whose quasi-static evolution is driven by time-dependent boundary conditions. The interaction of the particles is modeled by classical interaction potentials where we implement a suitable irreversibility condition modeling the breaking of atomic bonding. This leads to a delay differential equation depending on the complete history of the deformation at previous times. We prove existence of solutions and provide numerical tests for the prediction of quasi-static crack growth in particle systems.

## 1. Introduction

The theory of brittle fracture is based on the fundamental idea that the formation of cracks may be seen as the result of the competition between the elastic bulk energy of the body and the work needed to produce a new crack. Despite its long history in mechanics dating back to [1], a rigorous mathematical formulation of the problem is much more recent: in the variational model of quasi-static crack growth proposed in [2], displacements and crack paths are determined from an energy minimization principle, reflecting suitably the three foundational ingredients of Griffith's theory: (1) a surface energy associated to discontinuities of the deformation, (2) a propagation criterion for those surfaces, and (3) an irreversibility condition for the fracture process.

The mathematical well-posedness of the variational model [2] has been the subject of several contributions over the last two decades, see e. g. [3–6]. The proof of continuous-time evolutions is based on approximation by time-discretized versions resulting from a sequence of minimization problems of so-called Griffith functionals, being variants of the Mumford and Shah functional [7]. Functionals of this type comprising elastic bulk contributions for the sound regions of the body and surface terms along the crack have been studied extensively in the last years in the natural weak framework of special functions of bounded variation. We refer to [8] for a thorough overview of the variational approach to fracture. In particular, it has been shown that such continuum models can be identified as effective limits derived from atomistic systems as the interatomic distance tends to zero [9–11]. Asymptotic analysis of this kind is notoriously difficult, and is not based on simply taking pointwise limits but rather on a variational convergence, called Γ-convergence [12], which in this setting ensures convergence of minimizers of the atomistic system to the ones of the continuum problem.

Although studies on atomistic-to-continuum passages are flourishing, most results are static and the evolutionary nature of processes is mostly neglected. Our goal is to advance this understanding by establishing a rigorous connection between atomistic and continuum models in brittle fracture for the prediction of quasi-static crack growth. In this contribution, we perform the first step in this direction by setting up a suitable quasi-static model on the atomistic level respecting the irreversibility condition of Griffith's theory. The passage to continuum models of quasi-static crack growth will be discussed in a forthcoming work [13].

We consider atomistic systems consisting of interacting particles arranged in an atomic lattice occupying a bounded region representing the reference domain of a material. The interaction of the atoms is modeled by classical potentials in the frame of Molecular Mechanics, e. g. by Lennard-Jones potentials. Based on an energy minimization principle, the deformation of the particles is driven by time-dependent boundary conditions. This leads to an evolution of gradient-flow type. Whereas the study of interacting particles motion is classical, the novelty of our contribution lies in implementing an irreversibility condition along the evolution. As long as the length of interactions does not exceed a certain threshold, interactions are considered to be 'elastic' and can recover completely after removal of loading. Otherwise, interactions are supposed to be 'damaged', and the system is affected at the present and all future times. Here, we suitably adapt the maximal opening memory

* Corresponding author at: Department of Mathematics, Friedrich-Alexander Universität Erlangen-Nürnberg, Cauerstr. 11, Erlangen D-91058, Germany.
*E-mail addresses:* rufat.badal@fau.de (R. Badal), manuel.friedrich@fau.de (M. Friedrich), joscha.seutter@fau.de (J. Seutter).

https://doi.org/10.1016/j.finmec.2022.100138
Received 29 July 2022; Received in revised form 27 October 2022; Accepted 28 October 2022
Available online 5 November 2022

SOFT MATERIALS
2022, VOL. 20, NO. 4, 428–443
https://doi.org/10.1080/1539445X.2022.2061513



# Accelerating molecular dynamics simulations by a hybrid molecular dynamics-continuum mechanical approach

Christof Bauer, Maximilian Ries, and Sebastian Pfaller

Institute of Applied Mechanics, Department of Mechanical Engineering, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

**ABSTRACT**

In this contribution, molecular dynamics (MD) simulations in combination with continuum mechanical (CM) approaches are performed to investigate particle movements under uniaxial deformations of an amorphous polymer at particle resolution. A coarse-grained (CG) model of atactic polystyrene is used as an exemplary model system. We propose a hybrid molecular dynamics-continuum mechanical (MD-CM) approach to simulate the deformation behavior of the polymer. As a reference, purely molecular dynamics systems are used. The methods are compared with regard to the local displacement of the particles and the global stress-strain behavior of the overall system. The good reproducibility of the system's mechanical behavior with the hybrid molecular dynamics-continuum mechanical method is shown. Furthermore, it is demonstrated that CPU time can be significantly reduced with the hybrid calculation model.

**ARTICLE HISTORY**
Received 22 October 2021
Accepted 30 March 2022

**KEYWORDS**
Continuum mechanics; molecular dynamics simulation; simulation of polymers; polystyrene; deformation simulation

## Introduction

### *Multiscale Simulations of Polymers*

Polymers offer great potential since their properties can be tailored to specific applications. A major challenge is the numerical investigation of polymers particularly in the case of inhomogeneities as they appear, e.g., in polymer composites or polymer fracture problems. From an engineering point of view, the material response under mechanical loadings is of specific interest, which requires a holistic consideration to capture the large range of resolutions involved. In order to appropriately describe the overall macroscopic material behavior, mechanisms at atomistic scales have to be taken into account, but should be confined only to those regions that are of particular relevance in order to constrain the computational effort. In this regard, so-called domain decomposition techniques are well-suited to run multiscale simulations at a reasonable computational cost, where only distinguished parts have to be treated at atomistic resolution, cf. e.g. Ref. [1]The remaining regions, which should be as large as possible, use coarse-scale techniques as, e.g., continuum mechanics at a significantly less computational cost.

In the simplest case, the regions to be considered at fine and coarse resolution are defined a priori, i.e., are based on expectations about the loadings they will be exposed to in the subsequent deformation procedure. This, however, requires knowledge about how deformation evolves throughout the entire system and which parts will be higher or lower strained. In the case of fracture simulations, a complex strain state occurs, which renders the a priori definition impossible. Figure 1 shows one of our first multiscale studies of polymer fracture,[2] in which we choose a particle-based resolution in the vicinity of the crack tip and a much coarser continuum-based treatment elsewhere. For these simulations, we use our domain decomposition "Capriccio" method, whose original version has been introduced and further developed by our group in recent years, cf. Refs. [3–7] The Capriccio method couples a continuum, described by the finite element method (FEM), with a particle-based domain relying on molecular dynamics (MD) and employing stochastic boundary conditions.[8] Aside from polymer fracture as referred to here, it has shown its capabilities in the context of polymer nanocomposites.[9–12]

As evident from fracture investigations in general, the highest loads appear near the crack tip, such that they will move throughout the domain according to the crack propagation. In this case, it is desirable to introduce adaptivity and to select computationally expensive fine-scale regions based on the effective load they are exposed to. In this concept, the coarse-scale description can be kept wherever only low strains occur, such that significant parts of the deformation history could be described

CONTACT Christof Bauer christof.bauer@fau.de Institute of Applied Mechanics Friedrich-Alexander Universität Erlangen-Nürnberg Germany
Supplemental data for this article can be accessed on the publisher's website

OPEN ACCESS

Journal of Statistical Mechanics: Theory and Experiment
An IOP and SISSA journal

PAPER: Disordered systems, classical and quantum

# Statistical aspects of interface adhesion and detachment of hierarchically patterned structures

**Nosaibeh Esfandiary, Michael Zaiser and Paolo Moretti***

Department of Materials Science, Friedrich-Alexander Universität Erlangen-Nürnberg, WW8-Materials Simulation, Dr Mack-Str. 77, 90762 Fürth, Germany
E-mail: paolo.moretti@fau.de

Received 21 December 2021
Accepted for publication 27 January 2022
Published 24 February 2022

Online at stacks.iop.org/JSTAT/2022/023301
https://doi.org/10.1088/1742-5468/ac52a4

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

**Keywords:** fracture, elasticity

*Author to whom any correspondence should be addressed.



1742-5468/22/023301+18$33.00

J. Stat. Mech. (2022) 023301

nature COMMUNICATIONS

ARTICLE

https://doi.org/10.1038/s41467-022-30530-1 OPEN

# Predicting the failure of two-dimensional silica glasses

Francesc Font-Clos[1,4], Marco Zanchi[1,4], Stefan Hiemer[2,4], Silvia Bonfanti[1,3], Roberto Guerra[1], Michael Zaiser[2] & Stefano Zapperi[1,2,3]✉

Being able to predict the failure of materials based on structural information is a fundamental issue with enormous practical and industrial relevance for the monitoring of devices and components. Thanks to recent advances in deep learning, accurate failure predictions are becoming possible even for strongly disordered solids, but the sheer number of parameters used in the process renders a physical interpretation of the results impossible. Here we address this issue and use machine learning methods to predict the failure of simulated two dimensional silica glasses from their initial undeformed structure. We then exploit Gradient-weighted Class Activation Mapping (Grad-CAM) to build attention maps associated with the predictions, and we demonstrate that these maps are amenable to physical interpretation in terms of topological defects and local potential energies. We show that our predictions can be transferred to samples with different shape or size than those used in training, as well as to experimental images. Our strategy illustrates how artificial neural networks trained with numerical simulation results can provide interpretable predictions of the behavior of experimentally measured structures.

[1] Center for Complexity and Biosystems, Department of Physics, University of Milan, via Celoria 16, 20133 Milan, Italy. [2] Institute of Materials Simulation, Department of Materials Science Science and Engineering, Friedrich-Alexander-University Erlangen-Nuremberg, Dr.-Mack-Str. 77, 90762 Fürth, Germany. [3] CNR - Consiglio Nazionale delle Ricerche, Istituto di Chimica della Materia Condensata e di Tecnologie per l'Energia Via R. Cozzi 53, 20125 Milan, Italy. [4] These authors contributed equally: Francesc Font-Clos, Marco Zanchi, Stefan Hiemer. ✉email: stefano.zapperi@unimi.it

Hiemer *et al. Materials Theory* (2023) 7:1
https://doi.org/10.1186/s41313-022-00050-y

Materials Theory

RESEARCH Open Access

# Relating plasticity to dislocation properties by data analysis: scaling vs. machine learning approaches

Stefan Hiemer[1], Haidong Fan[2] and Michael Zaiser[1*]

*Correspondence:
michael.Zaiser@fau.de

[1] Department of Materials Science, WW8-Materials Simulation, Friedrich-Alexander Universität Erlangen-Nürnberg, Dr.-Mack-Str. 77, 90762 Fürth, Germany
[2] Department of Mechanics, Sichuan University, Chengdu, People's Republic of China

**Abstract**

Plasticity modelling has long relied on phenomenological models based on ad-hoc assumption of constitutive relations, which are then fitted to limited data. Other work is based on the consideration of physical mechanisms which seek to establish a physical foundation of the observed plastic deformation behavior through identification of isolated defect processes ('mechanisms') which are observed either experimentally or in simulations and then serve to formulate so-called physically based models. Neither of these approaches is adequate to capture the complexity of plastic deformation which belongs into the realm of emergent collective phenomena, and to understand the complex interplay of multiple deformation pathways which is at the core of modern high performance structural materials. Data based approaches offer alternative pathways towards plasticity modelling whose strengths and limitations we explore here for a simple example, namely the interplay between rate and dislocation density dependent strengthening mechanisms in fcc metals.

**Keywords:** Dislocation plasticity, Scaling invariance, Machine learning

## Introduction

Plasticity modelling has long proceeded along two independent lines. On the one hand, engineers are seeking tools to predict the behavior of engineering components during processing and under in-service loads. In this case, the material is assumed as given and the task is to predict, based on available experimental data, as accurately as possible the behavior of this material within complex-shaped parts with equally complex boundary loadings. This has led to phenomenological models which seek, often with an abundance of parameters, to reproduce a set of experimental data as accurately as possible. The task of these models is to reproduce the behavior of a given material under a typically rather limited range of deformation conditions, and in meeting this task they often achieve an impressive degree of accuracy. Their predictive power beyond the material and range of deformation conditions for which they have been parametrized, on the other hand, is extremely limited. Therefore, materials scientists tasked with the development of new and improvement of existing materials tend to use a different approach. By analysing deformation on the level of the defect microstructure, they seek to identify the physical

Forces in Mechanics 9 (2022) 100141

Contents lists available at ScienceDirect

Forces in Mechanics

journal homepage: www.sciencedirect.com/journal/forces-in-mechanics

# Predicting creep failure by machine learning - which features matter?

Stefan Hiemer [a], Paolo Moretti [a], Stefano Zapperi [a,b,c], Michael Zaiser [*,a]

[a] Institute of Materials Simulation, Department of Materials Science Science and Engineering, Friedrich-Alexander-University Erlangen-Nuremberg, Dr.-Mack-Str. 77, Fürth 90762, Germany
[b] Center for Complexity and Biosystems, Department of Physics, University of Milan, via Celoria 16, Milan 20133, Italy
[c] CNR - Consiglio Nazionale delle Ricerche, Istituto di Chimica della Materia Condensata e di Tecnologie per l'Energia, Via R. Cozzi 53, Milan 20125, Italy

ARTICLE INFO

*Keywords:*
Fracture
Machine learning
Random fuse model
Subcritical failure

ABSTRACT

Spatial and temporal features are studied with respect to their predictive value for failure time prediction in subcritical failure with machine learning (ML). Data are generated from simulations of a novel, brittle random fuse model (RFM), as well as elasto-plastic finite element simulations (FEM) of a stochastic plasticity model with damage, both models considering stochastic thermally activated damage/failure processes in disordered materials. Fuse networks are generated with hierarchical and nonhierarchical architectures. Random forests - a specific ML algorithm - allow us to measure the feature importance through a feature's average error reduction. RFM simulation data are found to become more predictable with increasing system size and temperature. Increasing the load or the scatter in local materials properties has the opposite effect. Damage accumulation in these models proceeds in stochastic avalanches, and statistical signatures such as avalanche rate or magnitude have been discussed in the literature as predictors of incipient failure. However, in the present study such features proved of no measurable use to the ML models, which mostly rely on global or local strain for prediction. This suggests the strain as viable quantity to monitor in future experimental studies as it is accessible via digital image correlation.

## 1. Introduction

Creep failure is an example of a subcritical failure process, where an applied load which is insufficient to instantaneously break the sample drives time dependent damage accumulation. This gradual accumulation of damage deteriorates the strength of the material and ultimately results in delayed failure [1].

It is in general unfeasible to design structures in such a manner as to avoid the damage processes that lead to subcritical failure. Predicting the residual lifetime of a structure under subcritical load is therefore an important issue that is actively investigated by both physicists and engineers. Reliable lifetime predictions may help to avoid catastrophic in-service failure of components and systems and harness substantial economic benefits by adapting and where possible extending replacement cycles.

To assist prediction, it is desirable to obtain sample specific information about the damage accumulation process through non destructive means. Such information can be obtained from the macroscopic sample response, i.e., the time dependent creep strain or strain rate as accessible by surface monitoring. Additional and more detailed information can be drawn from analysis of the spatio-temporal pattern of energy releases as local creep damage accumulates, as microcrack formation is accompanied by elastic energy release which can be recorded by monitoring the acoustic emission (AE) of the sample.

Several empirical approaches have been proposed to predict sample specific failure times from macroscopic creep strain data. The simplest possible approach is to correlate the time $t_m$ of minimum strain rate with the catastrophic failure time $t_f$, in the simplest case by assuming a linear relationship between both [2,3]. A variant consists in relating the failure time to the duration of the primary (decelerating) creep stage [4].

A slightly different approach towards failure time prediction based on macroscopic strain (strain rate) focuses, instead, on the rapid increase of creep strain and strain rate in the run-up to failure, which typically is characterized by a creep strain (strain rate) that increases like an inverse power of the time-to-failure. Fitting such a power law to the data recorded until a given moment implies a prediction of the residual lifetime – an approach which has been promoted by D. Sornette and applied, in different variations, to catastrophic phenomena from material rupture over financial crises to childbirth [5] to the catastrophic breakdown of civilization as we know it [6].

* Corresponding author.
*E mail address:* michael.zaiser@fau.de (M. Zaiser).

https://doi.org/10.1016/j.finmec.2022.100141
Received 12 August 2022; Received in revised form 25 October 2022; Accepted 31 October 2022
Available online 5 November 2022

RETURN TO ISSUE | < PREV MOLECULAR MECHANICS NEXT >

# Addressing Surface Effects at the Particle-Continuum Interface in a Molecular Dynamics and Finite Elements Coupled Multiscale Simulation Technique

Yash Jain*, Maximilian Ries*, Sebastian Pfaller, and Florian Müller-Plathe

Cite this: *J. Chem. Theory Comput.* 2022, 18, 4, 2375−2387
Publication Date: March 1, 2022
https://doi.org/10.1021/acs.jctc.1c00940





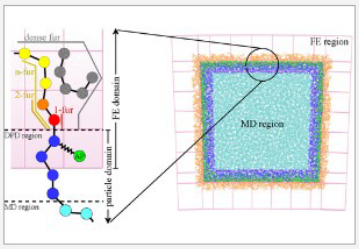
Journal of Chemical Theory and Computation



**SUBJECTS:** Deformation, Energy, Interfaces, Nanoparticles, Stress

## Abstract

Atomistic-to-continuum coupling methods are used to unravel molecular mechanisms of polymers and polymer composites. These multiscale techniques advantageously combine the computational efficiency of continuum approaches while keeping the accuracy of particle-based methods. The Capriccio method [Pfaller et al. *Comput. Methods Appl. Mech. Eng.* 2013, *260*, 109−129.] is a well-proven multiscale technique, which connects finite elements (FE) with molecular dynamics (MD) in a partitioned-domain approach. A vital aspect of these multiscale methods is to provide physically sound boundary conditions to the particle domain suppressing any interface effects at the domain boundary occurring due to the coupling. These interfacial coupling artifacts still pose a significant problem, especially for amorphous polymers due to their highly irregular microstructure. We solve this problem by extending the particle-continuum interface by a layer of passive atoms which move with the outer continuum, thereby providing the missing interactions with a surrounding polymer bulk to the inner particle region. This solution allows us to successfully reproduce structural and mechanical properties obtained under conventional periodic boundary conditions, like density, stress, Young's modulus, and Poisson's ratio. Furthermore, we demonstrate the application of a nonaffine deformation by means of a simple bending test. In general, our revised method provides a framework to apply complex deformations for molecular scientists, while it allows the engineering community to examine challenging phenomena such as fracture behavior at a molecular level.



polymers

MDPI

*Article*

# Molecular Simulations and Network Analyses of Surface/Interface Effects in Epoxy Resins: How Bonding Adapts to Boundary Conditions

**Julian Konrad [1], Paolo Moretti [2] and Dirk Zahn [1,*]**

[1] Lehrstuhl für Theoretische Chemie/Computer Chemie Centrum, Friedrich-Alexander Universität Erlangen-Nürnberg, Nägelsbachstraße 25, 91052 Erlangen, Germany
[2] Institute of Materials Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Dr.-Mack-Str. 77, 90762 Fürth, Germany
* Correspondence: dirk.zahn@fau.de

**Abstract:** In this study, we unravel the atomic structure of a covalent resin near boundaries such as surfaces and composite constituents. For this, a molecular simulation analysis of epoxy resin hardening under various boundary conditions was performed. On the atomic level of detail, molecular dynamics simulations were employed to study crosslinking reactions and self-organization of the polymer network within nm scale slab models. The resulting structures were then coarsened into a graph theoretical description for connectivity analysis of the nodes and combined with characterization of the node-to-node vector orientation. On this basis, we show that the local bonding of epoxy resins near interfaces tends to avoid under-coordinated linker sites. For both epoxy–vacuum surface models and epoxy–silica/epoxy cellulose interfaces, we find almost fully cured polymer networks. These feature a local increase in network linking lateral to the surface/interface, rather than the dangling of unreacted epoxy groups. Consequently, interface tension is low (as compared to the work of separating bulk epoxy), and the reactivity of the resin surface appears negligible.

**Keywords:** composites; molecular dynamics; curing; interfaces



**Citation:** Konrad, J.; Moretti, P.; Zahn, D. Molecular Simulations and Network Analyses of Surface/Interface Effects in Epoxy Resins: How Bonding Adapts to Boundary Conditions. *Polymers* **2022**, *14*, 4069. https://doi.org/10.3390/polym14194069

Academic Editor: Keon-Soo Jang

Received: 14 September 2022
Accepted: 23 September 2022
Published: 28 September 2022



## 1. Introduction

Epoxy polymer-based composites are of increasing importance for many technological developments aiming at the combination of low syntheses costs and tailor-made material properties. While the thermosetting polymer offers excellent processing characteristics, the mechanical properties of pure epoxy resins are unsuited for most applications. This motivated concepts of polymer reinforcement, particularly by the embedding of fibers or (nano-) particles to increase toughness in a controlled manner. The range of such composite formulations is immense, and combinations of favorable effects are often employed. For example, toughening of epoxy resins by particle insertion may also provide better resilience to abrasion. In parallel, the embedding of fibers may account for improvements in the characteristics of wear and fracture [1–3].

To name just one example from the vast number of different devices made of toughened epoxy resins, wet clutches are typically based on epoxy composites including both particles (silica, clay, etc.) and fibers (cellulose, aramid, etc.). The production process is akin to that of paper, entailing soaking of the fibers by water–particle mixtures, followed by pressing and drying of sheets or discs. Once dried, this "base paper" is then soaked by epoxy and hardener species, leading to the curing of the resin within a matrix of fibers and particles [4–6]. The enormous industrial relevance led to extensive engineering of constituents and processing parameters. Parallel to this, atomic force and electron microscopy improved our understanding of the µm scale structure [6].

polymers

MDPI

*Article*

# Multi-Scale Modelling of Plastic Deformation, Damage and Relaxation in Epoxy Resins

**Julian Konrad [1], Sebastian Pfaller [2] and Dirk Zahn [1,*]**

[1] Lehrstuhl für Theoretische Chemie/Computer Chemie Centrum, Friedrich-Alexander-Universität Erlangen-Nürnberg, Nägelsbachstr. 25, 91052 Erlangen, Germany
[2] Lehrstuhl für Technische Mechanik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 5, 91058 Erlangen, Germany
* Correspondence: dirk.zahn@fau.de

**Abstract:** Epoxy resin plasticity and damage was studied from molecular dynamic simulations and interpreted by the help of constitutive modelling. For the latter, we suggested a physically motivated approach that aims at interpolating two well-defined limiting cases; namely, pulling at the vanishing strain rate and very rapid deformation; here, taken as 50% of the speed of sound of the material. In turn, to consider 0.1–10-m/s-scale deformation rates, we employed a simple relaxation model featuring exponential stress decay with a relaxation time of 1.5 ns. As benchmarks, deformation and strain reversal runs were performed by molecular dynamic simulations using two different strain rates. Our analyses show the importance of molecular rearrangements within the epoxy network loops for rationalizing the strain-rate dependence of plasticity and residual stress upon strain reversal. To this end, our constitutive model reasonably reproduced experimental data of elastic and visco-elastic epoxy deformation, along with the maximum stress experienced before fracturing. Moreover, we show the importance of introducing damage elements for mimicking the mechanical behavior of epoxy resins.

**Keywords:** epoxy resins; molecular dynamics; constitutive modelling



**Citation:** Konrad, J.; Pfaller, S.; Zahn, D. Multi-Scale Modelling of Plastic Deformation, Damage and Relaxation in Epoxy Resins. *Polymers* **2022**, *14*, 3240. https://doi.org/10.3390/polym14163240

Academic Editors: Melissa A. Pasquinelli and Farzin Rahmani

Received: 25 June 2022
Accepted: 4 August 2022
Published: 9 August 2022



## 1. Introduction

Epoxy resins and their composites with fibers and particles have become indispensable construction materials for a continuously growing range of industrial applications. These range from using reinforced polymers in lightweight, mechanically resilient devices to use as versatile repair materials [1–3]. Due to the enormous engineering efforts invested within many decades, state-of-the-art epoxies currently represent practically ideal chemical bonding and unreacted moieties, with thermosetting polymers amounting to less than 1%. Despite this near 100% degree of crosslinking, epoxy resins feature amorphous network structures with only limited ordering at the 1-nm-length scale [4–7]. This implies an interplay of local chemistry and more global material properties, the understanding of which is an ongoing challenge to both experiments and theories.

While we are still in the beginning stage of this endeavor, molecular simulation approaches recently showed significant advances in elaborating realistic models of crosslinked polymers, such as epoxy resins. Pioneering studies dating back to more than ten years ago reasonably reproduced elastic moduli and bulk density, albeit reaching hardly more than 70% of crosslinking in the underlying network models [5,8,9]. On this basis, the fundamental aspects of epoxy characteristics beyond the elastic regime, such as glass transition points and yielding, could be assessed at least from a qualitative point of view [10]. More recently, however, improved crosslinking algorithms paved the way to models with up to 99%-reacted epoxy resins [4,11,12]. On this basis, we can reproduce key experimental data, such as the degree of curing, heat of polymerization reactions, elastic moduli, yield stress, and ultimate stress before fracturing [13].

Forces in Mechanics 9 (2022) 100135

Contents lists available at ScienceDirect

Forces in Mechanics

journal homepage: www.sciencedirect.com/journal/forces-in-mechanics

# A graded interphase enhanced phase-field approach for modeling fracture in polymer composites

Paras Kumar [*,a,b], Paul Steinmann [a,c], Julia Mergheim [a]

[a] Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany
[b] Competence Unit for Scientific Computing, Friedrich-Alexander-Universität, Erlangen-Nürnberg, Erlangen, Germany
[c] Glasgow Computational Engineering Centre, University of Glasgow, Glasgow, UK

ARTICLE INFO

*Keywords:*
Phase-field fracture
Polymer composites
Graded interphases
Micro-scale modeling

ABSTRACT

The superiority of nanosized filler particles in improving the elastic and fracture behavior of polymers, in comparison to microsized inclusions, has been substantiated by several experimental observations. Accurate modeling of crack propagation in such heterogeneous materials, however, involves resolution of complex crack topologies while taking into account the coalescence and branching of multiple cracks. Such complexity renders the traditional sharp crack modeling approaches, such as those based on the idea of partition of unity, to be of limited suitability, especially in 3D, since these involve explicit tracking of the evolving crack surfaces. Consequently, phase-field fracture approaches have come up as an attractive alternative to the traditional sharp crack models, especially when complex crack topologies need to be handled. Furthermore, standard two-phase continuum models, owing to their lack of the necessary length scale, are unable to capture the previously mentioned *smaller is stronger* size effect. In order to remedy this shortcoming, in context of finite strain hyperelasticity, a graded interphase based enhancement of the standard first-order continuum model was introduced in our previous work. The present contribution extends the idea of graded interphases to the phase-field fracture approach. Herein, an interphase region around filler particles, as observed experimentally, having continuously varying or graded material properties is considered. Fracture behavior of the composite material can be controlled by means of the degree of grading employed in determining the elastic and fracture properties within the interphase region. An optimal combination of the graded interphase parameters yields a tougher macroscopic response, as observed in case of tougher interphases, in comparison to the one obtained with a standard phase-field fracture model, The appropriateness of the introduced technique for modeling a wide spectrum of experimentally observed fracture behaviors, depending upon the degree of adhesion between the filler and the matrix phases, is depicted by means of extensive numerical experimentation.

## 1. Introduction

The ever increasing demand on engineering components to survive extreme loading scenarios stemming from cutting edge applications has impelled the development of materials with *tailor-made* micro-structures adapted to the application at hand. An important class of such materials comprises of polymer (nano-)composites which are employed in a plethora of use cases ranging from aerospace structures to bio-compatible implants [1,2]. The experimentally observed *smaller is stronger* size effect implies better structural reinforcement capability of nanosized filler particles than their microsized counterparts [3,4]. This fact has further invigorated the development of robust modeling approaches capable of accurately predicting the (in)elastic as well as fracture behavior of such unprecedented materials [5].

Traditionally, within the computational fracture mechanics paradigm, cracks have been modeled as *sharp (cohesive) interfaces*, i.e. lower dimensional manifolds, which evolve under the applied loads. Since the crack path is usually not known a priori, these approaches either involve remeshing so as to ensure that the element edges/faces are aligned with the crack faces, or some *enriched* finite element formulation to capture the displacement discontinuities caused by the crack cutting through an element, cf. [6,7] for instance. Further, these approaches need to be augmented with an ad-hoc criterion, which could be based on the classical critical stress intensity factors, the maximum energy release

* Corresponding author.
*E-mail address:* paras.kumar@fau.de (P. Kumar).

https://doi.org/10.1016/j.finmec.2022.100135
Received 17 August 2022; Received in revised form 5 October 2022; Accepted 16 October 2022
Available online 8 November 2022

Received: 14 February 2022 | Accepted: 20 March 2022
DOI: 10.1002/nme.6975

RESEARCH ARTICLE

WILEY

# A nonlocal interface approach to peridynamics exemplified by continuum-kinematics-inspired peridynamics

**Marie Laurien**[1] | **Ali Javili**[2] | **Paul Steinmann**[1]

[1]Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany
[2]Department of Mechanical Engineering, Bilkent University, Ankara, Turkey

**Correspondence**
Marie Laurien, Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 5, 91058 Erlangen, Germany.
Email: marie.laurien@fau.de

**Funding information**
Deutsche Forschungsgemeinschaft, Grant/Award Number: 377472739; Scientific and Technological Research Council of Turkey (TÜBITAK), Grant/Award Number: 218M700

**Abstract**

In this contribution, we present a novel approach on how to treat material interfaces in nonlocal models based on peridynamics (PD) and in particular continuum-kinematics-inspired peridynamics (CPD), a novel variationally consistent peridynamic formulation. Our method relies on a nonlocal interface where the material subdomains overlap. Within this region, a kinematic coupling of the two constituents is enforced. The contact is purely geometrical as interaction forces act only between points of the same material. We provide a detailed description of the computational implementation within the framework of CPD, that is in principle applicable to all formulations of PD. A variety of numerical examples for modeling bimaterial interfaces illustrate the utility of the technique for both two-dimensional and three-dimensional problems, including examples at large deformations. Our model approaches a local model when the nonlocality parameter, the horizon size, is decreased. The proposed methodology offers a viable alternative to previous approaches in PD, which are essentially imposing mixture rules for the interfacial material parameters.

**KEYWORDS**
continuum kinematics, material interface, nonlocality, peridynamics

## 1 | INTRODUCTION

Peridynamics (PD) is a nonlocal continuum formulation that was introduced by Silling in 2000.[1] Providing a tool to describe long-range forces within a continuum framework, the theory is increasingly applied to model physical phenomena that are not accurately captured through the consideration of local contact forces in classical (local) continuum models. This is achieved by incorporating integral terms into the governing equations of PD that comprise the interaction forces acting across a finite distance. Thus, PD enriches a continuum model by including long-range interactions. Conceptually speaking, PD borrows certain concepts from both classical continuum mechanics (CCM) and molecular dynamics (MD). Due to the replacement of spatial derivatives with integral operators, PD is inherently capable of modeling discontinuities, such as cracks, within a continuum framework. It is therefore widely used in fracture mechanics,[2] but has expanded to a multitude of application fields, such as multiscale modeling,[3-7] multiphysics,[8-10] and biological systems.[11-14] In the basic version of PD, that is, bond-based PD, the Poisson ratio is restricted to $\nu = 1/4$ in three-dimensional

Forces in Mechanics 10 (2023) 100124

Contents lists available at ScienceDirect

Forces in Mechanics

journal homepage: www.sciencedirect.com/journal/forces-in-mechanics

# Peridynamic modeling of nonlocal degrading interfaces in composites

Marie Laurien [*,a,c], Ali Javili [b], Paul Steinmann [a]

[a] Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 5, 91058 Erlangen, Germany
[b] Department of Mechanical Engineering, Bilkent University, 06800 Ankara, Turkey
[c] Competence Unit for Scientific Computing, Friedrich-Alexander-Universität Erlangen-Nürnberg, Martensstr. 5a, 91058 Erlangen, Germany

ARTICLE INFO

*Keywords:*
Nonlocal materials
Nonlocal interface
Composites
Peridynamics
Continuum-kinematics-inspired peridynamics

ABSTRACT

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

## 1. Introduction

A well-established technique in commercial polymer manufacturing to optimize the effective chemical, thermal and mechanical properties of a composite is the incorporation of particles or fibers. The stiffness of brittle polymers, for instance, is often enhanced by means of micro- and nanoparticles with the focus increasingly shifting to the latter [1]. When modeling physical systems at such small scales, the incorporation of a length-scale parameter and the consideration of nonlocal effects are essential. Continuous models based on classical continuum mechanics (CCM) consider only contact forces and are thus not aware of any length-scale. Employing molecular dynamics (MD), it is possible to model interactions of discrete particles over finite distances at the molecular scale, which is, however, computationally expensive and entails additional complexity for polymers. Peridynamics (PD) bridges the gap between CCM and MD in the sense that it is a continuum formulation that possesses an inherent length-scale and can therefore be considered an "upscaling" of MD. In PD, the behavior of a continuum point is governed by the nonlocal interaction forces exerted by surrounding points. These are determined by an integral over the neighborhood of the point, in which the size of the neighborhood defines the level of nonlocality of the model and allows for capturing scale-dependence. PD therefore serves as a tool to capture nonlocal effects that are assumed to play a major role on small length-scales. The basic version of PD, i.e. bond-based PD [2], is restricted to a fixed Poisson ratio. Recently, Javili et al. [3] have overcome this restriction by transferring the kinematic measures of CCM to a nonlocal setting, resulting in the geometrically exact theory of continuum-kinematics-inspired peridynamics (CPD). CPD has been applied in multiple works, see [4–12], among others. An overview of PD in general is provided in [13].

Nonlocal effects can be observed, for example, as a result of material interfaces, i.e. when two subdomains of potentially dissimilar materials meet. In a fully nonlocal model, also this interface is inherently nonlocal, giving rise to the term "nonlocal (material) interface". Here, the influence of the interface "spreads" into the surrounding bulk material due to nonlocal interactions. Moreover, the interface-to-volume ratio of embedded particles – and thus the influence of the interface – is comparatively pronounced at small scales. This motivates an

* Corresponding author.
*E-mail addresses:* marie.laurien@fau.de (M. Laurien), ajavili@bilkent.edu.tr (A. Javili), paul.steinmann@fau.de (P. Steinmann).

https://doi.org/10.1016/j.finmec.2022.100124
Received 28 July 2022; Received in revised form 2 September 2022; Accepted 17 September 2022
Available online 19 September 2022

Forces in Mechanics 9 (2022) 100127

Contents lists available at ScienceDirect

Forces in Mechanics

journal homepage: www.sciencedirect.com/journal/forces-in-mechanics

# LEFM☆ is agnostic to geometrical nonlinearities arising at atomistic crack tips

Tarakeshwar Lakshmipathy [*,a], Paul Steinmann [b], Erik Bitzek [c]

[a] Department of Materials Science and Engineering, Institute I, & Competence Unit for Scientific Computing (CSC), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Martensstr. 5, Erlangen, 91058, Germany
[b] Department of Mechanical Engineering, Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Egerlandstraße 5, Erlangen, 91058, Germany
[c] Department Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, 40237, Germany

ARTICLE INFO

*Keywords:*
LEFM
Fracture toughness
Lattice trapping
Atomistic simulation
Harmonic potential

ABSTRACT

Various fields such as mechanical engineering, materials science, etc., have seen a widespread use of linear elastic fracture mechanics (LEFM) at the continuum scale. LEFM is also routinely applied to the atomic scale. However, its applicability at this scale remains less well studied, with most studies focusing on non-linear elastic effects. Using a harmonic "snapping spring" nearest-neighbor potential which provides the closest match to LEFM on a discrete lattice, we show that the discrete nature of an atomic lattice leads to deviations from the LEFM displacement field during energy minimization. We propose that these deviations can be ascribed to geometrical nonlinearities since the material does not have a nonlinear elastic response prior to bond breaking. We demonstrate that crack advance and the critical stress intensity factor in an incremental loading scenario is governed by the collectively loaded region, and can not be determined analytically from the properties (max. elongation, max. sustained force, etc.) of the stressed crack tip bond alone.

## 1. Introduction

Linear elastic fracture mechanics (LEFM) has a long history in structural integrity and the design of fracture-resistant materials, and is well established in literature [1]. The roots of LEFM trace back to the works of Inglis [2] who introduced the concept of a stress concentration factor to describe the stresses due to an elliptical hole with respect to an applied macroscopic stress. Later, Griffith [3] assumed a linear elastic material to establish a thermodynamic criterion for perfectly brittle crack advance. According to this model, a crack would propagate when the the stored elastic energy released by crack propagation exceeds the energy required to create two new crack surfaces. The energy release rate $G$, which can be defined as the rate of change in potential energy with crack area, can then be related to Griffith's criterion as follows:

$$G \leq G_{\mathrm{G}} = 2\gamma, \tag{1}$$

where $G_{\mathrm{G}}$ is Griffith's theoretical resistance of the material that needs to be overcome to create two crack new surfaces, with $\gamma$ being their surface energy. Williams [4] and Irwin [5] then used a stress-based approach to establish the concept of a stress intensity factor (SIF). This factor $K$ is a single loading parameter that describes the scaling of the amplitude of the stress field around the crack. The stress intensity factor is related to the energy release rate as follows:

$$K = \sqrt{GE^{\star}}, \tag{2}$$

where $E^{\star}$ is the orientation dependent elastic modulus. Applying the Griffith criterion to the stress-based approach using Eqs. (1) and (2), we obtain the theoretical SIF $K_{\mathrm{G}}$ required for crack advance:

$$K_{\mathrm{G}} = \sqrt{G_{\mathrm{G}}E^{\star}}. \tag{3}$$

In atomistic simulations of fracture [6,7], a SIF-controlled loading approach is usually employed by displacing atoms according to the linear elastic *anisotropic* solution in plane strain in mode I [8]. The LEFM displacement field is given by:

$$u_x(r,\theta) = \frac{K_{\mathrm{I}}\sqrt{2r}}{\sqrt{\pi}}[f_x(\theta)], \tag{4}$$

Linear Elastic Fracture Mechanics.

* Corresponding author.
*E-mail address:* tara.ll.lakshmipathy@fau.de (T. Lakshmipathy).

https://doi.org/10.1016/j.finmec.2022.100127
Received 3 August 2022; Received in revised form 21 September 2022; Accepted 22 September 2022
Available online 23 September 2022

Forces in Mechanics 10 (2023) 100161

Contents lists available at ScienceDirect

Forces in Mechanics

journal homepage: www.sciencedirect.com/journal/forces-in-mechanics

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

Dhananjay Phansalkar [a,b,*], Deepak B. Jadhav [a,b], Kerstin Weinberg [c], Michael Ortiz [d], Sigrid Leyendecker [a]

[a] Institute of Applied Dynamics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Immerwahrstrasse 1, Erlangen 91058, Germany
[b] Central Institute for Scientific Computing, Friedrich-Alexander-Universität Erlangen-Nürnberg, Martensstrasse 5a, Erlangen 91058, Germany
[c] Chair of Solid Mechanics, Universität Siegen, Paul-Bonatz-Strasse 9–11, Siegen 57076, Germany
[d] Division of Engineering and Applied Sciences, California Institute of Technology, Pasadena, CA 91125, USA

ARTICLE INFO

*Keywords:*
Brittle fracture
Phase-field model
Spatial variation of the regularisation length
Adaptive mesh refinement

ABSTRACT

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

## 1. Introduction

The mathematical theory of a variational-based formulation for brittle fracture dates back to late 1990's, especially to the work of Francfort and Marigo [1]. This formulation is later regularised in the works of Bourdin et al. [2,3]. It provides a general criterion for crack propagation with a consistent numerical solution strategy to simulate complex fracture phenomena such as crack branching, coalescence, initiation and brutal propagation. The variational problem is best studied within the context of spaces of special functions of bounded variations (SBV) and their variants, where it is categorised as a free discontinuity problem in the contemporary theory of the calculus of variations.

For a variational-based discrete brittle fracture, Dal Maso and Toader [4] proved the existence of a result for the quasi-static evolution of a fracture by using the time-discretization method in the two-dimensional case of anti-plane shear, and Chambolle [5] for plane elasticity with vectorial displacement fields. It is shown that, in the limit for the length parameter $\epsilon \to 0$ the phase-field energy functional approaches the discrete brittle fracture energy in the sense of $\Gamma$-convergence [6,7]. Thus, it is required to choose a relatively small $\epsilon$ for a good approximation of the discrete solution. Various studies [3,8] suggest that a relatively fine mesh size compared to $\epsilon$ is needed, i.e., $h < \epsilon$. Additionally, in the work of [9], a numerical study shows that there exists an optimal mesh size $h$ for a given $\epsilon$, in particular $h \propto \epsilon^2$, i.e., the optimal $h$ leads to minimum potential. This lead to our work [10] in which we deal with these challenges by introducing a variational formulation to determine an optimal field $\epsilon(x)$ to develop a spatially adaptive phase-field formulation.

Our initial investigations [10] on this subject did not consider unilateral contact at the crack lips. The regularised model chosen by Bourdin et al. [2,3] exhibits symmetric behaviour in traction and compression and permits negative displacement jumps, i.e. material interpenetration in fractures associated with compressive forces. This

* Corresponding author.
*E-mail address:* dhananjay.phansalkar@fau.de (D. Phansalkar).

https://doi.org/10.1016/j.finmec.2022.100161
Received 15 December 2022; Accepted 16 December 2022
Available online 23 December 2022

Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 395 (2022) 114880
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

# A spatially adaptive phase-field model of fracture

Dhananjay Phansalkar[a,b,*], Kerstin Weinberg[c], Michael Ortiz[d], Sigrid Leyendecker[a]

[a] Institute of Applied Dynamics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Immerwahrstrasse 1, Erlangen 91058, Germany
[b] Central Institute for Scientific Computing, Friedrich-Alexander-Universität Erlangen-Nürnberg, Martensstrasse 5a, Erlangen 91058, Germany
[c] Chair of Solid Mechanics, Universität Siegen, Paul-Bonatz-Strasse 9-11, Siegen 57076, Germany
[d] Division of Engineering and Applied Sciences, California Institute of Technology, Pasadena, CA 91125, USA

Received 21 September 2021; received in revised form 28 January 2022; accepted 10 March 2022
Available online 16 May 2022

**Abstract**

Phase-field models of fracture introduce smeared cracks of width commensurate with a regularisation length parameter $\epsilon$ and obeying a minimum energy principle. Mesh adaptivity naturally suggests itself as a means of supplying spatial resolution where needed while simultaneously keeping the computational size of the model as small as possible. Here, a variational-based spatial adaptivity is proposed for a phase-field model of fracture.

An extension of the conventional phase-field model is achieved by allowing spatial variation of the regularisation length $\epsilon$ in the energy functional. Similar to the displacement and phase fields, the optimal regularisation length is obtained by minimising the energy functional. This extended phase-field model serves as the foundation for an adaptive mesh refinement strategy, in which the mesh size is determined locally by the optimal regularisation length. The resulting solution procedure is implemented in the framework of the finite element library FEniCS. According to the selected numerical experiment, the spatially adaptive phase-field model converges marginally faster than the conventional phase-field model but with a vastly superior constant, resulting in significant computational savings.



*Keywords:* Brittle fracture; Phase-field model; Spatial variation of the regularisation length; Adaptive mesh refinement

## 1. Introduction

Understanding a material's fracture is essential to design mechanical systems, particularly for components with a low safety factor. However, reliable fracture computations are difficult for a variety of reasons, including the tracking of complex crack paths, the singularity of stress at the crack tip, and the dependency of the solution on the discretisation method and mesh size. To overcome these difficulties, non-local methods like phase-field models have gained popularity. In such a method, the crack is 'smeared' over a certain width $\epsilon$, regularising the sharp interface problem of the discrete crack. Phase-field models are easy to use and implement, and, in contrast to discrete crack models, they do not require mesh manipulation for crack initiation, kinking, and branching.

Phase-field models are typically derived from a variational principle [1]. The direct, monolithic solution of the resulting fully-coupled non-linear Euler–Lagrange equations has problems usually solved with a viscous

* Corresponding author.
*E-mail address:* dhananjay.phansalkar@fau.de (D. Phansalkar).

https://doi.org/10.1016/j.cma.2022.114880

Received: 1 June 2022 | Revised: 1 September 2022 | Accepted: 18 September 2022

DOI: 10.1002/app.53209

RESEARCH ARTICLE

Applied Polymer SCIENCE WILEY

# A novel study on the sandwich-structure strain sensor using ethylene-vinyl acetate-based hot-melt adhesive mesh web: Fabrication, properties, and modeling

**Muchao Qu**[1] | **Jiaqiang Fang**[1] | **Chenzhong Mu**[2] | **Yanfeng Li**[1] | **Shaojuan Huang**[1] | **Lei Han**[1] | **Stefan Hiemer**[3] | **Wei Xu**[1] | **Yijing Qin**[4]

[1]School of Automobile and Transportation Engineering, Guangdong Polytechnic Normal University, Guangdong, People's Republic of China

[2]State Key Laboratory of Special Functional Waterproof Materials, Beijing Oriental Yuhong Waterproof Technology Co., Ltd., Beijing, China

[3]Friedrich-Alexander-Universität Erlangen-Nürnberg, Institute of Materials Simulation, Department of Materials Science and Engineering, Fürth, Germany

[4]Center for Engineering Materials and Reliability, Guangzhou HKUST Fok Ying Tung Research Institute, Guangzhou, China

**Correspondence**
Wei Xu, School of Automobile and Transportation Engineering, Guangdong Polytechnic Normal University, Guangdong 510000, People's Republic of China.
Email: xuy_wei@126.com

Yijing Qin, Center for Engineering Materials and Reliability, Guangzhou HKUST Fok Ying Tung Research Institute, Guangzhou, China.
Email: yjqin@ust.hk

**Funding information**
Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), Grant/Award Number: 377472739/GRK/2423/1-2019; Scientific and Technological Plan of Guangdong Province, China, Grant/Award Number: 2019B090905005; Start-up funding Project from Guangdong Polytechnic Normal University, Grant/Award Numbers: 2021SDKYA017, 991641261

**Abstract**

In this study, a flexible strain sensor consisting of carbon nanotubes (CNTs) and ethylene-vinyl acetate (EVA)-based hot-melt adhesive web (HAW) is proposed with the advantages of low cost and easy fabrication. Six different weight fractions of the CNTs were employed in producing the three-layer sandwich-structure composite membrane. The morphology and internal particle structure of the cross section of the EVA/CNTs composite membranes was studied using scanning electron microscopy. The mechanical properties as well as the mechanical–electrical behavior of the EVA/CNTs sensors were investigated, showing a gauge factor up to 477. In addition, two mathematical equations to establish the relationship between the output electrical signal and the input strain signal during the monotonic and cyclic measurements were proposed, respectively. Overall, this study provides a solvent-free one-step approach for the preparation of flexible strain sensors with innovative and broad application prospects, and offers some insight into the mathematical prediction of the strain sensing behavior.

**KEYWORDS**

membranes, morphology, nanotubes, theory and modeling

## 1 | INTRODUCTION

Flexible conductive polymeric composites (FCPCs) are commonly applied as flexible strain sensors[1,2] due to their flexibility and high electrical conductivity, which enable FCPCs to monitor electrical signals in real-time continuously.[3,4] Thus, they are used in a wide range of applications such as electronic skin, healthcare, and sports equipment.[5] Until now, lots of conductive fillers have been investigated for their performance in the

Jiaqiang Fang contributed equally to this work and should be considered as co-first author.

Mathematics and Mechanics of Solids
OnlineFirst

https://doi.org/10.1177/10812865221108099

SAGE journals

*Article*

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

**Maximilian Ries** [1], **Christof Bauer** [2], **Felix Weber** [3], **Paul Steinmann** [4], **and Sebastian Pfaller** [5]

**Abstract**

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

**Keywords**

Molecular dynamics, continuum mechanics, material characterization, anisotropy, elasticity

[1]Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany
[2]Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany
[3]Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany
[4]Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany
[5]Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

**Corresponding author(s):**
Maximilian Ries, Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91054 Erlangen, Germany.
Email: maximilian.ries@fau.de

## 1. Introduction

The versatility of polymers can be further expanded by the addition of fillers. In particular, filler particles at the nanoscale have been found to significantly improve the polymers' mechanical [1,2], thermal [3,4],

*Express Polymer Letters Vol.16, No.12 (2022) 1304–1321*
*Available online at www.expresspolymlett.com*
*https://doi.org/10.3144/expresspolymlett.2022.94*

*Research article*

# Applying a generic and fast coarse-grained molecular dynamics model to extensively study the mechanical behavior of polymer nanocomposites

*Maximilian Ries**, *Jakob Seibert*, *Paul Steinmann*, *Sebastian Pfaller*

Institute of Applied Mechanics, Friedrich-Alexander-Universität, Erlangen-Nürnberg, Germany

*Received 14 April 2022; accepted in revised form 9 August 2022*

**Abstract.** The addition of nano-sized filler particles enhances the mechanical performance of polymers. The resulting properties of the polymer nanocomposite depend on a complex interplay of influence factors such as material pairing, filler size, and content, as well as filler-matrix adhesion. As a complement to experimental studies, numerical methods, such as molecular dynamics (MD), facilitate an isolated examination of the individual factors in order to understand their interaction better. However, particle-based simulations are, in general, computationally very expensive, rendering a thorough investigation of nanocomposites' mechanical behavior both expensive and time-consuming. Therefore, this paper presents a fast coarse-grained MD model for a generic nanoparticle-reinforced thermoplastic. First, we examine the matrix and filler phase individually, which exhibit isotropic elasto-viscoplastic and anisotropic elastic behavior, respectively. Based on this, we demonstrate that the effect of filler size, filler content, and filler-matrix adhesion on the stiffness and strength of the nanocomposite corresponds very well with experimental findings in the literature. Consequently, the presented computationally efficient MD model enables the analysis of a generic polymer nanocomposite. In addition to the obtained insights into mechanical behavior, the material characterization provides the basis for a future continuum mechanical description, which bridges the gap to the engineering scale.

***Keywords:*** *mechanical properties, nanocomposites, modelling and simulation, interphase, size effect*

## 1. Introduction

The properties of polymers can be tailored to meet the increasingly application-specific requirements by adding filler particles. Particularly, nano-sized additives yield considerable gains in optical [1], electrical [2], thermal [3, 4], and mechanical [5] properties. The filler particles influence the characteristics of the matrix polymer in their immediate vicinity [6], creating a region with diverging properties denoted as *interphase* [7]. In the case of non-overlapping interphases, the volume fraction of the interphase is directly proportional to the filler-matrix interface and thus dependent on the surface/volume fraction of the filler particles (at constant filler content). In the case of overlapping interphases, the proportionality depends on the extent of overlaps. Due to their substantial surface-to-volume ratio, nano-sized particles, *i.e.*, one dimension ≤100 nm [8], yield a high interphase volume fraction which affects the overall properties considerably. Consequently, the material behavior of nanocomposites is strongly filler size sensitive, in contrast to conventional (micro)composites [9, 10]. This dependence on the filler size, often called the *size effect*, has been experimentally confirmed in many cases, including calcium carbonate-induced polypropylene [11], magnesium hydroxide-reinforced rubber [12], and ground tire rubber-filled polyethylene [13]. In addition to the filler size,

*Corresponding author, e-mail: maximilian.ries@fau.de

Composites Part A: Applied Science and Manufacturing
Volume 161, October 2022, 107094

# A quantitative interphase model for polymer nanocomposites: Verification, validation, and consequences regarding size effects

Maximilian Ries, Felix Weber, Gunnar Possart, Paul Steinmann, Sebastian Pfaller

Show more



https://doi.org/10.1016/j.compositesa.2022.107094



## Abstract

The enhanced mechanical behavior of polymer nanocomposites with spherical filler particles is attributed to the formation of matrix-filler interphases. The nano-scale leads to particularly high interphase volume fractions while rendering experimental investigations extremely difficult. Previously, we introduced a molecular dynamics-based interphase model capturing the crucial spatial profiles of elastic and inelastic properties inside the interphase. This contribution demonstrates that our model captures polymer nanocomposites' essential characteristics reported from experiments. To this end, we thoroughly verify and validate the model before discussing the resulting local plastic strain distribution. Furthermore, we obtain a reinforcement in terms of the overall stiffness for smaller particles and higher filler contents, while the influence of particle spacing seems negligible, matching experimental observations in the literature. This paper proposes a methodology to unravel the underlying complex mechanical behavior of polymer nanocomposites and to translate the findings into engineering quantities accessible to a broader audience and technical applications.

Forces in Mechanics 9 (2022) 100132

Contents lists available at ScienceDirect

Forces in Mechanics

journal homepage: www.sciencedirect.com/journal/forces-in-mechanics

# An energetically consistent surface correction method for bond-based peridynamics

Jonas Ritter [a,b,*], Shucheta Shegufta [a,b], Paul Steinmann [c], Michael Zaiser [a]

[a] Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), Department of Materials Science, WW8-Materials Simulation, Dr.-Mack-Straße 77, 90762 Fürth, Germany
[b] Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), Central Institute for Scientific Computing (ZISC), Martensstraße 5a, 91058 Erlangen, Germany
[c] Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), Department of Mechanical Engineering, Applied Mechanics, Egerlandstraße 5, 91058 Erlangen, Germany

ARTICLE INFO

*Keywords:*
Peridynamics
Surface effect
Indentation

ABSTRACT

A novel surface correction method is proposed for bond-based peridynamics which ensures energy consistency with a classical reference body for general affine deformations. This method is validated for simple geometries and then applied to a typical surface-dominated problem, namely the indentation of a surface in the shallow to moderate-depth regime.

## 1. Introduction

Peridynamics is a nonlocal formulation of continuum mechanics that was introduced by Silling [1] but which has close relations to Eringen's nonlocal elasticity theory [2] and earlier work dating back to the 1960s (see e.g. Kröner [3]) while its treatment of fracture problems shows close analogies to damage mechanics [4]. In its simplest form, so-called bond-based peridynamics, each material point is envisaged to interact with all material points within a finite domain, the so-called horizon, through central 'bond' forces whose magnitudes are proportional to the bond elongation times a phenomenological bond strength. Local fracture can then be simply described by setting the strength of a bond to zero upon fulfilment of a failure criterion. No specific traction boundary conditions are needed at surfaces or crack surfaces, which renders the method most useful for geometrically complex fracture problems such as fragmentation [5] or fracture of highly porous media [6,7].

A generic feature of peridynamics is the so-called surface effect: near-surface regions behave elastically softer than the bulk of the material. This is not always a desirable feature, as the peridynamic surface softening may misrepresent the behavior of actual materials, where both surface softening and surface stiffening are observed. Here we present a new energy-based method to correct this surface effect if needed (for an overview and comparative discussion of alternative correction methods, see Ref. [8]). We give a brief introduction into bond-base peridynamics in Section 2, including a discussion of the origin of the surface effect. We then present our correction scheme in Section 3 and give examples of its application in Section 4 before concluding in Section 5.

## 2. Theoretical Background

For completeness of presentation, we give a brief overview of the bond-based peridynamics model which we consider in the following; for original reference, see [9], our presentation follows mainly Ref. [7]. We characterize the deformation of a $D$ dimensional continuous body $\mathscr{B}$ of density $\rho(\boldsymbol{x})$ by the displacement field $\boldsymbol{u}(\boldsymbol{x})$ where $\boldsymbol{x}$ are material coordinates. The force balance equation for the point $\boldsymbol{x}$ is written in the form

$$\rho(\boldsymbol{x})\ddot{\boldsymbol{u}}(\boldsymbol{x}) = \int_{\mathscr{H}_x} \boldsymbol{f}(\boldsymbol{x},\boldsymbol{x}')\mathrm{d}\boldsymbol{x}' + \boldsymbol{b}(\boldsymbol{x}), \tag{1}$$

where $\boldsymbol{f}(\boldsymbol{x},\boldsymbol{x}')$ is the pair force between $\boldsymbol{x}'$ and $\boldsymbol{x}$, $\boldsymbol{b}$ is a body force field, and interactions of the material point $\boldsymbol{x}$ with other material points are restricted to the so-called horizon $\mathscr{H}_x$ which we take to be a $D$ dimensional sphere of radius $\delta$ around $\boldsymbol{x}$, $(|\boldsymbol{x}-\boldsymbol{x}^*| \leq \delta)\ \forall\ \boldsymbol{x}^* \in \mathscr{H}_x$.

The pair force is specified constitutively. Considering linear elasticity and small deformations, we write the pair force as

$$\begin{aligned} &\boldsymbol{f}(\boldsymbol{x},\boldsymbol{x}') = \widehat{\boldsymbol{f}}(\boldsymbol{x},\boldsymbol{x}') + \widehat{\boldsymbol{f}}(\boldsymbol{x}',\boldsymbol{x}) \quad , \quad \text{where} \\ &\widehat{\boldsymbol{f}}(\boldsymbol{x},\boldsymbol{x}') = \frac{1}{2}\boldsymbol{C}(\boldsymbol{x},\boldsymbol{\xi})[\boldsymbol{u}(\boldsymbol{x}') - \boldsymbol{u}(\boldsymbol{x})], \\ &\widehat{\boldsymbol{f}}(\boldsymbol{x}',\boldsymbol{x}) = \frac{1}{2}\boldsymbol{C}(\boldsymbol{x}',\boldsymbol{\xi})[\boldsymbol{u}(\boldsymbol{x}') - \boldsymbol{u}(\boldsymbol{x})]. \end{aligned} \tag{2}$$

Here $\boldsymbol{\xi} = \boldsymbol{x}' - \boldsymbol{x}$. $\boldsymbol{C}(\boldsymbol{x},\boldsymbol{\xi})$ is called the micro-modulus tensor. It is of the form

* Corresponding author at: Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), Department of Materials Science, WW8-Materials Simulation, Dr.-Mack-Straße 77, 90762 Fürth, Germany

https://doi.org/10.1016/j.finmec.2022.100132
Received 31 August 2022; Received in revised form 6 October 2022; Accepted 16 October 2022
Available online 17 October 2022

Forces in Mechanics 10 (2023) 100157

Contents lists available at ScienceDirect

Forces in Mechanics

journal homepage: www.sciencedirect.com/journal/forces-in-mechanics

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

Maurice Rohracker [*,a,b], Paras Kumar [a,b], Julia Mergheim [a]

[a] Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany
[b] Competence Unit for Scientific Computing, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

ARTICLE INFO

*Keywords:*
Phase-field fracture simulations
Spatial adaptivity
Brittle fracture
Single edge notched shear test

ABSTRACT

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

## 1. Introduction

In recent years, the phase-field method is used extensively for the simulation of fracture in brittle materials, see e. g. [1,2]. Thereby, a sharp discontinuous crack $\Gamma$ is approximated by a smeared continuous zone in the body using the phase-field variable $z \in [0,1]$, cf. Fig. 1. The phase-field variable $z$ takes the value 0 on $\Gamma$, rises smoothly to 1 in a subset of $\mathscr{B}\backslash\Gamma$, and then takes the value 1 in the rest of the domain as can be seen in the 1-dimensional representation in Fig. 1b. With this definition, the limits $z = 0$ and $z = 1$ represent the fully broken and the intact (undamaged) material phases, respectively, whereas the intermediate range $z \in (0,1)$ mimics the transition zone between them. In the phase-field method for fracture, the crack length scale parameter $l_c$ governs the regularization which converges to the sharp discontinuous crack as $l_c \to 0$.

The smeared approximation of the crack requires suitable mesh sizes in the region of crack propagation to resolve the small length scale inherent to the diffusive crack. A too coarse mesh might lead to wrong results or no crack propagation at all. To overcome this problem a pre-refinement of the assumed regions of crack propagation can be applied [3,4]. This, however, can be computationally very expensive because of the high number of elements. Furthermore, the crack paths are not always known beforehand. A better and more common solution is the usage of adaptive spatial refinement (ASR) strategies based on appropriate refinement and coarsening criteria. The criteria used for ASR are very different. In Burke et al. [5,6], different adaptive finite element algorithms for the phase-field fracture problem in brittle materials are introduced. Mesh refinement takes place depending on a residual-based local refinement criterion. In [5], the standard Ambrosio-Tortorelli functional [7] is minimized to solve the crack problem, whereas in [6], generalized Ambrosio-Tortorelli functionals are considered and an irreversibility constraint is taken into account. It was observed that the adaptive algorithms are capable of computing the evolving crack paths accurately and reliably. However, the crack path can be sensitive to the choice of parameters. Artina et al. [8] extended the work of [5] for anisotropic adaptive meshes. Wick [9] developed an

* Corresponding author.
*E-mail address:* mau.rohracker@fau.de (M. Rohracker).

https://doi.org/10.1016/j.finmec.2022.100157
Received 26 September 2022; Received in revised form 18 November 2022; Accepted 7 December 2022
Available online 15 December 2022

ARTICLE

# Bone fracture healing within a continuum bone remodelling framework

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

Pages 1040-1050 | Received 06 Jul 2021, Accepted 20 Oct 2021, Published online: 03 Nov 2021

Download citation https://doi.org/10.1080/10255842.2021.1998465 Check for updates

Full Article Figures & data References Citations Metrics Reprints & Permissions Get access

## Abstract

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

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

*Geological Magazine*

**www.cambridge.org/geo**

## Original Article

**Cite this article:** Smith RY, Lesueur M, Kelka U, Poulet T, and Koehn D. Using fractured outcrops to calculate permeability tensors: implications for geothermal fluid flow and the influence of seismic-scale faults. *Geological Magazine* https://doi.org/10.1017/S0016756822000309

Received: 31 January 2022
Revised: 29 March 2022
Accepted: 31 March 2022

**Keywords:**
natural fractures; geothermal; numerical modelling; fluid flow; outcrop; permeability tensors

**Author for correspondence:**
Ruaridh Y. Smith, Email: ruaridh.smith@fau.de



CAMBRIDGE UNIVERSITY PRESS

# Using fractured outcrops to calculate permeability tensors: implications for geothermal fluid flow and the influence of seismic-scale faults

Ruaridh Y. Smith[1], Martin Lesueur[2], Ulrich Kelka[3], Thomas Poulet[3] and Daniel Koehn[1]

[1]Geozentrum Nordbayern, Friedrich-Alexander Universität (FAU), Erlangen-Nürnberg, Germany; [2]School of Earth Sciences, University of Western Australia, Perth, Australia and [3]CSIRO Mineral Resources, Kensington WA, Australia

**Abstract**

Faulted and fractured systems form a critical component of fluid flow, especially within low-permeable reservoirs. Therefore, developing suitable methodologies for acquiring structural data and simulating flow through fractured media is vital to improve efficiency and reduce uncertainties in modelling the subsurface. Outcrop analogues provide excellent areas for the analysis and characterization of fractures within the reservoir rocks where subsurface data are limited. Variation in fracture arrangement, distribution and connectivity can be obtained from 2D fractured cliff sections and pavements. These sections can then be used for efficient discretization and homogenization techniques to obtain reliable predictions on permeability distributions in the geothermal reservoirs. Fracture network anisotropy in the Malm reservoir unit is assessed using detailed structural analysis and numerical homogenization of outcrop analogues from an open pit quarry within the Franconian Basin, Germany. Several events are recorded in the fracture networks from the Late Jurassic the Alpine Orogeny and are observed to be influenced by the Kulmbach Fault nearby with a reverse throw of 800 m. The fractured outcrops are digitized for fluid flow simulations and homogenization to determine the permeability tensors of the networks. The tensors show differences in fluid transport direction where fracture permeability is controlled by orientation compared to a constant value. As a result, it is observed that the orientation of the tensor is influenced by the Kulmbach Fault, and therefore faults within the reservoirs at depth should be considered as important controls on the fracture flow of the geothermal system.

## 1. Introduction

Faults and fractures are abundant discontinuity features in rocks that govern fluid flow in the subsurface (Caine *et al.* 1996; Sibson, 1996; Curewitz & Karson, 1997; Connolly and Cosgrove 1999; Sanderson & Zhang, 2004; Kurz *et al.* 2008; Zhang *et al.* 2008; Bense *et al.* 2013; Morley & Nixon, 2016; La Bruna *et al.* 2021; Pisani *et al.* 2022). These structural features develop at a variety of scales from large-scale regional faults to outcrop scale, fracture and stylolite networks, all of which can either enhance or impede flow in the subsurface (Caine *et al.* 1996; Odling *et al.* 1999; Bour *et al.* 2002; Sanderson & Zhang, 2004; Manzocchi *et al.* 2010; Bense *et al.* 2013; Bruna *et al.* 2019; Giuffrida *et al.* 2019; Araújo *et al.* 2021). Analysing these networks and characterizing their impact on flow and transport, is paramount for a variety of subsurface applications, e.g. geothermal energy extraction (Lipsey *et al.* 2016; Vidal *et al.* 2017; Smeraglia *et al.* 2021), hydrocarbon production (Nelson, 2001), mineral exploration (e.g. Cox, 1999), $CO_2$ sequestration (CSS; e.g. Stork *et al.* 2015) and hydrogen storage (Saxena *et al.* 2018). This is especially important in geothermal reservoirs where host-rock permeability is generally low, e.g. granite geothermal systems (Wibberley & Shimamoto, 2002), and fluid flow is controlled at first order by fracture network geometry (Hollinsworth *et al.* 2019).

Efficient discretization and simulation techniques are required to obtain reliable prediction of permeability distributions within geothermal reservoirs. We use a field example from an open pit quarry near Kulmbach, Germany, to show how fracture network anisotropy in geothermal reservoirs can be assessed using detailed analysis of outcrop analogues. Specifically, we analyse variation of fracture networks in a cross-section towards the seismic-scale Kulmbach Fault. We present the results of the structural analysis, followed by introducing a mixed-dimensional approach for quick discretization of the network for the numerical analysis of flow in the dense fracture networks. Based on our field data we will demonstrate the importance of linking geological field work to numerical model development. Finally, we propose a new approach to numerical permeability homogenization that is informed by detailed field observations.

https://doi.org/10.1017/S0016756822000309 Published online by Cambridge University Press

Received: 5 July 2022 | Revised: 4 October 2022 | Accepted: 7 November 2022

DOI: 10.1002/nme.7168

RESEARCH ARTICLE

WILEY

# Robust design optimization for enhancing delamination resistance of composites

**Sukhminder Singh**[1,2] | **Lukas Pflug**[1] | **Julia Mergheim**[3] | **Michael Stingl**[2]

[1]Competence Unit for Scientific Computing (CSC), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany

[2]Chair of Applied Mathematics (Continuous Optimization), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany

[3]Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany

**Correspondence**
Sukhminder Singh, Chair of Applied Mathematics (Continuous Optimization), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Cauerstr. 11, 91058 Erlangen, Germany.
Email: sukhminder.singh@fau.de

**Funding information**
Deutsche Forschungsgemeinschaft, Grant/Award Number: 377472739/GRK 2423/1-2019

**Abstract**

Recent developments in the field of computational modeling of fracture have opened up possibilities for designing structures against failure. A special case, called interfacial fracture or delamination, can occur in loaded composite structures where two or more materials are bonded together at comparatively weak interfaces. Due to the potential crack growth along these interfaces, the structural problem suffers from snap-back/snap-through instabilities and bifurcations with respect to the model parameters, leading to noisy and discontinuous responses. For such a case, the design optimization problem for a selected quantity of interest is ill-posed, since small variations in the design parameters can lead to large jumps in the structural response. To this end, this article presents a stochastic optimization approach to maximize delamination resistance that is less sensitive to small perturbations of the design and thereby leads to a robust solution. To overcome the intractability of Monte Carlo methods for estimating the expected value of the expensive-to-evaluate response function, a global, piecewise-constant surrogate is constructed based on nearest-neighbor interpolation that is iteratively refined during the optimization run. We found that by taking a large stochastic region at the beginning of the optimization and gradually reducing it to the desired one can help overcome poor local optima. Our results demonstrate the effectiveness of the proposed framework using an example of shape optimization of hard inclusions embedded in a double-cantilever beam, which significantly enhances delamination resistance.

**KEYWORDS**

composite structures, delamination, nearest-neighbor interpolation, robust design, stochastic optimization

## 1 | INTRODUCTION

Structural defects in the form of sharp cracks tend to grow in highly stressed regions and in those regions that provide easy pathways for crack propagation, for instance, adhesive interfaces in laminated composites. In the latter case, introducing architected heterogeneities or voids at the micro- or meso-scale along the interfaces is expected to retard or even stop the growth of the crack, thereby increasing the resistance to interfacial fracture or *delamination*. The size, shape and

Forces in Mechanics 9 (2022) 100137

Contents lists available at ScienceDirect

Forces in Mechanics

journal homepage: www.sciencedirect.com/journal/forces-in-mechanics

# Generalized interfaces enabling macroscopic modeling of structural adhesives and their failure

Lucie Spannraft *, Gunnar Possart, Paul Steinmann, Julia Mergheim

*Institute of Applied Mechanics, Universität Erlangen-Nürnberg, Egerlandstr. 5, Erlangen 91058, Germany*

ARTICLE INFO

*Keywords:*
Interface (in)elasticity
Anisotropic cohesive zone
Generalized interfaces
Damage
Structural adhesives

ABSTRACT

This contribution presents a geometrically linear and thermodynamically consistent model for generalized mechanical interfaces. The interface's response is kinematically non-coherent, i.e. allows for a displacement jump and for anisotropic cohesive failure, and kinetically non-coherent, i.e. allows for traction jumps across the interface and membrane damage. The traction jump ensues from an interfacial (in)elasticity formulation which introduces additional membrane stiffness and membrane stresses under in-plane stretch in the interface. The cohesive and membrane degradations are coupled via damage variables determined by the different deformation modes to account for their interaction. A numerical example applies the presented model to brittle interfaces adhesively bonding two substrates. By subjecting the interface to a small in-plane stretch prior to performing a peel test, the influence of damage coupling on the mechanical response is illustrated.

## 1. Introduction

The bonding of a wide variety of materials by means of structural adhesives has been steadily increasing for decades, both for applications in lightweight construction and in vehicle and aircraft production [17]. Force- and form-fitting connections are often realized with cheap and easy-to-apply polymer-based adhesives, e.g. epoxies, whose stiffness is in the range of a few GPa and whose failure behavior can be adjusted from comparatively ductile to very brittle, depending on the formulation and, if necessary, additives, see [11]. The design of such structural bonds is increasingly supported by continuum mechanical modeling and finite element simulations. For reasons of efficiency and because of the usually small thickness of the adhesive layers, so-called interface elements and cohesive zone models are used, which model the adhesive as a two-dimensional interface and not as bulk, e.g. [8,9,46]. So far, modeling of this kind only takes into account tangential and normal jumps in the relative displacements of the substrates to each other in order to describe force transmission or, in the further course, also the damage behavior of the adhesive layer. Above all, the (in)elasticity of the adhesive with regard to membrane deformations, i.e. in-plane distortions without displacement jumps, is ignored. Especially with brittle adhesives, however, even small in-plane distortions can lead to pre-damage and thus negatively feed back to the remaining cohesive normal and tangential strength. In order to take these effects into account, we present a thermodynamically consistent, generalized interface model for small strains, which extends the conventional approaches by a membrane component and also allows a full coupling of all possible damage modes. A numerical example of the bonding of substrates with brittle epoxies demonstrates the performance and versatility of our model.

## 2. Classification of zero-thickness element models

Zero-thickness interfaces are characterized as two-sided surfaces which represent a thin layer of material. They are of lower dimension than the surrounding bulk. Accurate modeling of the interface behavior, especially for failure, is essential, since the interface, whose properties differ from the surrounding bulk, is often the weak link in a component. The deformation localizes in the interface which can result in decohesion or membrane degradation.

A mechanical interface can be considered as generalized if it allows for both, a jump[1] in the displacement $[\![\boldsymbol{u}]\!] \neq \boldsymbol{0}$ and the traction $[\![\boldsymbol{t}]\!] := [\![\boldsymbol{\sigma}]\!]\cdot\bar{\boldsymbol{m}} \neq \boldsymbol{0}$ across the interface, with the jump in the bulk Cauchy stress $[\![\boldsymbol{\sigma}]\!]$ and the interface normal vector $\bar{\boldsymbol{m}}$, see Table 1.

Cohesive zone models (CZM) [5,6,16] allow for displacement jumps $[\![\boldsymbol{u}]\!] \neq \boldsymbol{0}$ assuming that initially identical material points can separate. At

* Corresponding author.
*E-mail address:* lucie.spannraft@fau.de (L. Spannraft).

[1] The jump of a quantity is defined as $[\![\bullet]\!] = \bullet^{+} - \bullet^{-}$.

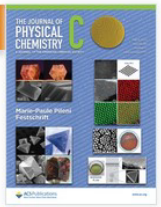
https://doi.org/10.1016/j.finmec.2022.100137
Received 17 August 2022; Received in revised form 25 October 2022; Accepted 25 October 2022
Available online 30 October 2022

# Resolution of Intramolecular Dipoles and a Push-Back Effect of Individual Molecules on a Metal Surface

Sergey Trishin, Tobias Müller, Daniela Rolf, Christian Lotze, Philipp Rietsch, Siegfried Eigler, Bernd Meyer*, and Katharina J. Franke*

Cite this: *J. Phys. Chem. C* 2022, 126, 17, 7667−7673
Publication Date: April 25, 2022
https://doi.org/10.1021/acs.jpcc.2c00334



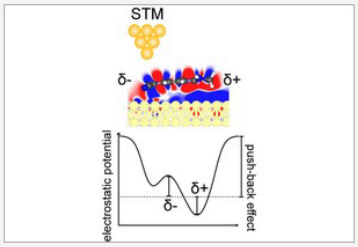



The Journal of Physical Chemistry C

**SUBJECTS:** Adsorption, Metals, Molecular structure, Molecules, Scanning tunneling microscopy

## Abstract

Molecules consisting of a donor and an acceptor moiety can exhibit large intrinsic dipole moments. Upon deposition on a metal surface, the dipole may be effectively screened and the charge distribution altered due to hybridization with substrate electronic states. Here, we deposit ethyl-diaminodicyanoquinone molecules, which exhibit a large dipole moment in the gas phase, on a Au(111) surface. Employing a combination of scanning tunneling microscopy and noncontact atomic force microscopy, we find that a significant dipole moment persists in the flat-lying molecules. Density functional theory calculations reveal that the dipole moment is even increased on the metal substrate as compared to the gas phase. We also show that the local contact potential across the molecular islands is decreased by several tens of meV with respect to the bare metal. We explain this by the induced charge-density redistribution due to the adsorbed molecules, which confine the substrate's wavefunction at the interface. Our local measurements provide direct evidence of this so-called push-back or cushion effect at the scale of individual molecules.



Forces in Mechanics 10 (2023) 100159

Contents lists available at ScienceDirect

Forces in Mechanics

journal homepage: www.sciencedirect.com/journal/forces-in-mechanics

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

Felix Weber [a,*], Maximilian Ries [b], Christof Bauer [a], Christian R. Wick [c], Sebastian Pfaller [b]

[a] Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Institute of Applied Mechanics & Competence Unit for Scientific Computing (CSC), Egerlandstrasse 5, 91058 Erlangen, Germany
[b] Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Institute of Applied Mechanics, Egerlandstrasse 5, 91058 Erlangen, Germany
[c] Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Institute for Theoretical Physics, PULS Group, Interdisciplinary Center for Nanostructured Films (IZNF) & Competence Unit for Scientific Computing (CSC), Cauerstrasse 3, 91058 Erlangen, Germany

ARTICLE INFO

*Keywords:*
Molecular dynamics
Finite element method
Multiscale modeling
Particle-continuum coupling
Simulation of polymers

ABSTRACT

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

## 1. Introduction

Due to the usage of polymers within an evermore enlarging range of engineering applications, a thorough understanding of their features relevant to fracture is vital. To influence the material behavior to exhibit specific properties, for instance, an increased fracture toughness [1] or the ability to self-heal [2], insights into molecular processes are indispensable. Numerical studies are very well suited to bridge the different time and length scales involved and to examine influencing factors isolated from each other, see e.g. [3,4]. However, numerical studies of fracture in polymers at atomistic or molecular resolution require powerful multiscale simulation techniques enabling non-affine boundary conditions, which are essential to appropriately capture the kinematics of the numerical specimen. In addition, such techniques can treat regions outside the vicinity of the crack tip at much coarser resolution and thus may significantly reduce the numerical effort.

Following a classification proposed by 5 [5], multiscale techniques can be classified as sequential and concurrent approaches. Contrary to sequential methods, concurrent coupling techniques establish an ongoing information transfer between the coarse and fine resolutions. The latter can be further subdivided into hierarchical and partitioned-domain techniques. In case of hierarchical methods, both scales exist simultaneously throughout the entire domain with the fine resolution typically subjected to periodic boundary conditions (PBC) and providing the constitutive relation for the coarse resolution. As a consequence, the highly localized character of a crack tip is hard to capture. A prominent example of such a hierarchical technique is the $FE^2$ method, see e.g. the study conducted by 6 [6], which can well capture

* Corresponding author.
*E-mail addresses:* felix.w.weber@fau.de (F. Weber), maximilian.ries@fau.de (M. Ries), christof.bauer@fau.de (C. Bauer), christian.wick@fau.de (C.R. Wick), sebastian.pfaller@fau.de (S. Pfaller).

https://doi.org/10.1016/j.finmec.2022.100159
Received 9 August 2022; Received in revised form 1 December 2022; Accepted 14 December 2022
Available online 21 December 2022

Forces in Mechanics 9 (2022) 100143

Contents lists available at ScienceDirect

Forces in Mechanics

journal homepage: www.sciencedirect.com/journal/forces-in-mechanics

# Evaluating the predictive character of the method of constrained geometries simulate external force with density functional theory

Christian R. Wick [a,c,*], Ece Topraksal [a], David M. Smith [b], Ana-Sunčana Smith [a,b,*]

[a] Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Institute for Theoretical Physics, PULS Group, Interdisciplinary Center for Nanostructured Films (IZNF), Cauerstrasse 3, Erlangen 91058, Germany
[b] Group for Computational Life Sciences, Division of Physical Chemistry, Ruđer Bošković Institute, Bijenička cesta 54, Zagreb 10000, Croatia
[c] Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Competence Unit for Scientific Computing (CSC), Martensstr. 5a, Erlangen 91058, Germany

ARTICLE INFO

*Keywords:*
COGEF
Density Functional Theory (DFT)
Mechanical force
Mechanochemistry
Molecular fracture
Mechanical bond scission
Mechanoradicals

ABSTRACT

Mechanochemistry is a fast-developing field of interdisciplinary research with a growing number of applications. Therefore, many theoretical methods have been developed to quickly predict the outcome of mechanically induced reactions. Constrained geometries simulate External Force (CoGEF) is one of the earlier methods in this field. It is easily implemented and can be conducted with most DFT codes. However, recently, we observed totally different predictions for model systems of epoxy resins in different conformations and with different density functionals. To better understand the conformational and functional dependence in typical CoGEF calculations we present a systematic evaluation of the CoGEF method for different model systems covering homolytic and heterolytic bond cleavage reactions, electrocyclic ring opening reactions and scission of non-covalent interactions in hydrogen-bond complexes. From our calculations we observe that many mechanochemical descriptors strongly depend on the functional used, however, a systematic trend exists for the relative maximum Force. In general, we observe that the CoGEF procedure is forcing the system to high energetic regions on the molecular potential energy profiles, which can lead to unexpected and uncorrelated predictions of mechanochemical reactions. This is questioning the true predictive character of the method.

## Introduction

It is well understood that mechanical forces induce versatile chemical reactions in polymeric materials at the molecular scale [1–5]. The types of reactions that can be triggered by mechanical energy range from simple heterolytic or homolytic bond breaking to unexpected and otherwise forbidden chemical reactions [3,4,6,7]. This opened up the field for synthesis of compounds with predetermined mechanochemical reactivity, so-called mechanophores [2,8–10]. However, the prediction of mechanochemical reactivity of polymer chains or mechanophores is very difficult by experimental means, so that computational methods became indispensable to investigate the induction of chemical reactivity by mechanical force and to streamline the design of new mechanophoric components [11–15]. While most computational methods that allow incorporation of an external force afford a priori knowledge of the expected reaction mechanism, the Constrained Geometries Simulate External Force method (CoGEF) only requires knowledge of the reactants [16]. The CoGEF method allows to investigate the mechanochemical strength of covalent bonds by density functional theory and, recently, it was validated as a predictive tool for mechanochemical reactivity [17]. While multidimensional approaches are also available [18], the classical 1D-CoGEF method is a prominent approach to study mechanochemical reactions due to its simplicity and broad availability. Indeed, similar approaches were already utilized to study the molecular response to external forces before the name CoGEF [16] was suggested by Beyer in 2000 [14].

While investigating the mechanochemical response of epoxy resins with the CoGEF method, we observed that the CoGEF prediction can strongly depend on the initial conformation and the density functional used. Therefore, in this contribution we present an evaluation of the functional dependence of the CoGEF method covering a broad spectrum of different mechanochemical reactivities and force ranges. The results indicate that multiple reactions or reaction cascades can become accessible at the high energetic regions typically observed in 1D-CoGEF calculations. Nevertheless, general relative trends of the mechanochemically interesting descriptors remain mostly independent on the

* Corresponding authors.
*E mail addresses:* christian.wick@fau.de (C.R. Wick), ana-suncana.smith@fau.de (A.-S. Smith).

https://doi.org/10.1016/j.finmec.2022.100143
Received 2 August 2022; Received in revised form 2 November 2022; Accepted 2 November 2022
Available online 8 November 2022

RETURN TO ISSUE | ‹ PREV **RESEARCH ARTICLE** NEXT ›

# Improving the Performance of Supported Ionic Liquid Phase Catalysts for the Ultra-Low-Temperature Water Gas Shift Reaction Using Organic Salt Additives

Patrick Wolf, Christian R. Wick, Julian Mehler, Dominik Blaumeiser, Simon Schötz, Tanja Bauer, Jörg Libuda, David Smith, Ana-Sunčana Smith, and Marco Haumann*

**Cite this:** *ACS Catal.* 2022, 12, 9, 5661−5672
Publication Date: April 27, 2022
https://doi.org/10.1021/acscatal.1c05979


Article Views 414 | Altmetric 6 | Citations -
LEARN ABOUT THESE METRICS
Share Add to Export RIS

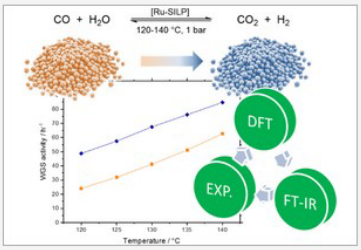
ACS Catalysis



**SUBJECTS:** Additives, Anions, Catalysts, Free energy, Precursors

## Abstract

The water gas shift reaction (WGSR) is catalyzed by supported ionic liquid phase (SILP) systems containing homogeneous Ru complexes dissolved in ionic liquids (ILs). These systems work at very low temperatures, that is, between 120 and 160 °C, as compared to >200 °C in the conventional process. To improve the performance of this ultra-low-temperature catalysis, we investigated the influence of various additives on the catalytic activity of these SILP systems. In particular, the application of methylene blue (MB) as an additive doubled the activity. Infrared spectroscopy measurements combined with density functional theory (DFT) calculations excluded a coordinative interaction of MB with the Ru complex. In contrast, state-of-the-art theoretical calculations elucidated the catalytic effect of the additives by non-covalent interactions. In particular, the additives can significantly lower the barrier of the rate-determining step of the reaction mechanism *via* formation of hydrogen bonds. The theoretical predictions, thereby, showed excellent agreement with the increase of experimental activity upon variation of the hydrogen bonding moieties in the additives investigated.




**KEYWORDS:** water gas shift reaction, supported ionic liquid phase, ruthenium, methylene blue, electronic interaction

### 2.2.2 Submitted / accepted / in press and other publications

(in alphabetical order)

| | |
|---|---|
| 1 | **B. Mathur**, R. Prabhakaran and D. Koehn, "Evolving geometries, topologies, and apertures in fracture networks: quantitative insights from lattice modeling," submitted to FRASCAL Special Issue in Forces in Mechanics, 2022; preprint available at https://opus4.kobv.de/opus4-fau/frontdoor/index/index/docId/20174 |
| 2 | D. T. Huamani, **W. Zhao**, and S. Pfaller, "A particle-continuum coupling method for amorphous polymers with multiple particle-based domains", submitted to *Proceedings in Applied Mathematics and Mechanics* https://doi.org/10.1002/pamm.202200245 |
| 3 | **J. Konrad**, D. Zahn, "Interaction Forces in reinforced Epoxy Resins: from molecular Scale Understanding towards mesoscale Interfaces", submitted to FRASCAL Special Issue in Forces in Mechanics, 2022 |
| 4 | M. Livraghi, K. Höllring, **C. R. Wick**, D. M. Smith, A.-S. Smith: PULS-Group/Percolation-Analyser v1.0.0 (publication_v1.0), Zenodo, 2022; software snapshot release available at https://doi.org/10.5281/zenodo.5838104 |
| 5 | M. Livraghi, S. Pahi, D. M. Smith, **C. R. Wick** and A.-S. Smith, "Block chemistry for accurate modeling of epoxy resins," submitted, 2022. https://doi.org/10.26434/chemrxiv-2022-d5cwr |
| 6 | **M. Ries**, **C. Bauer**, **F. Weber**, P. Steinmann, S. Pfaller: Characterization of the material behavior and identification of effective elastic moduli based on molecular dynamics simulations of coarse- grained silica: dataset (2022) Zenodo https://doi.org/10.5281/zenodo.5557076 |
| 7 | **M. Ries**, V. Dötschel, J. Seibert, S. Pfaller: "A self-avoiding random walk algorithm (SARW) for generic thermoplastic polymers and nanocomposites" (2022) Zenodo https://doi.org/10.5281/zenodo.6245699 |
| 8 | **M. Ries**, J. Seibert, P. Steinmann, S. Pfaller, "Applying a generic and fast coarse-grained molecular dynamics model to extensively study the mechanical behavior of polymer nanocomposites: supplementary information and dataset," dataset (2022) Zenodo. https://doi.org/10.5281/zenodo.6245701 |
| 9 | **M. Ries**, **F. Weber**, G. Possart, P. Steinmann, S. Pfaller: A quantitative interphase model for polymer nanocomposites: Verification, validation, and consequences regarding size effects: dataset (2022) Zenodo. https://doi.org/10.5281/zenodo.7024651 |
| 10 | **J. Ritter**, M Zaiser: "High Strain Rate Compressive Failure of Porous Brittle Snow Microstructures Simulated by Peridynamics" (2022), EGU General Assembly 2022, Vienna, Austria, 23–27 May 2022, EGU22-12376 https://doi.org/10.5194/egusphere-egu22-12376 |
| 11 | **A. Santarossa**, O. D'Angelo, A. Sack, T. Poeschel: "Effect of Particle Size on the Suction Mechanism in Granular Grippers," accepted for Granular Matter, 2022. https://doi.org/10.48550/arXiv.2209.04342 |
| 12 | **L. Spannraft**, P. Steinmann, J. Mergheim: "A generalized anisotropic damage interface model for finite strains, submitted, 2022. https://nbn-resolving.org/urn:nbn:de:bvb:29-opus4-201567 |
| 13 | **A. M. Velasco**, J. D. Muñoz, T. Pöschel: "Adaptative Resolution Increase for the Fracture of Brittle Solids with a Multi-sphere Discrete Element Method," in: 15th World Congress on Computational Mechanics, page 331, 2022. https://www.wccm2022.org/dl/index/book_of_abstracts.pdf |
| 15 | N. R. Varela-Rosales, **A. Santarossa,** M. Engel, T. Poeschel: "Effect of size Dispersity on the Efficiency of Granular Dampers," (oral presentation), ESMC 2022 - 11th European Solid Mechanics Conference, 4-8 July, 2022, Galway, Ireland. https://az659834.vo.msecnd.net/eventsairwesteuprod/production-abbey-public/73adf436c1e747ca87d4ead5620f0d49 |
| 15 | **F. Weber**, **M. Ries**, **C. Bauer**, **C. R. Wick**, S. Pfaller On equilibrating non-periodic molecular dynamics samples for coupled particle-continuum simulations of amorphous polymers: dataset https://doi.org/10.5281/zenodo.6868243 |
| 16 | **C. R. Wick**, E. Topraksal, D. M. Smith, A.-S. Smith: cogef.py: Tools to run COnstraint Geometries simulate External Force calculations (v1.8.0), Zenodo, 2022; software snapshot release available at https://doi.org/10.5281/zenodo.7079733 |
| 17 | **C. R. Wick**, E. Topraksal, D. M. Smith, A.-S. Smith, "Predicting mechanochemical reactivity with the method of constrained geometries simulate external force" dataset (2022) Zenodo. https://doi.org/10.5281/zenodo.6948605 |

### 2.2.3 Patents

"Granulat aus mit weichem Material ummantelten harten Teilchen zur Verwendung in Greifern für Roboter"
Patent application DE10 2022 200 732.8. Authors: Holger Götz, Patric Müller, **Angel Santarossa**, Achim Sack, Thorsten Pöschel

"Granulat-Greifer mit Saugwirkung"
Patent application DE 10 2022 204 185.2. 2022. Authors: **Angel Santarossa**, Achim Sack, Olfa d'Angelo, Walter Pucheanu, Thorsten Pöschel

## 2.3 Participation in conferences and workshops

**Christof Bauer**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 04.04.2022 / 06.04.2022 | EMMC18 | Oxford, UK (hybrid) | Talk: *An adaptive discrete-to-continuum coupling scheme for scale bridging simulations of amorphous polymers* |
| 05.06.2022 / 09.06.2022 | ECCOMAS CONGRESS 2022 | Oslo, Norway | Talk: *An adaptive multiscale coupling method for thermo-plastic polymers* |

**Deepak Jadhav**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 27.06.2022/ 01.07.2022 | ECF23, European Conference on Fracture 2022 | Funchal, Portugal | Participation only |

**Paras Kumar**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 04.06.2022 / 09.06.2022 | ECCOMAS CONGRESS 2022 | Oslo, Norway | Talk: *Phase-Field Fracture Models for Polymer Nano-Composites*<br>Co-Organization of MS (jointly with D. Phansalkar, P. Carrara, S. Leyendecker, J. Mergheim, L. De Lorenzis and P. Steinmann): Recent developments and current issues in the phase-field modeling of fracture [https://www.eccomas2022.org/frontal/ProgMS.asp?id=95] |
| 31.07.2022 / 05.08.2022 | WCCM-APCOM 2022 | Yokohama, Japan (virtual) | Participation only<br>Co-Organization of MS (jointly with D. Phansalkar, J. Mergheim, S. Leyendecker and P. Steinmann): Computational Fracture Modeling in Heterogeneous Materials - Recent Advances and Future Challenges [https://www.wccm2022.org/minisymposia0123.html] |

**Marie Laurien**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 15.08.2022 / 19.08.2022 | 92nd GAMM | Aachen, Germany | Talk: *Nonlocal degrading interfaces* |

**Tobias Müller**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 02.07.2022 / 08.07.2022 | WATOC 2022 | Vancouver, Canada | Poster: *Kinetic trapping in brittle crack opening* |
| 04.09.2022 / 09.09.2022 | DPG 2022 | Regensburg, Germany | Poster: *Kinetic trapping in brittle crack opening* |

**Dhananjay Phansalkar**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 05.06.2022 / 09.06.2022 | ECCOMAS CONGRESS 2022 | Oslo, Norway | Talk: *A spatially adaptive phase-field model for dynamic fracture*<br>Co-Organization of MS (jointly with P. Kumar, P. Carrara, S. Leyendecker, J. Mergheim, L. De Lorenzis and P. Steinmann): Recent developments and current issues in the phase-field modeling of fracture [https://www.eccomas2022.org/frontal/ProgMS.asp?id=95] |
| 31.07.2022 / 05.08.2022 | WCCM-APCOM 2022 | Yokohama, Japan (virtual) | Participation only<br>Co-Organization of MS (jointly with P. Kumar, J. Mergheim, S. Leyendecker and P. Steinmann): Computational Fracture Modeling in Heterogeneous Materials - Recent Advances and Future Challenges [https://www.wccm2022.org/minisymposia0123.html] |

**Maximilian Ries**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 15.08.2022 / 19.08.2022 | 92nd GAMM | Aachen, Germany | Talk: *Interphase characterization in polystyrene-silica nanocomposites based on molecular dynamics simulations.* |
| 21.09.2022 / 23.09.2022 | 9th GACM 2022 | Essen, Germany | Talk: *Studying the mechanical behavior of polymer nanocomposites with a generic and fast molecular dynamics model* |

**Jonas Ritter**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 23.05.2022 / 27.05.2022 | EGU General Assembly 2022 | Vienna, Austria | Talk: *High Strain Rate Compressive Failure of Porous Brittle Snow Microstructures Simulated by Peridynamics* |

**Christian Ritterhoff**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 08.06.2022 / 10.06.2022 | From Electrons to Phase Diagrams | Bochum, Germany | Participation only |

| | | | |
|---|---|---|---|
| 22.08.2022 / 25.08.2022 | Psi-k conference | Lausanne, Switzerland | Poster: *Accelerating plane-wave-based ab initio molecular dynamics by optimization of Fast-Fourier Transforms for modern HPC architectures* |
| 04.09.2022 / 09.09.2022 | DPG 2022 | Regensburg, Germany | Poster: *Accelerating plane-wave-based ab initio molecular dynamics by optimization of Fast-Fourier Transforms for modern HPC architectures* |

**Maurice Rohracker**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 21.09.2022 / 23.09.2022 | 9th GACM 2022 | Essen, Germany | Talk: *Comparison of Adaptive Spatial Refinement Strategies in Phase-Field Simulations for Brittle Fracture* |

**Ina Schmidt**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 26.06.2022 / 29.06.2022 | ESB2022 | Porto, Portugal | Poster: *Epiphyseal bone healing within continuum bone remodelling* |
| 02.11.2022 / 04.11.2022 | 5th AfriComp | Cape Town, South Africa | Talk: *Continuum bone remodelling considering mechanical stimulation and epiphyseal bone healing* |

**Ruaridh Smith**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 23.05.2022 / 27.05.2022 | EGU General Assembly 2022 | Vienna, Austria | Talk: *Using fractured outcrops to calculate permeability tensors. Implications for geothermal fluid flow within naturally fractured reservoirs* https://doi.org/10.5194/egusphere-egu22-11868 |

**Joscha Seutter**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 04.10.2022 / 07.10.2022 | Annual Meeting of GRK 2339 (IntComSin) | Kloster Weltenburg, Germany | Talk: *Existence of quasi-static crack evolution for atomistic systems* |

**Sukhminder Singh**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 31.07.22 / 05.08.22 | WCCM-APCOM 2022 | Yokohama, Japan (virtual) | Talk: *Surrogate-based stochastic optimization for enhancing interfacial fracture resistance of heterogeneous structures* |

**Felix Weber**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 28.09.2022 / 30.09.2022 | ISPN 2022 | Lorient, France | Talk: *Modeling size effects in polymer nanocomposites with a quantitative interphase model* |

**Christian Wick**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 03.05.2022 / 05.05.2022 | Intern. CataLysis Networking Conference 2022 | Kassel, Germany | Poster presentation: *Modelling SILP Catalysis: The Water-Gas-Shift Reaction* |
| 27.06.2022 / 29.06.2022 | 55. Jahrestreffen Deutscher Katalytiker, 2022 | Weimar, Germany | Poster presentation: *Modelling SILP Catalysis: The Water-Gas-Shift Reaction* |
| 28.11.2022 / 29.11.2022 | NHR-Atomistic Simulation Symposium 2022 | Paderborn, Erlangen, Berlin, Germany (online) | Participation only |

**Wuyang Zhao**

| From / to | Name of conference | Location | Title of own presentation / title of own poster presentation / participation only |
|---|---|---|---|
| 05.06.2022 / 09.06.2022 | ECCOMAS CONGRESS 2022 | Oslo, Norway | Talk: *An atomistic-to-continuum coupling method for fracture simulations of amorphous polymers* |
| 15.08.2022 / 19.08.2022 | 92nd GAMM | Aachen, Germany | Talk: *Investigation of time-temperature superposition for amorphous thermoplastics at finite strain based on molecular dynamics simulations* |
| 05.09.2022 / 08.09.2022 | CMM - SolMech 2022 | Świnoujście, Poland | Talk: *A domain-decomposition MD-FE coupling method for fracture simulations of amorphous polymers* |

## 2.4 Collaborations with other research institutions

**Christof Bauer**

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

**Tarakeshwar Lakshmipathy**

| Partner institute | Researchers involved | Research topic |
|---|---|---|
| ICAMS, Ruhr-Universität Bochum; Germany | Alexander Hartmaier | Influence of crack tip radius on fracture behaviour |

| | | |
|---|---|---|
| ICAMS, Ruhr-Universität Bochum, Germany | Thomas Hammerschmidt | Benchmarking of interatomic potentials in fracture simulations |
| Division of Mechanics, Lund University, Sweden | Pär A. T. Olsson | Benchmarking of interatomic potentials in fracture simulations |

**Maximilian Ries**

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

**Angel Santarossa**

| Partner institute | Researchers involved | Research topic |
|---|---|---|
| Universidad Nacional de Sur, Departamento de Física, Bahía Blanca, Argentina | Leopoldo Gómez, Laureano Ortellado | Crack Front Segmentation in Mixed Mode I+III Hydraulic Fracture in Hydrogels |

**Ina Schmidt**

| Partner institute | Researchers involved | Research topic |
|---|---|---|
| Technische Hochschule Nürnberg, Mechanical Engineering and Building Services Engineering | Areti Papastavrou | Biomechanics |

**Lucie Spannraft**

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

**Anna Titlbach**

| Partner institute | Researchers involved | Research topic |
|---|---|---|
| Glasgow Computational Engineering Centre (GCEC), University of Glasgow, United Kingdom | Andrew McBride | Modelling and Simulation of the flexoelectric effect in human bone using a coupled micromorphic approach |

**Felix Weber**

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

**Christian Wick**

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

**Wuyang Zhao**

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

# 3 Qualification Concept

## 3.1 Qualification programme

The qualification programme comprises

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

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

### 3.1.1 Qualification days

During each lecture period (typically from October to February and from April to July), one day per week is reserved for “qualification days” covering FRASCAL mini lectures including special seminars and FRASCAL schools, soft skills trainings, and seminars. Furthermore, all presentations of student theses supervised by FRASCAL doctoral researchers take place within the framework of the so-called student seminar series of FRASCAL ($S^3$ FRASCAL). Social events accompanying qualification days encourage close exchange between the doctoral researchers and the mentoring teams.

**FRASCAL Mini Lectures**

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

The mini lectures are usually given by FRASCAL PAs, but occasionally also by FRASCAL doctoral researchers, scientists from the participating departments or external experts.

With the start of the 2nd year of FRASCAL in 2022, the mini lecture series has also started all over again. However, since Manuel Friedrich could be won as a new PA for FRASCAL, the mini lecture programme was expanded and a lecture on the topic of mathematical skills ("Introduction to the Approximation of Free Discontinuous Problems") was offered.

*Table 10: Mini lectures*

| | Date | Title | Lecturer |
|---|---|---|---|
| 01 | 21 April 2022 | Introduction to Tensor Calculus | P. Steinmann |
| 02 | 25 April 2022 | Introduction to Approximation of Free-Discontinuity Problems | M. Friedrich |
| 03 | 03 June 2022 | Introduction to the Finite Element Method | S. Pfaller |
| 04 | 24 June 2022 | Introduction to Numerics | R.T. Sato de Almagro, D. Huang, G. Capobianco |
| 05 | 08 July 2022 | Introduction to Concurrent Modelling | S. Pfaller |
| 06 | 25 November 2022 | Introduction to Mesoscopic Modelling | P. Moretti |

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


*Figure 56: Impressions of the two mini lectures and photo of the mini lecture notes.*

## 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.

In 2022, we were able to gain two excellent scientists for this purpose: Dr. László Mészáros on the initiative of the associated doctoral researcher Maximilian Ries and Prof. Reza Soheilifard, who was working as a visiting researcher with PA Dirk Zahn at the time.

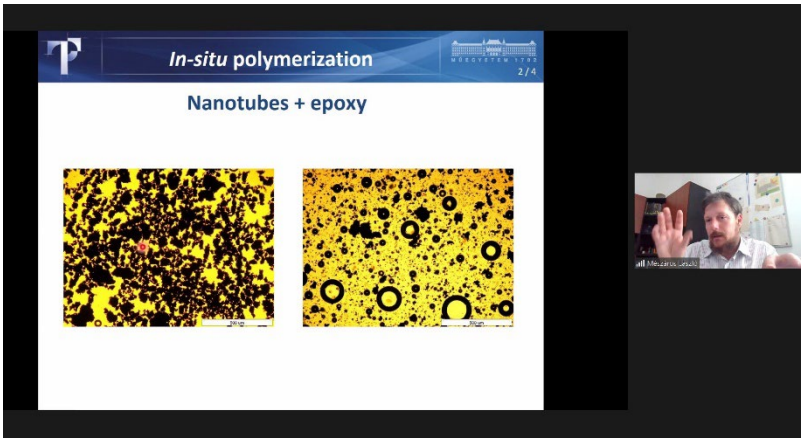



*Figure 57: László Mészáros during his virtual special seminar.*

*Table 11: Special seminars*

| | Date | Title | Lecturer |
|---|---|---|---|
| 01 | 01 July 2022 | Introduction to Polymer Nanocomposites (virtual) | Dr. László Mészáros, Budapest Univ. of Technology & Economics, HU |
| 02 | 02 September 2022 | Fibre Fracture: Atomic Mechanisms and Overall Mechanisms | Prof. Reza Soheilifard, Hakim Sabzevari University, IR |

## FRASCAL schools

The FRASCAL schools format, newly established in 2022, enables doctoral researchers to organise completely independently workshops lasting several days, preferably away from home, on a topic of their choice, in order to expand important competences for their research and to strengthen the FRASCAL team spirit. The FRASCAL schools are to be held in loose succession as needed.

*Table 12: FRASCAL schools*

| From / to | Name of school | Location |
|---|---|---|
| 13.10.2022 / 14.10.2022 | 1st FRASCAL Autumn School: Software Development | Hotel Fuchsbräu, Beilngries, Germany |

The researchers of all thirteen FRASCAL research projects independently organised a two-day hybrid autumn school on software development at the Hotel Fuchsbräu in Beilngries and on Zoom. The aim of this two-day event was not only to improve software development in C++, but also to re-establish social contacts after the pandemic years had subsided, which succeeded perfectly in the charming ambience of the medieval baroque town of Beilngries, located about an hour from Erlangen in the middle of the Altmühltal Nature Park directly on the Main-Danube Canal.

The 1st FRASCAL Autumn School was split into two parts:On the first day, expert and full-time professor Prof. Dr.-Ing. Harald Köstler (FAU) introduced the doctoral researchers to the features of modern C++. He regularly teaches at the Chair of Computer Science 10, which develops various types of software, e.g. HPC simulation software for physical applications, but also software engi-

*Figure 58: Impressions of the 1st FRASCAL Autumn School in Beilngries.*

neering for HPC including code generation and continuous benchmarking on HPC systems. He explained the powerful standard template library (STL) of C++ and gave useful tips for implementation.

On the second day, Dr.-Ing. Klaus Iglberger (freelance C++ trainer and consultant) focused on different design patterns for software development in C++. Dr.-Ing. Klaus Iglberger is a former colleague of Prof. Köstler and one of the leading experts in software development in modern C++. In addition to his consulting work in the German industry, he is an international C++ trainer, initiator and lead designer of the C++ mathematical library Blaze, organiser of the Munich C++ user group, and initiator and co-chair of the Cppcon Software Design Track.

During his class on the second day, the young researchers were exemplarily introduced to different design patterns by solving a similar problem using different design patterns resulting in readable and efficient software, a major goal for sustainable software. As a result, we presented that there is no one solution for software development since each design pattern has its pros and cons. However, the students were taught to decide on their own to choose the best-suited design pattern for the software development of their application to solve their specific problems efficiently and correctly.

In the remaining evening hours, the participants set off for a walk to the Schloss Hirschberg, fresh air and good conversations sweetened the hard day's work and a social get-together at the Hotel Fuchsbräu rounded off the programme.

The newly conceived series of FRASCAL schools was successfully opened with the workshop on „Software Development“ with new and profound programming knowledge and a strong team spirit.

**FRASCAL Soft Skills Trainings**

In 2022, four soft skills seminars (numbers 01 - 03 and 05 in Table 13) were held, which were specially designed for FRASCAL doctoral students and tailored to their needs and wishes. The seminars on “Research Data Management” and “Good Scientific Practice” were compulsory for all FRASCAL doctoral researchers. In addition, the workshop "Strategies to Handle your Stage Fright" took place with FRASCAL participation, which was organised by the Graduate School EAM - initiated by the FRASCAL coordination. Finally, the FRASCAL doctoral researchers had the opportunity to participate in a workshop organised by the Faculty of Engineering's research coordinator: “How does Science Slam Work". The lecturer Stefan Rieger from ZIWIS (FAU) prepared the participants to be able to present their research topic to a layperson within three minutes in an entertaining, lively and generally understandable way, so to speak.

*Table 13: Soft skills trainings*

| | Date | Title | Lecturer |
|---|---|---|---|
| 01 | 16 February 2022 | How to Write a Scientific Paper | Prof. J. Saramäki, Aalto, Finland |
| 02 | 29 April 2022 | Research Data Management | Dr. J. Rohrwild, FAU |
| 03 | 20 May 2022 | Good Scientific Practice | Dr. C. Schmitt-Engel, FAU |
| 04 | 21 - 22 September 2022 | Strategies to Handle your Stage Fright | P. Gründel (Nürnberg) |
| 05 | 12 October 2022 | FRASCAL RDM Workshop | PD Dr. S. Pfaller, FAU |
| 06 | 11 November 2022 | How does Science Slam Work | S. Rieger, FAU |

The seminar "How to Write a Scientific Paper" was initiated by the associated doctoral researcher Maximilian Ries. He read the book "How to Write a Scientific Paper" by Jari Saramäki (full professor at the Department of Computer Science, Aalto University, Finland), which helped him a lot in writing his own publications. This led to the idea of inviting Jari Saramäki to a seminar to teach all FRASCAL doctoral researchers his step-by-step top-down approach, which makes it easier to turn results into research papers that are focused, exciting and worth reading. Shortly after Maximilian Ries contacted Jari Saramäki, the seminar took place in virtual form. The event was very well received and

not only FRASCAL doctoral researchers attended, but also some of the principal advisors and a large number of FASCAL external interested parties.

The seminar focused on the process of writing rather than technicalities, breaking this process down into manageable sections. How do you choose the main topic of your paper? How does one write the abstract sentence by sentence? How does one structure the essay? How do you turn the outline into a first draft and then into a finished manuscript? What to do if you get stuck? And finally, how do you deal with critical reviews?

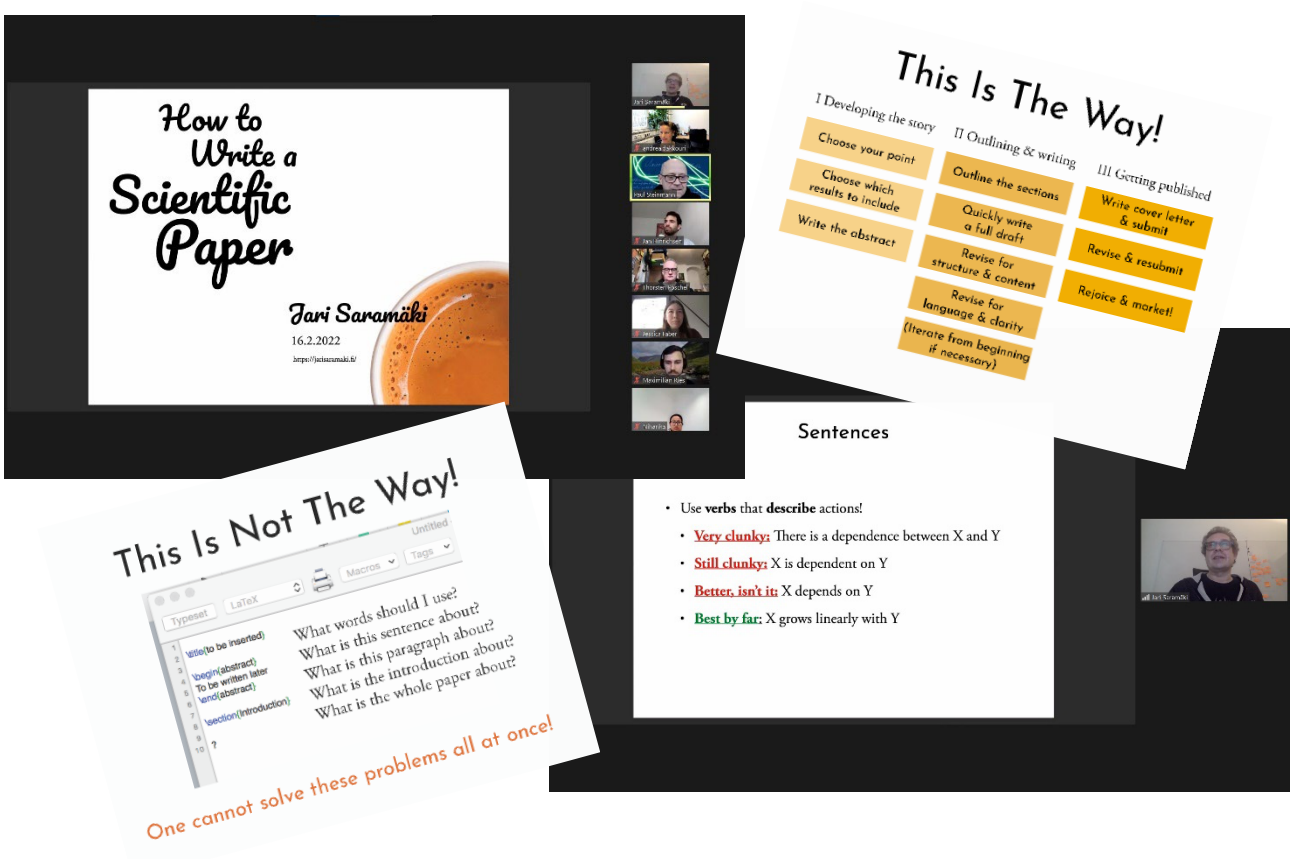



*Figure 59: Soft skills seminar "How to Write a Scientific Paper" with Jari Saramäki.*

Although the seminar was primarily aimed at doctoral researchers, the principal advisors were also able to take away some insights for themselves. A repetition of this seminar for the next cohort is firmly planned.

### FRASCAL Seminars

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

In 2022, one FRASCAL seminar took place as a hybrid event, where the doctoral researchers and associated doctoral researchers of the second cohort had the opportunity to present the research results of their first doctoral year.

*Table 14: FRASCAL seminars*

| | Date | Subject | Mode |
|---|---|---|---|
| 01 | 19 December 2022 | 7. FRASCAL Seminar | Presentations by six doctoral researchers and three associated doctoral researchers |

Programme see Appendix 1

**FRASCAL Retreats**

After approximately 3 and 18 months, two FRASCAL retreats are held for each cohort, in which each doctoral researcher must participate, focusing on the internal evaluation of FRASCAL's scientific progress. For this purpose, the doctoral researchers and associated doctoral researchers report on their scientific activities to all members of FRASCAL, which enables further assessment of the scientific progress of the doctoral projects. The FRASCAL retreats take place as two-day seminars at suitable, selected locations outside the FAU campus and are accompanied by workshops, reports on career paths and social activities for informal get-togethers.

*Table 15: FRASCAL retreats*

| | Date | Type | Location |
|---|---|---|---|
| 01 | 4 - 5 May 2022 | 2. FRASCAL retreat | Hotel Arvena, Bad Windsheim |

Programme see Appendix 2

The second FRASCAL retreat took place on 5 and 6 May 2022 at the Hotel Arvena Reichsstadt in the small historic town of Bad Windsheim.

The spokesperson Paul Steinmann initiated the programme on the first day with a brief welcome and introductory speech. This was followed by the presentations of the doctoral researchers of the second cohort on their latest research updates and their master thesis. Following the presentations, one of the FRASCAL principal advisors, Manuel Friedrich, introduced his outstanding academic and professional career to the group.

*Figure 60: FRASCAL members at the 2nd FRASCAL retreat in Bad Windsheim. (Image: A. Dakkouri-Baldauf)*

*Figure 61: Stimulating discussions at the RDM workshop. (Image: A. Dakkouri-Baldauf)*

In the afternoon session, a workshop on “Research Data Management (RDM)” was held where Sebastian Pfaller discussed different data management schemes with the doctoral researchers. In parallel, a workshop was held with the FRASCAL principal advisors to develop strategies for the preparation of the upcoming renewal proposal.

The workshops were followed by a walking tour of the beautiful Franconian Open-Air Museum where the researchers got a chance to bond in smaller groups.

After a sumptuous dinner, the evening event began with the presentation of certificates awards – the “FRASCAL Glass Award“ – to the doctoral researchers of the first cohort for outstanding achievements in their research fields. Afterwards, the results of the RDM workshop were presented by the sub-groups from the workshop.

Day 2 started with the remaining presentations by the doctoral researchers of the second cohort, followed by a poster session with poster blitz by the doctoral researchers from the first cohort. Everyone had exactly one minute to present her/his poster before the poster session, which was partly done in a very entertaining way. The posters showed a kind of visual outline of their dissertation, true to the motto „Tell the story of your dissertation …“. The poster session catalysed the dialogues and knowledge exchange between various research groups.

*Figure 62: Presentation of the certificate and the glass FRASCAL award. (Image: F. Weber)*

*Figure 63: Poster session at the 2nd FRASCAL retreat of FRASCAL. (Image: A. Dakkouri-Baldauf)*

Later, the workshop groups presented the results of their brainstorming session during the RDM workshop in an attempt to develop a sustainable and user-friendly data management system. Finally, the retreat ended with the closing session talk by Paul Steinmann.

The second FRASCAL retreat at Bad Windsheim was informative as well as refreshing. Interactions between the researchers from varied backgrounds encouraged collaborations and incubated new research ideas.

(Text: Bakul Mathur)

Part 2 of the RDM workshop took place in the afternoon session with a detailed discussion on the structure of the RDM systems. Right before the workshop, the doctoral candidates expressed their gratitude to Andrea Dakkouri-Baldauf for her exceptional and continuous support to the FRASCAL group. Following the workshop, FRASCAL principal advisors Michael Stingl and Daniel Koehn enriched the group with their life stories and professional achievements.

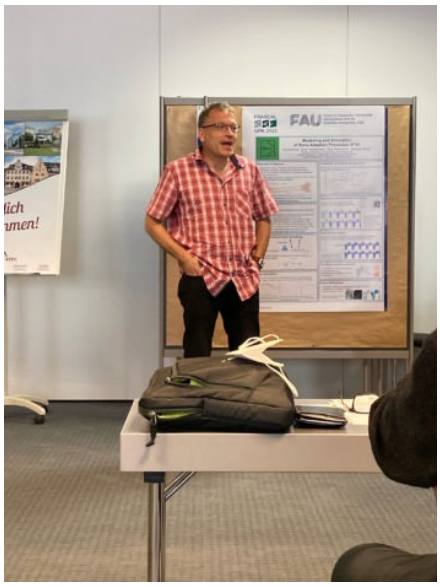



*Figure 64: FRASCAL PA Daniel Koehn. (Image: J. Deserno)*


*Figure 65: The FRASCAL doctoral researchers of the first cohort proudly present their certificates and awards. (Image: A. Dakkouri-Baldauf)*

## TOPZ

The digital format called FRASCAL TOPZ (Topical Overview Presentation Zoomposium), typically, once per week, was used for an informal get-together in ZOOM, where the PAs, the spokespersons, the doctoral and associated doctoral researchers, the postdoc, and the scientific coordinator were present. Typically, the latest scientific progress and open questions from one doctoral project were briefly presented and jointly discussed. Moreover, FRASCAL TOPZs provided an informal atmosphere to discuss any organisational, administrational, and topical issues related to FRASCAL in a relaxed manner. Active participation in the TOPZ was expected of every doctoral researcher. In 2022, a total of 19 TOPZ took place, so that on average each doctoral project was presented twice.

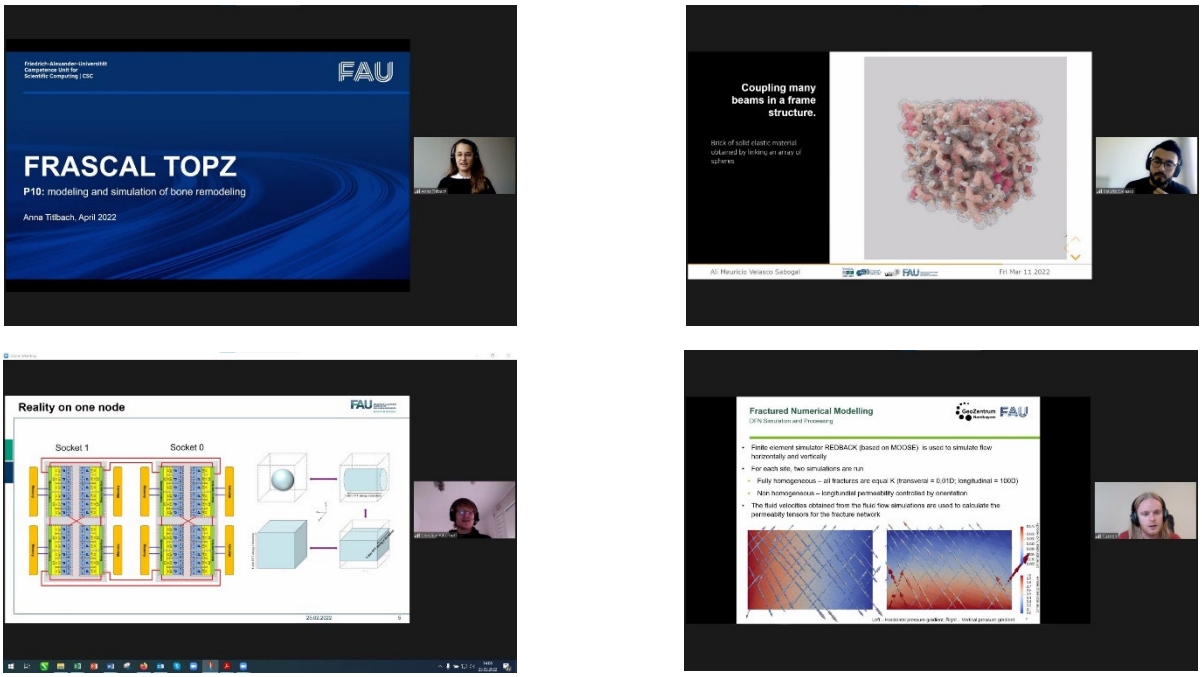



*Figure 66: Topical Overview Presentation Zoomposium (TOPZ): Anna Titlbach (top left), Ali Mauricio Velasco Sabogal (top right), Christian Ritterhoff (bottom left) and Ruaridh Smith (bottom right).*

## Language Coaching in Scientific English

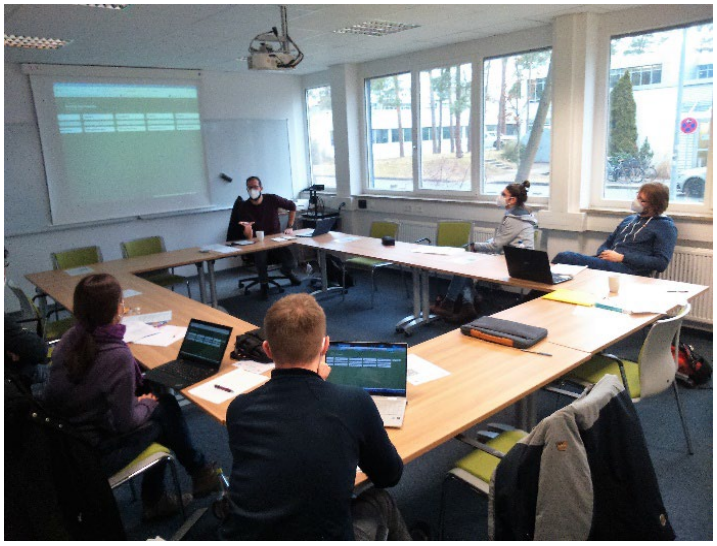


*Figure 67: English coaching with Paul Gahman. (Image: J. Ritter)*

Publications in international journals, presentations at international conferences, and scientific exchange with international researchers require proficiency in scientific English. Paul Gahman from the “FAU Language Centre”, a professional English language coach was available for the FRASCAL participants to train oral presentations, to proofread English publications, and to give English classes in each lecture period. Attendance of English classes is optional.

Since both the first and second cohorts of FRASCAL doctoral researchers participated in English coaching in 2022, the group was divided according to their different needs in the summer semester, and tailored courses were offered in rotation.

*Table 16: Language coaching in scientific English*

| Lecture period | Topic |
|---|---|
| Winter semester 2021/2022 | Practising the Q&A Session |
| | Continued Practice with Common Mistakes and Varying Sentence Structure; Targeting Written Language Mistakes, Advanced Transitional Phrases |
| | Intent vs Purpose, Course Recap, Course Planning:<br>Advanced Transitional Phrases, Forgetting What to Say, Targeting Written Language Mistakes |
| Summer semester 2022 | Group 1 (Newer group): Identifying and tactics for overcoming pronunciation issues due to L1 (native tongue) interference |
| | Group 2 (Experienced Group): Paraphrasing and re-writing for the lit review section |
| | Group 1: What to Say When at a Loss for Words:<br>Phraseology for buying time when speaking and unsure of what to say. We will also be taking a deep dive in intonation and rhythm in English |
| | Group 2: Paraphrasing and Sentence Reformulation:<br>Employing transitional word variety to achieve greater sentence complexity |
| | Group 1: Practicing Q&A Sessions, Articulation & Enunciation:<br>Targeting hurdles in Q&A sessions; mock Q&A sessions based on your current/previous research; work on typical English articulation and enunciation techniques via assimilation to improve fluency |
| | Group 2: Punctuation Review and Maintaining a Through-line in Writing:<br>Reviewing commas rules; ensuring coherence when writing |
| | Group 1: Reviewing Problematic Sounds and Punctuation:<br>Expansion work on pronunciation/enunciation issues based on those identified in first lecture; review of punctuation rules (commas and hyphens) in English |
| Winter semester 2022/2023 | Presenting Your Research: Pitfalls and things to look out for while presenting; presenting your research succinctly; practice with elevator pitches |
| | Individual Consultations |
| | Mock Presentation: The presentation will also have a Q&A session with feedback and further practice. Otherwise, additional speaking practice will be given during the lecture |
| | Individual Consultations |
| | Mock Presentation: The presentation will also have a Q&A session with feedback and further practice |

## 3.2 Visiting researcher programme

*Table 17: Visiting researchers*

| From / to | Guest | Topic |
|---|---|---|
| 15.02.2022 | **Prof. Juri Saramäki**, Dept. of Computer Science, Aalto University, Finland | Soft skills seminar: "How to write a scientific paper?"<br>**Organiser:** Maximilian Ries (P6) |
| 01.07.2022 | **Dr. László Mészáros**, Budapest University of Technology and Economics, Department of Polymer Engineering, Hungary | Special seminar: "Introduction to polymer nanocomposites", preparation and structure of polymer matrix nano- and hybrid composites |
| 13.10.2022 | **Prof. Harald Köstler,** FAU Erlangen-Nuremberg, Department of Computer Science, Erlangen, Germany | FRASCAL Autumn School: "Features of Modern C++"<br>**Organiser:** Felix Weber (P6) |
| 14.10.2022 | **Dr. Klaus Iglberger**, Freelancer, Germany | FRASCAL Autumn School: "Software Development in Modern C++"<br>**Organiser:** Felix Weber (P6) |
| 09.11.2021 / 13.11.2021 | **Prof. Michael Ortiz**, California Institute of Technology, Pasadena, CA, USA | Collaboration with S. Leyendecker, D. Phansalkar (P9) and D. Jadhav (P9): discussion about<br>- dynamic fracture<br>- phase field models<br>- adaptive simulation in space and time<br>- numerical convergence analysis in statics and dynamics |

## 3.3 Additional qualification measures

### 3.3.1 Research stays

**Stefan Hiemer**

| From / to | Institute visited | Local supervisor (if applicable) | Research activities performed and skills acquired during stay |
|---|---|---|---|
| 25.04.2022 / 26.05.2022 | Università degli Studi di Milano, Italy | Stefano Zapperi | Development of a new theoretical model of thermally activated creep in fiber bundles, Machine Learning in atomistic glasses |

### 3.3.2 Student fieldtrips

**Ruaridh Smith**

| From / to | Fieldtrip topic | Location |
|---|---|---|
| 02.09.2022 / 10.09.2022 | Structural and Regional Geology – Structural mapping and measuring and creating cross-sections | Scotland, UK |

### 3.3.3 Summer schools / Autumn schools

**Christof Bauer**

| From / to | Name of school | Location |
|---|---|---|
| 13.10.2022 / 14.10.2022 | 1st FRASCAL Autumn School: Software Development | Hotel Fuchsbräu, Beilngries, Germany |

**Christian Greff**

| From / to | Name of school | Location |
|---|---|---|
| 13.10.2022 / 14.10.2022 | 1st FRASCAL Autumn School: Software Development | Hotel Fuchsbräu, Beilngries, Germany |

**Lennart Igel**

| From / to | Name of school | Location |
|---|---|---|
| 13.10.2022 / 14.10.2022 | 1st FRASCAL Autumn School: Software Development | Hotel Fuchsbräu, Beilngries, Germany |

**Deepak Jadhav**

| From / to | Name of school | Location |
|---|---|---|
| 25.06.2022 / 26.06.2022 | Sommer school: Fracture Mechanics and Structural Integrity | Funchal, Portugal |
| 13.10.2022 / 14.10.2022 | 1st FRASCAL Autumn School: Software Development | Hotel Fuchsbräu, Beilngries, Germany |

**Jonas Ritter**

| From / to | Name of school | Location |
|---|---|---|
| 13.10.2022 / 14.10.2022 | 1st FRASCAL Autumn School: Software Development | Hotel Fuchsbräu, Beilngries, Germany |

**Christian Ritterhoff**

| From / to | Name of school | Location |
|---|---|---|
| 13.10.2022 / 14.10.2022 | 1st FRASCAL Autumn School: Software Development | Hotel Fuchsbräu, Beilngries, Germany |

**Maurice Rohracker**

| From / to | Name of school | Location |
|---|---|---|
| 13.10.2022 / 14.10.2022 | 1st FRASCAL Autumn School: Software Development | Hotel Fuchsbräu, Beilngries, Germany |

**Ina Schmidt**

| From / to | Name of school | Location |
|---|---|---|
| 13.10.2022 / 14.10.2022 | 1st FRASCAL Autumn School: Software Development | Hotel Fuchsbräu, Beilngries, Germany |

**Joscha Seutter**

| From / to | Name of school | Location |
|---|---|---|
| 20.6.2022 / 24.6.2022 | Lake Como School of Advanced Studies: Mathematical Models for Bio-Medical Sciences | Como, Italy |

**Shucheta Shegufta**

| From / to | Name of school | Location |
|---|---|---|
| 13.10.2022 / 14.10.2022 | 1st FRASCAL Autumn School: Software Development | Hotel Fuchsbräu, Beilngries, Germany |

**Sukhminder Singh**

| From / to | Name of school | Location |
|---|---|---|
| 13.10.2022 / 14.10.2022 | 1st FRASCAL Autumn School: Software Development | Hotel Fuchsbräu, Beilngries, Germany |

**Ruaridh Smith**

| From / to | Name of school | Location |
|---|---|---|
| 13.10.2022 / 14.10.2022 | 1st FRASCAL Autumn School: Software Development | Hotel Fuchsbräu, Beilngries, Germany |

**Anna Titlbach**

| From / to | Name of school | Location |
|---|---|---|
| 20.06.2022 / 24.06.2022 | Numerical solution of PDEs u-sing the finite element method | SISSA Trieste, Italy |
| 13.10.2022 / 14.10.2022 | 1st FRASCAL Autumn School: Software Development | Hotel Fuchsbräu, Beilngries, Germany |

**Felix Weber**

| From / to | Name of school | Location |
|---|---|---|
| 13.10.2022 / 14.10.2022 | 1st FRASCAL Autumn School: Software Development | Hotel Fuchsbräu, Beilngries, Germany |

### 3.3.4 Academic activity training

In addition to the qualification programme, doctoral researchers could take on extra tasks in their host department, especially in the context of teaching. This so-called academic activity training comprises, for example: supervision of bachelor, project, or master theses, supervision of seminar papers, mentoring of academic courses, exam support etc.
In this context, the so-called Student Seminar Series of FRASCAL ($S^3$ FRASCAL) was established in 2021: Bachelor, project, and master theses supervised by FRASCAL doctoral and associated doctoral researchers and postdocs were part of the qualification programme. The students' presentations, as part of their theses, took place at the respective chairs of the supervisors and examiners, but were at the same time part of $S^3$ FRASCAL, with all FRASCAL members invited to the presentation and subsequent discussion.


*Figure 68: Felix Weber during his project thesis presentations at $S^3$ FRASCAL.*

*Table 18: $S^3$ FRASCAL (Bachelor theses (BT), project theses (PT), master theses (MT), master seminar (MS)*

| Student | Topic | Supervision / Date |
|---|---|---|
| Felix Weber | PT: A quantitative interphase model for polymer nanocomposites: Verification and validation in terms of size effects | Maximilian Ries / 10.01.2022 |
| Kok Siong Siah | PT: Computational Modeling of Large Strain Nonlinear Viscoelastic Materials | Paras Kumar / 22.02.2022 |
| Maurice Rohracker | MT: Some Computational Aspects of Phase-Field Models for Brittle Fracture<br>MS: Modeling Irreversibility in Phase-Field Models for Brittle Fracture | Paras Kumar / 29.03.2022 |
| Jakob Seibert | BT: Investigation of the Influence of Nano-Sized Particles on the Entanglement Distribution of Generic Polymer Nanocomposite Using Molecular Dynamics | Maximilian Ries / 14.04.2022 |
| David Torres Huamani | PT: Untersuchungen der Konnektivität von teilchenbasierten Gebieten in der Capriccio Methode | Wuyang Zhao / 20.05.2022 |
| Sampanna Pahi | MT: Modelling mechanochemical bond scission of Epoxy resins under stress | Christian Wick / 27.07.2022 |
| Eva Richter | BT: Continuum-mechanical Analysis of a Polystyrene-Silica Nanocomposite using Multi-Particle Volume Elements | Maximilian Ries / 25.10.2022 |

### 3.3.5 Student projects and theses

Student work completed in 2022 that were supervised by FRASCAL doctoral researchers.

*Table 19: Bachelor theses (BT), project theses (PT), master theses (MT) completed in 2022.*

| Type | Student | Topic | Supervision |
|---|---|---|---|
| MT | Pahi, Sampanna | Modelling Mechanochemical Bond Scission of Epoxy Resins under Stress | C. Wick |
| PT | Reber, Sebastian | Untersuchung der mechanischen Eigenschaften von "grafted" Polymernanokompositen mithilfe molekulardynamischer Simulationen | M. Ries |
| BT | Richter, Eva | Continuum-mechanical Analysis of a Polystyrene-Silica Nano-composite using Multi-Particle Volume Elements | M. Ries |

| | | | |
|---|---|---|---|
| MT | Rohracker, Maurice | Some Computational Aspects of Phase-Field Models for Brittle Fracture | P. Kumar |
| BT | Seibert, Jakob | Investigation of the Influence of Nano-Sized Particles on the Entanglement Distribution of Generic Polymer Nanocomposite Using MD | M. Ries |
| PT | Siong Siah, Kok | Computational Modeling of Large Strain Nonlinear Viscoelastic Materials | P. Kumar |
| PT | Weber, Felix | A quantitative interphase model for polymer nanocomposites: Verification and validation in terms of size effects | M. Ries |
| MT | Weber, Felix | Systematic analysis and parameter optimization of the multiscale Capriccio method | M. Ries |

# 4 Equal Opportunity Measures

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

## 4.1 Workshops, seminars

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

*Table 20: Workshops organized by F$^3$G with participation of GRK 2423 FRASCAL members*

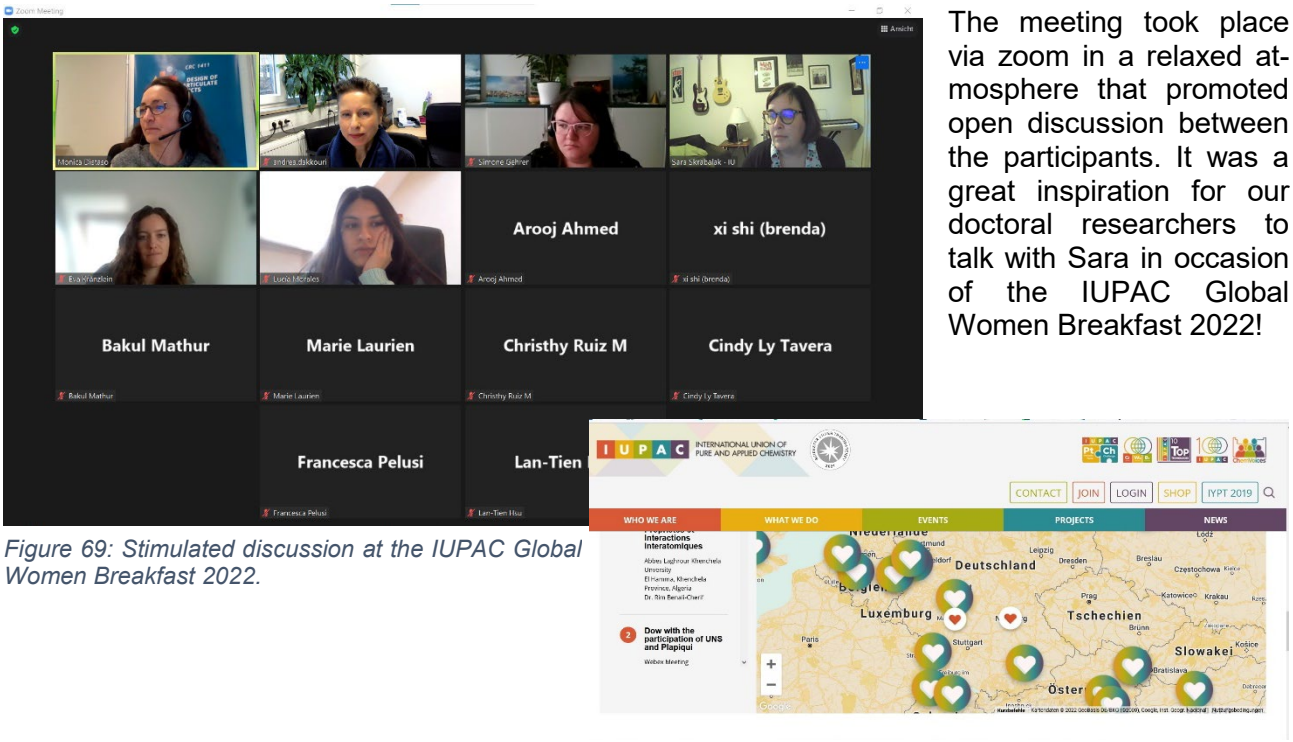
| | Date | Title | Lecturer |
|---|---|---|---|
| 01 | 24 – 27 January 2022 | Self-presentation and networking | Dr. Karin Bodewits (München) |
| 02 | 17 – 18 February 2022 | Thesis Defense Training | Dr. Malte Engel (Schönwalde) |
| 03 | 25 March 2022 | Good Scientific Practice | Dr. Anne Hamker (Leipzig) |

## 4.2 IUPAC Global Women Breakfast

The International Union of Pure and Applied Science has launched since a couple of years the Global Women Breakfast initiative under the motto: “Empowering Diversity in Science”.

Initiated by the scientific coordinator of the iRTG of CRC 1411, all the Research Training Groups affiliated to the Graduate School EAM have decided to participate in the IUPAC Breakfast 2022 as part of their gender activities. For this purpose, Prof. Sara Skrabalak from Indiana University was invited to be available to answer our questions after a short description of her professional career.

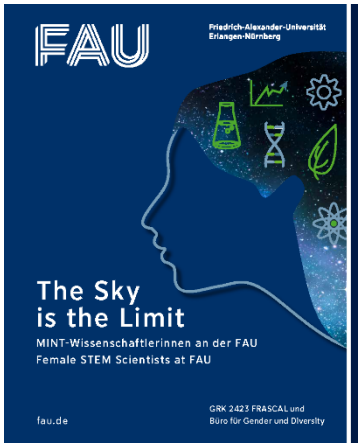
Considering that very few women reach top academic positions, there is often a lack of positive role models that can inspire young generations and bridge the gender gap in science and technology. Therefore, FRASCAL was glad to take active part in the GWB 2022 and connect with Prof. Sara Skrabalak for an informal chat with doctoral researchers.




The meeting took place via zoom in a relaxed atmosphere that promoted open discussion between the participants. It was a great inspiration for our doctoral researchers to talk with Sara in occasion of the IUPAC Global Women Breakfast 2022!

*Figure 69: Stimulated discussion at the IUPAC Global Women Breakfast 2022.*

## 4.3 The Sky is the Limit - Female STEM Scientists at FAU




In a joint project of the *GRK 2423 FRASCAL* and the *Office for Gender and Diversity*, female STEM scientists at FAU and their success stories are presented as part of the "Innovationsbündnis Hochschule 4.0".

The aim of the publication project was to interest schoolgirls and (potential) young female scientists in an academic career and to motivate them through concrete role models and examples. Just one day after it appeared in printed form, the publication was presented to over 6,000 visitors at FAU's “Schlossgartenfest”, and a few days later it was used at the study information day of the Department of Mechanical Engineering, at the "Nacht der Wissenschaft" at the Marie-Therese-Gymnasium in Erlangen and at the ”Schnupperuni” of Materials Science and Engineering/Nanotechnology (FAU). Many other FAU-internal and external events related to the role models presented in the publication are already planned (especially at Gymnasien). The publication also attracted attention outside FAU and was mentioned on the homepage (and social media channels) of the Bundeskonferenz der Frauen- und Gleichstellungsbeauftragten an Hochschulen e.V.[2] and Freie Universität Berlin[3], among

*scan me to get the pdf*


*Figure 70: Dr. Magda Luthay (BGD) and Prof. Dr. Paul Steinmann present the publication "The Sky is the Limit - Female STEM Scientists at FAU" to the public for the first time at FAU's Schlossgartenfest.*

[2] https://bukof.de/bukof-pinnwand/
[3] https://www.mi.fu-berlin.de/fb/beauf-aussch/beauf-frauen/News/_The-Sky-is-The-Limit--MINT-Wissenschaftlerinnen-an-der-FAU_.html

others, and print copies were requested by the Equal Opportunities Office of Heinrich Heine University Düsseldorf and the Büro der Gleichstellungsstelle der Stadt Nürnberg, among others.

*Figure 71: "Science Night" at the Marie Therese Gymnasium in Erlangen: very interested schoolgirls are engrossed in the publication "The Sky is the Limit". (Image: H. Stollberg)*


*Figure 72: Celebrating the project closing (from left to right): Dr. Susanne Stemmler (journalist), Dr. Andrea Dakkouri-Baldauf (editorial team), Dr. Imke Leicht (editorial team), Giulia Iannicelli (photographer), Prof. Paul Steinmann (idea), Bärbel Rhades (graphic designer), Dr. Magda Luthay (editor-in-chief).*


*Figure 73: Impressions of the project closing party. (Images: A. Dakkouri-Baldauf and G. Iannicelli)*

## 4.4 Further measures

- Financial support for vacation care for the children of our FRASCAL members.
- Financial support for specific F$^3$G projects in FAU holiday childcare programmes.
- Pedagogic improvement of the infrastructure at FAU day care facilities for children.
- Participation in F$^3$G coordination costs.
- Contingent option for one occupancy place in the day care centre “Pfauennest II”.
- Support for specific projects for the day care centre "Pfauennest".
- Support (purchase of a 3D printer) for a STEM project at the Albert-Schweitzer-Gymnasium Erlangen to promote young girls.


*Figure 74: Keeping the children occupied in the office during the school holidays with games from the toy box. (Image: A. Dakkouri-Baldauf)*

# 5 Selected Highlights

## 5.1 Kick-off meeting of the 2nd cohort


On 4 February 2022, we welcomed the doctoral researchers of the second FRASCAL cohort.

This first joint meeting took place online, firstly due to COVID-19-related restrictions, and secondly to give new doctoral researchers who are not yet in Erlangen at that time the opportunity to attend the welcome meeting.

First, Paul Steinmann welcomed all new doctoral students and briefly introduced FRASCAL. This was followed by a short personal presentation of the FRASCAL-funded doctoral students of the first cohort, followed by a short self-presentation of the doctoral students of the second cohort, in which they told about their previous scientific path, but also revealed personal about themselves. In the end there was still enough time to ask questions of all kinds.

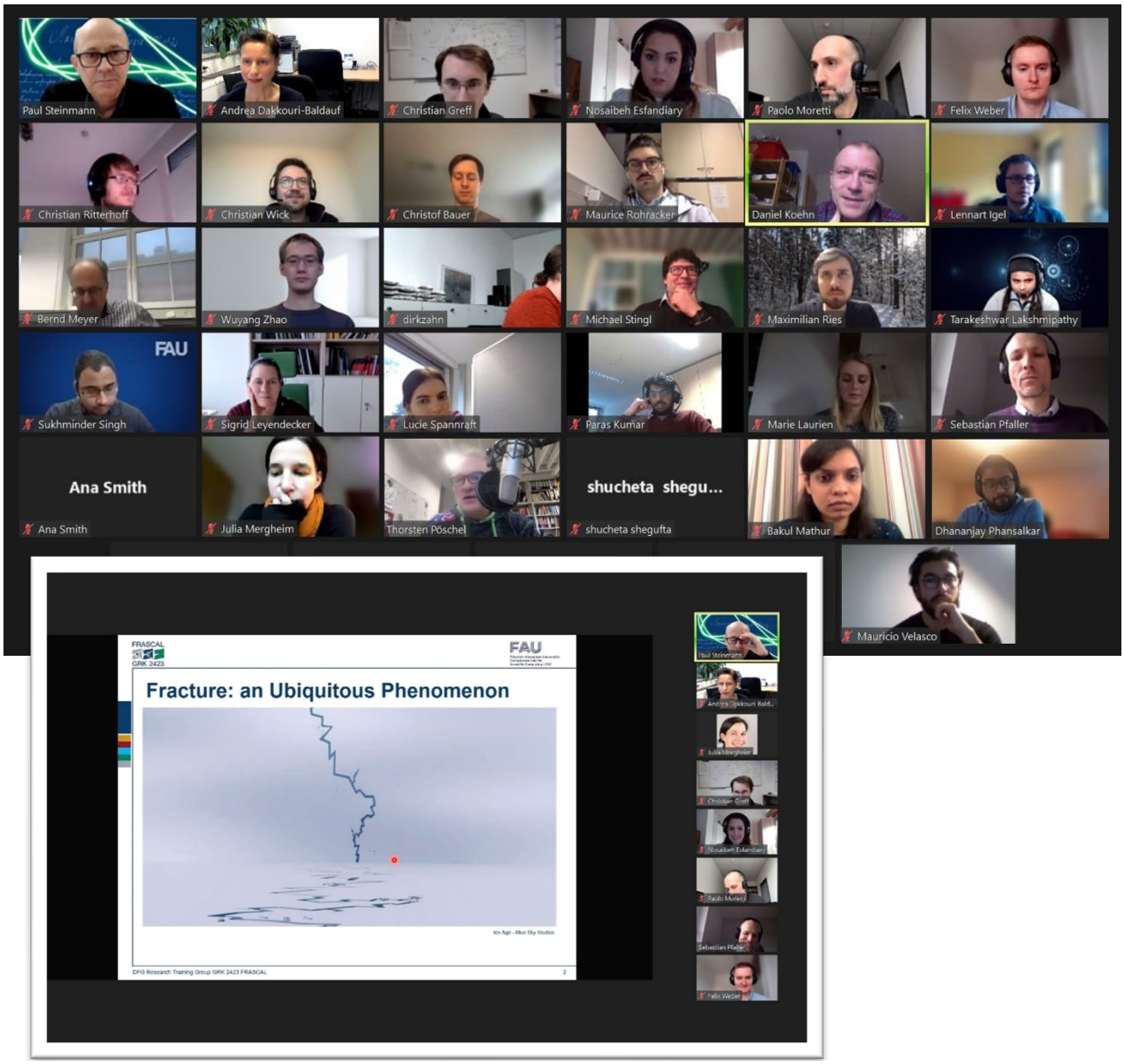


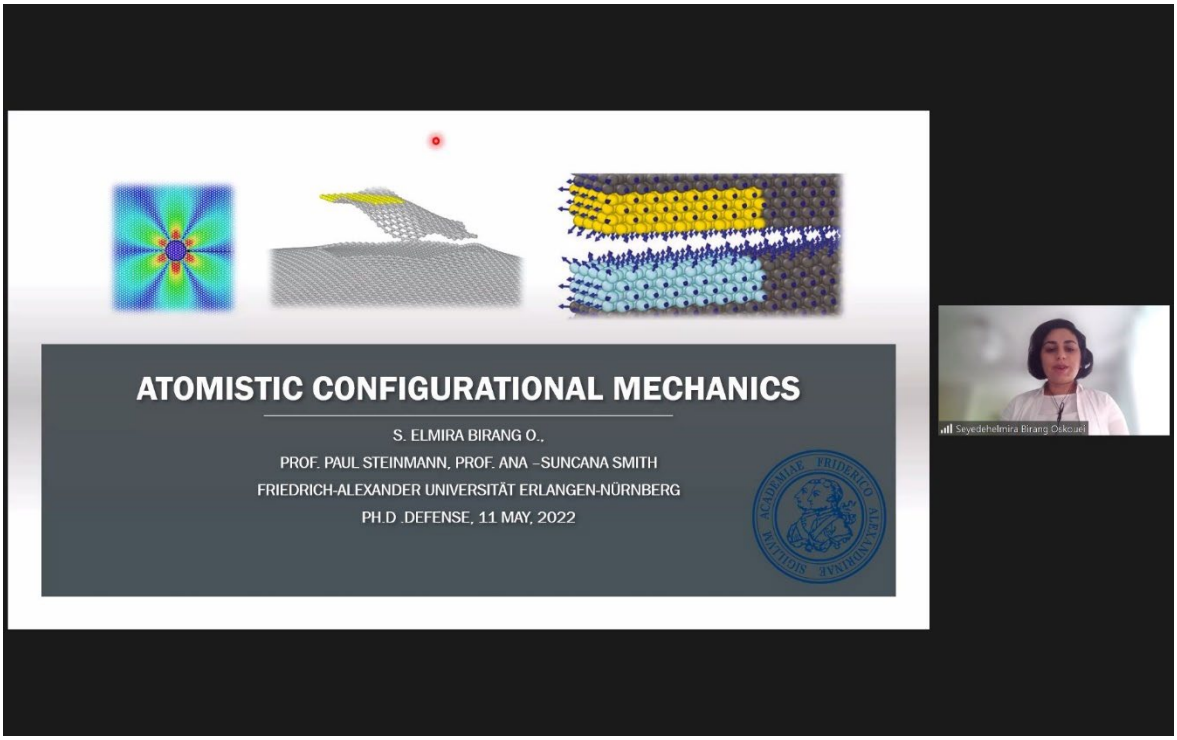

*Figure 75: Virtual kick-off meeting of the 2nd FRASCAL cohort.*

## 5.2 Doctoral degree

We are pleased to announce the first three successfully completed FRASCAL dissertation projects:

### Dr.-Ing. Seyedeh Elmira Birang Oskouei

Elmira Birang earned a doctoral degree after defending her thesis "*Atomistic Configurational Mechanics*" on 11 May 2022 in an online format. Her supervisor was Prof. Paul Steinmann, co-principal advisors were Ana-Sunčana Smith and Prof. Michael Stingl. Elmira is the first completed doctoral researcher of FRASCAL.



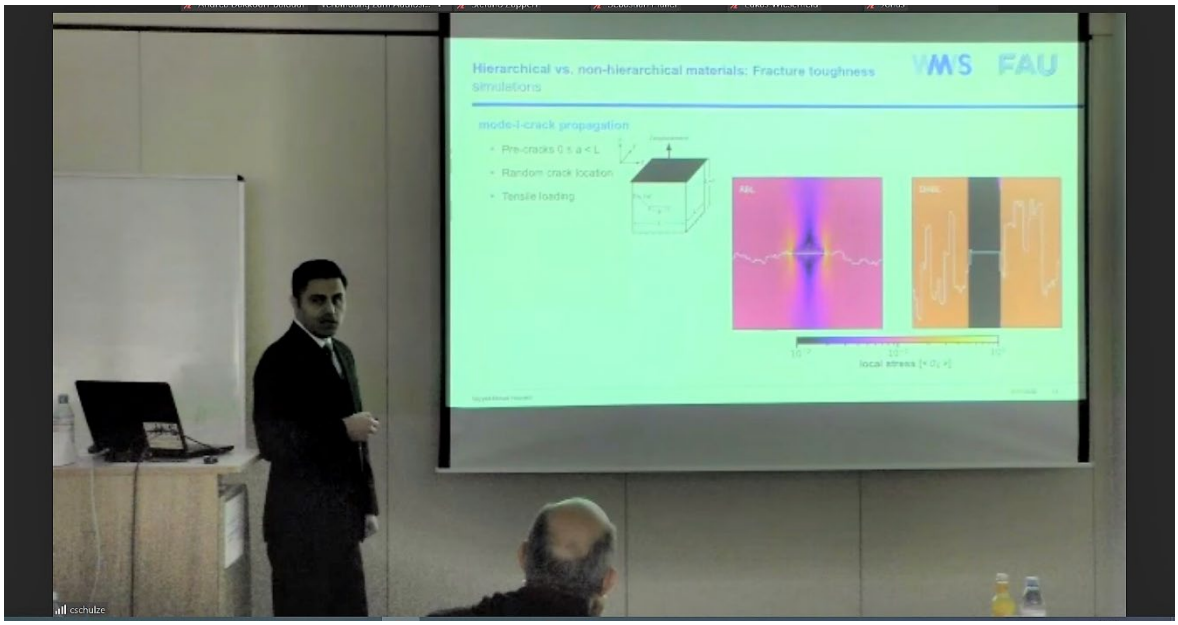

### Dr.-Ing. Ina Schmidt

On 01 August 2022, FRASCAL associate member Ina Schmidt (TH Nürnberg Georg Simon Ohm) successfully defended her dissertation entitled "*Modelling and Simulation of Bone Adaptation Processes*". Her dissertation project was supervised by Prof. Paul Steinmann and Prof. Areti Papastavrou (TH Nürnberg Georg Simon Ohm). Co-principal advisor was Prof. Michael Stingl.

*Figure 76: Ina Schmidt with her two supervisors Areti Papastavrou and Paul Steinmann. (Image. A. Dakkouri-Baldauf)*

### Dr.-Ing. Seyyed Ahmad Hosseini

Associate doctoral researcher Ahmad Hosseini successfully defended his dissertation in a hybrid examination on 21 November 2022. His dissertation dealt with the topic "*Fracture and Failure Properties of Hierarchical Materials*". His project was supervised by Prof. Michael Zaiser and co-supervised by Prof. Paul Steinmann.




## 5.3 Awards and distinctions

### Teaching Award of the Faculty of Engineering 2022

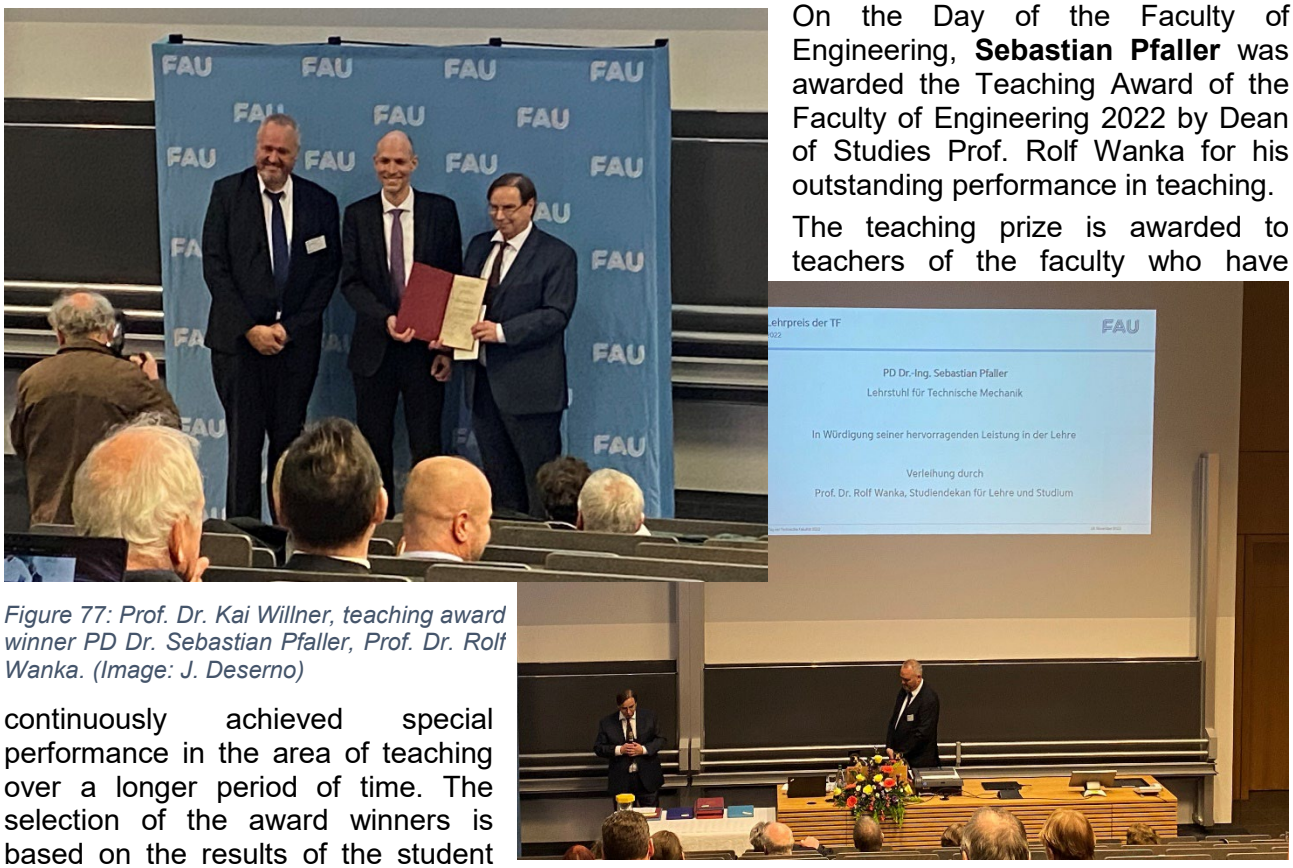



*Figure 77: Prof. Dr. Kai Willner, teaching award winner PD Dr. Sebastian Pfaller, Prof. Dr. Rolf Wanka. (Image: J. Deserno)*

On the Day of the Faculty of Engineering, **Sebastian Pfaller** was awarded the Teaching Award of the Faculty of Engineering 2022 by Dean of Studies Prof. Rolf Wanka for his outstanding performance in teaching.

The teaching prize is awarded to teachers of the faculty who have continuously achieved special performance in the area of teaching over a longer period of time. The selection of the award winners is based on the results of the student teaching evaluation of the past five years. The prize is endowed with 3,000 €.

Congratulations, Sebastian!

### Advanced Grant from the European Research Council (ERC)

**Paul Steinmann** has been awarded an Advanced Grant from the European Research Council (ERC). He will use the funding of 2.5 million for the next five years to study the fracture mechanics of soft materials such as rubber or fabric more intensively. Paul Steinmann already received an ERC Advanced Grant in 2011 for research into magnetic elastomers.

Congratulations to our spokesperson Paul Steinmann!

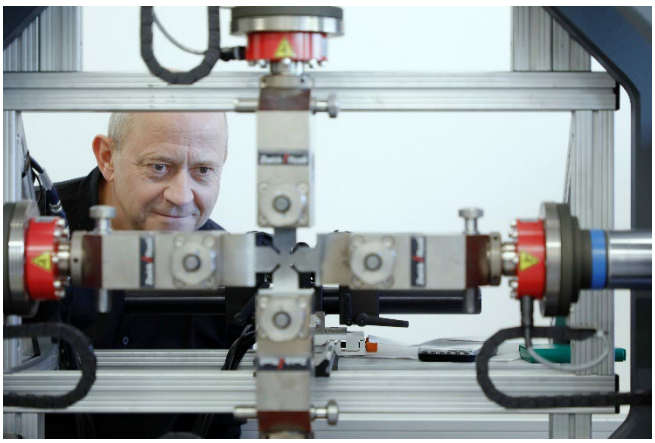


*Figure 78: Prof. Dr. Paul Steinmann (Institute of Applied Mechanics), spokesperson of GRK 2423 FRASCAL. (Image: G. Iannicelli)*

## 5.4 Mini-symposia at ECCOMAS CONGRESS 2022 and WCCM-APCOM 2022

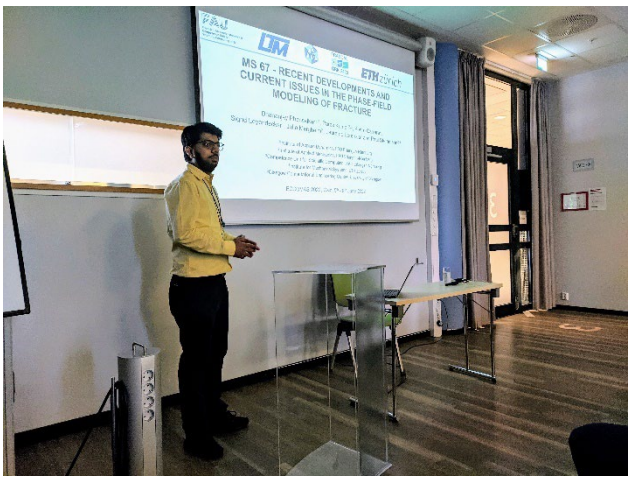



*Figure 79: Paras Kumar introducing the ECCOMAS mini-symposium.*

Participating in their first in-person conference after almost three years, the doctoral researchers Paras Kumar and Dhananjay Phansalkar, in collaboration with some FRASCAL PAs and the group of Prof. Laura De Lorenzis, organized a mini-symposium titled “Recent developments and current issues in the phase-field modelling of fracture” at the ECCOMAS 2022 conference in Oslo, Norway. The mini-symposium was spread across four sessions and comprised of 2 keynote lectures and 17 regular oral presentations. The event was a great success with fruitful discussions amongst the participants, in addition to be a learning opportunity for the involved doctoral researchers.

Asides, Paras and Dhananjay, under the tutelage of FRASCAL PAs, further organized a mini-symposium at the WCCM-APCOM 2022 conference which was initially planned to be held as an in-person conference in Yokohama, Japan, but was later shifted to virtual format due to another Covid-19 wave. The topic of this mini-symposium “Computational Fracture Modeling in Heterogeneous Materials - Recent Advances and Future Challenges” is in line with the core theme of FRASCAL and was received quite well by the participants. This culminated in an intense and enlightening online discussion session with varied perspectives towards the challenging problem of fracture modelling in heterogeneous materials.

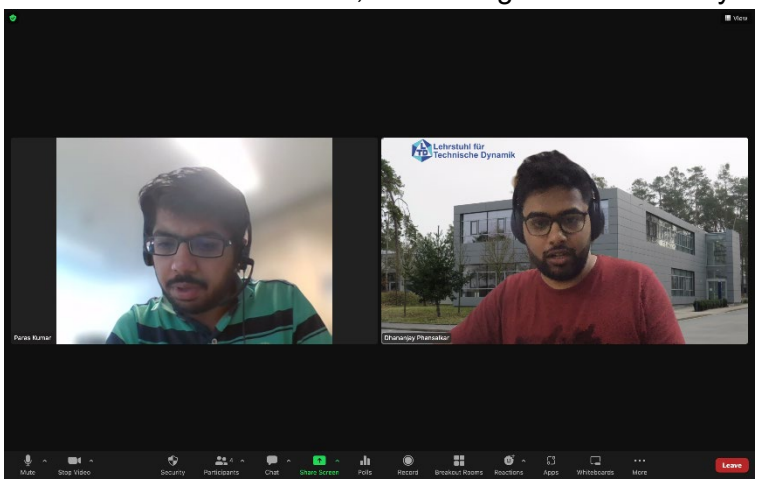



*Figure 80: Paras Kumar and Dhananjay Phansalkar welcoming participants to their WCCM-APCOM mini-symposium.*

(Text: Paras Kumar and Dhananjay Phansalkar)

## 5.5 Mini-retreat of FRASCAL project P6 (Capriccio group)

*Figure 81: Members of the Capriccio group hiking during their mini retreat. (Image: C. Bauer)*

On 27–29 July, we (Christof Bauer, Sebastian Pfaller, Felix Weber and Wuyang Zhao) held a Capriccio mini-retreat in Baiersdorf (next to Altkunstadt in Upper Franconia), focusing on our upcoming doctoral theses and the FRASCAL renewal proposal.

Starting with presentations by Wuyang and Christof on the current status of their dissertations, we intensively discussed the scientific and strategic issues of the doctoral projects and associated paper plans as well as handing over the research project to Felix. Beyond these fruitful discussions, Sebastian also shared important tips for writing dissertations with examples of his experiences. As another point, we finalized together the FRASCAL renewal proposal of subproject P6 in terms of topics across scales, collaborations, methods, and materials. Beyond the scientific part, we spent a nice time hiking at the Staffelberg.

(Text: Wuyang Zhao)

## 5.6 Poster event and get-together of GS EAM

On 15 September 2022, the Graduate School Engineering of Advanced Materials (GS EAM) invited doctoral and postdoctoral researchers to a scientific networking event.

After welcoming the participants, there was a short introduction to GS EAM and its associated Research Training Groups. FRASCAL was introduced to the participants in a short presentation by the two doctoral researchers' representatives Felix Weber and Maurice Rohracker.


*Figure 82: Impressions of the poster event and get-together of GS EAM. Top right: Maurice Rohracker introduces FRASCAL. (Images: GS EAM)*

In a subsequent poster presentation, science could be discussed in a relaxed atmosphere with food and drink and ample opportunity to meet and get to know other young scientists who contribute to the FAU research focus "New Materials and Processes".

## 5.7 Birthday celebration of FRASCAL's spokesperson Paul Steinmann

On the occasion of Prof. Paul Steinmann's 60th birthday, there was a ceremony on 11 February 2022, which had to take place online due to the restrictions imposed by the Covid-19 pandemic. An entertaining program offered greetings, a summary of the career and previous successes of Professor Steinmann with the appropriate title "Mechaniker aus Leidenschaft", a lecture by Prof. Ellen Kuhl from Stanford University on "Embracing Uncertainty".

FRASCAL surprised its spokesperson with FRASCAL-related gifts (see Figure 83): an engraved and singed beer mug (top left), a sketch showing the progression of the master of the Continuum mechanic that gets some laughs (top right) and a photo canvas of the FRASCAL members in pop art (bottom).

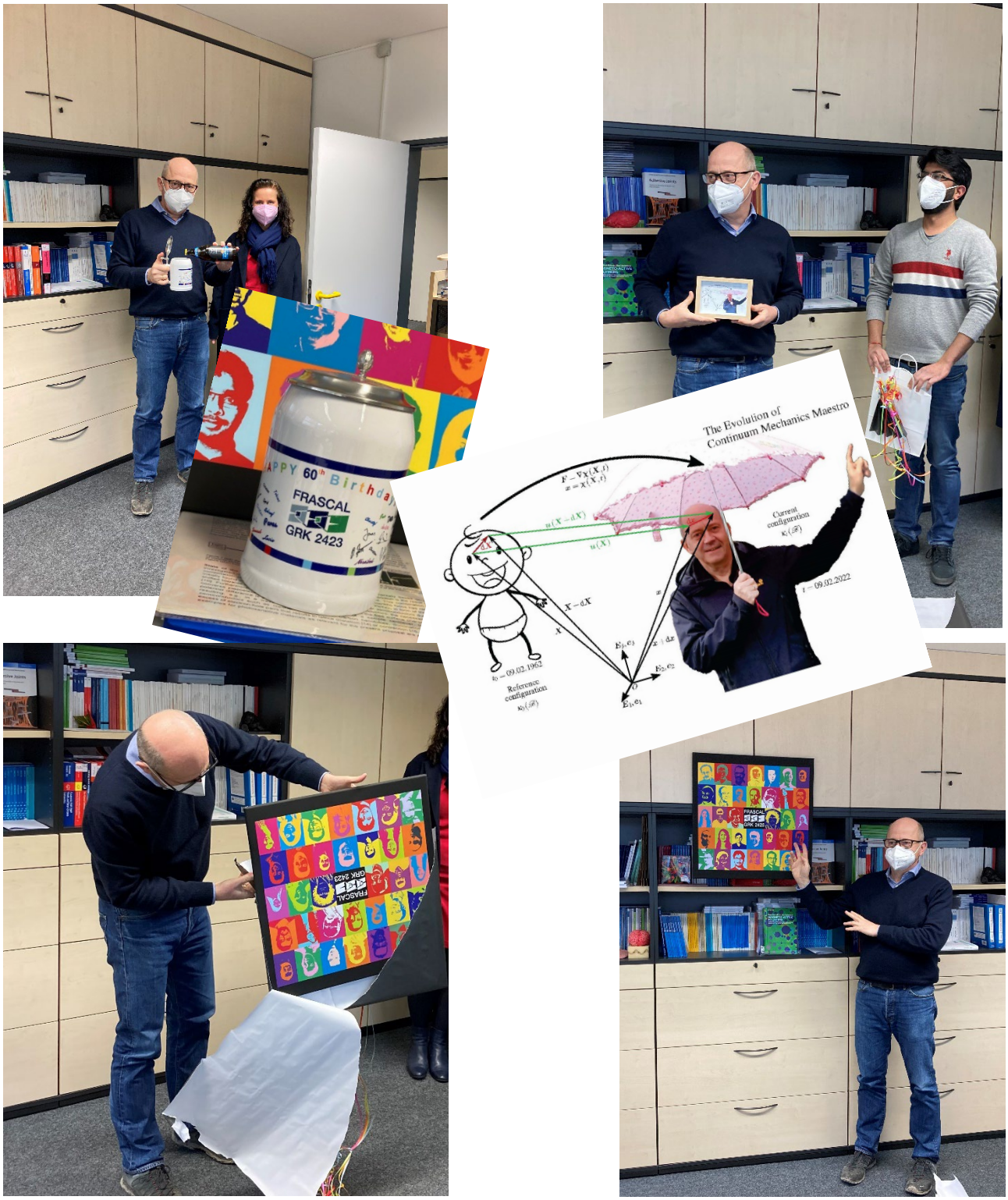



*Figure 83: Presents from FRASCAL for Paul Steinmann on the occasion of his 60th birthday. (Images: M. Ries)*

## 5.8 Preparing the continuation of FRASCAL

The year 2022 was dominated by the preparation of the FRASCAL renewal proposal and the progress report, as well as the preparation for the on-site review by the DFG in early 2023.

The main part of the progress report, in which each individual doctoral researcher, associate doctoral researcher and postdoctoral researcher has to report on the research results and the qualification programme they have completed, was organised by the doctoral researchers themselves with great effort.

The core organisational team of FRASCAL then worked out the renewal proposal and the progress report in detail in a seemingly endless number of face-to-face and online meetings, and with the input of the principal advisors and doctoral researchers, all the documents necessary for the renewal were finally uploaded online to the DFG on 30 September 2022. Both the renewal proposal including the research profiles of the PAs and the work report were also printed and are available as hard copies.

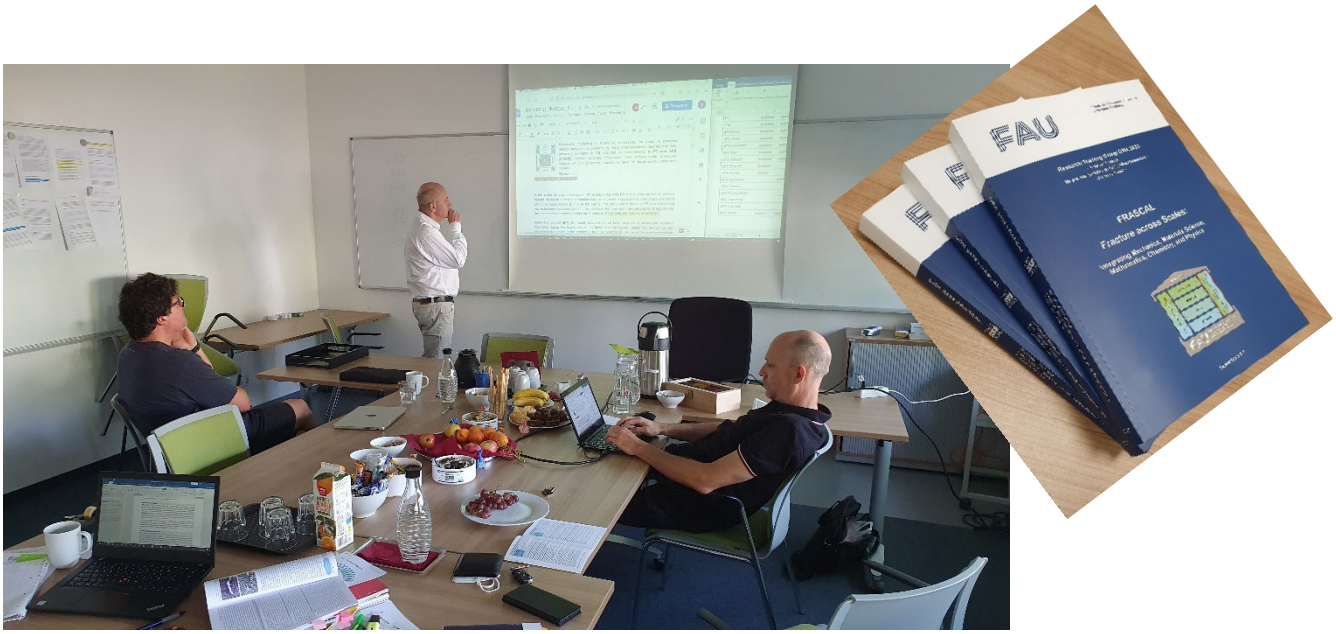



*Figure 84: Michael Stingl, Paul Steinmann and Sebastian Pfaller in one of the numerous meetings to prepare the renewal proposal and the progress report. (Image: A. Dakkouri-Baldauf)*

After the proposal was submitted, preparations began for the review process, in which the doctoral researchers play a key role. Since all doctoral researchers have to present a poster, this poster presentation was intensively practised in several sessions with the trainer Deborah Bennett.

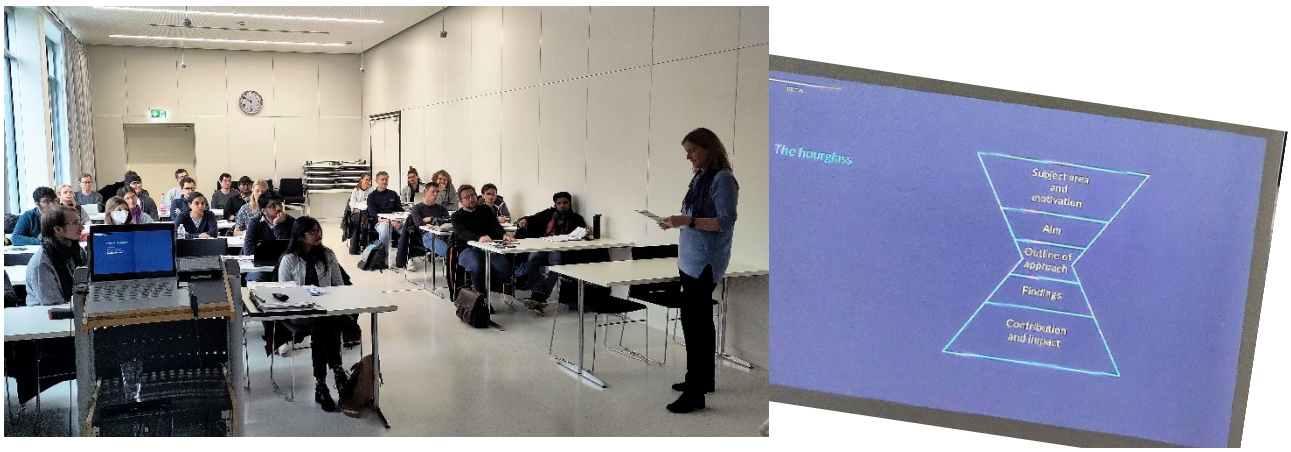



*Figure 85: Practising the poster session with Deborah Bennett. (Image: J. Ritter)*

## 5.9 FRASCAL library

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

94 new books have already been acquired in the first four years of FRASCAL.

For a complete list, see Appendix 3.

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


*Figure 86: FRASCAL library. (Image: A. Dakkouri-Baldauf)*

# 6 Appendices

## 6.1 Appendix 1: Programme of the 7th FRASCAL Seminar

| Programme of the 7th FRASCAL Seminar | | | |
|---|---|---|---|
| **Date** | 19 December 2022 | **Time** | 8:50 – 14:45 |
| **Location** | IZNF Seminarraum 00.156, Cauerstr. 3, 91058 Erlangen. | | |

| Time | Name | Title of Presentation |
|---|---|---|
| 8:50 – 9:00 | Welcome | |
| 9:00 – 9:20 | Marie Laurien (P10) | *Nonlocal degrading interfaces in continuum-kinematics-inspired peridynamics* |
| 9:20 – 9:40 | Christian Greff (P7) | *Failure in hierarchically structured 3D fuse and beam networks* |
| 9:40 – 10:00 | Anna Titlbach (P10) | *A micromorphic approach for bone density adaption* |
| 10:00 – 10:20 | COFFEE BREAK | |
| 10:20 – 10:40 | Christian Ritterhoff (P1) | *Accelerating QM-based atomistic crack tip calculations* |
| 10:40 – 11:00 | Lennart Igel (P11) | *A conditional stochastic gradient method for fracture* |
| 11:00 – 11:20 | Ruaridh Smith (P13) | *Homogenising fracture networks from outcrop and investigating scale relationships* |
| 11:20 - 12:40 | Q&A SESSION<br>Exercise for the DFG review | |
| 12:40 – 13:40 | LUNCH BREAK | |
| 13:40 – 14:00 | Bakul Mathur (P13) | *Modelling of fragmentation and fracturing processes in deformation bands* |
| 14:00 – 14:20 | Joscha Seutter (P14) | *Existence of quasi-static crack evolution for atomistic systems* |
| 14:20 - 14:40 | Angel Santarossa (P4) | *Crack front segmentation in mixed-mode I+III hydraulic fractures* |
| | Closing | |

## 6.2 Appendix 2: Programme of the 2nd FRASCAL Retreat

| Programme of the 2nd FRASCAL Retreat | | | |
|---|---|---|---|
| **Date** | 05 – 06 May 2022 | **Time** | 9:00 – 16:30 |
| **Location** | Hotel Arvena Reichsstadt, Bad Windsheim | | |

| Time | Name | Title of Presentation |
|---|---|---|
| 05 May 2022 | | |
| 9:00 – 9:20 | CHECK IN & COFFEE | |
| 9:20 – 9:30 | Welcome & Introduction | |
| 9:30 – 9:45 | Christian Ritterhoff (P1) | *Machine-Learned Potentials for Atomistic Crack Tip Investigations* |
| 9:45 – 10:00 | Shucheta Shegufta (P5) | *Failure of Highly Porous Material* |
| 10:00 – 10:15 | Felix Weber (P6) | *Systematic Analysis and Parameter Optimization of the Multiscale Capriccio Method* |
| 10:15 – 10:30 | Christian Greff (P7) | *Fracture Surface Geometry in 3D Hierarchical Material Adhesion* |
| 10:30 – 11:00 | COFFEE BREAK | |
| 11:00 – 11:15 | Maurice Rohracker (P8) | *Some Computational Aspects of Phase-Field Models for Brittle Fracture* |
| 11:15 – 11:30 | Deepak Jadhav (P9) | *Finite Element Modeling of Osteoporotic Pelvic Ring and Extension of Project P9 into Temporal Adaptivity* |
| 11:30 – 11:45 | Marie Laurien (P10) | *Peridynamic Fracture Mechanics* |
| 11:45 – 12:00 | *CVs and experiences of FRASCAL PAs: Manuel Friedrich* | |
| 12:00 – 13:15 | LUNCH BREAK | |
| 13:15 – 15:00 | *WORKSHOPS - PART 1*<br>**DR, aDR, PD**: *Workshop Research Data Management (RDM)*<br>**PAs**: *Workshop Renewal Proposal* | |
| 15:15 – 18:15 | Walk to and through the Franconian Open-Air Museum with snack | |
| 18:30 | DINNER | |
| 20:00 – 20:30 | *Presentation of the intermediate results of the RDM workshop* | |

| Time | Name | Title of Presentation |
|---|---|---|
| 06 May 2022 | | |
| 8:00 – 9:00 | BREAKFAST | |
| 9:15 – 9:30 | Lennart Igel (P11) | *Stochastic Optimization with High Dimensional Uncertainties with Application to Fracture Control* |
| 9:30 – 9:45 | Bakul Mathur (P13) | *Thermo-Hydro-Mechanical Simulation of Cooling-Induced Fault Reactivation* |
| 9:45 – 10:00 | Joscha Seutter (P14) | *Variational Models for Brittle Fracture and Crack Growth* |
| 10:00 – 10:20 | *Poster Blitz* | |
| 10:20 – 12:00 | Poster Session with COFFEE | |
| 12:00 – 13:15 | LUNCH BREAK | |
| 13:15 – 14:30 | *WORKSHOPS - PART 2*<br>**DR, aDR, PD**: *Workshop Research Data Management (RDM)*<br>**PAs**: *Workshop Renewal Proposal* | |
| 14:30 – 15:00 | COFFEE BREAK | |
| 15:00 – 15:30 | *CVs and experiences of FRASCAL PAs: Michael Stingl, Daniel Koehn* | |
| 15:30 – 16:30 | *Results of the Workshops* | |
| 16:30 - 17:00 | Closing & Departure | |

## 6.3 Appendix 3: List of book inventory

| | Author | Title | Publishing Year |
|---|---|---|---|
| 1 | Aboudi, Jacob; Arnold, Steven M.; Bednarcyk, Brett A. | Practical Micromechanics of Composite Materials | 2021 |
| 2 | Ambrosio, Luigi; Fusco, Nicola; Pallara, Diego | Functions of Bounded Variation and Free Discontinuity Problems | 2000 |
| 3 | Anandarajah, Annalingam | Computational Methods in Elasticity and Plasticity: Solids and Porous Media | 2010 |
| 4 | Antman, Stuart S. | Nonlinear Problems of Elasticity | 2005 |
| 5 | Başar, Yavuz; Weichert, Dieter | Nonlinear Continuum Mechanics of Solids: Fundamental Mathematical and Physical Concepts | 2010 |
| 6 | Bathe, Klaus-Jürgen | Finite Element Procedures | 2014 |
| 7 | Bažant, Zdeněk P. ; Le, Jia-Liang; Salviato, Marco | Quasibrittle Fracture Mechanics and Size Effect | 2021 |
| 8 | Bergström, Jörgen | Mechanics of Solid Polymers: Theory and Computational Modeling | 2015 |
| 9 | Bertram, Albrecht | Elasticity and Plasticity of Large Deformations | 2012 |
| 10 | Bertram, Albrecht; Glüge, Rainer | Solid Mechanics: Theory, Modeling, and Problems | 2015 |
| 11 | Bland, David Russell | The Theory of Linear Viscoelasticity | 2016 |
| 12 | Bobaru, Florin; Foster, John T.; Geubelle, Philippe H.; Silling, Stewart A. (eds.) | Handbook of Peridynamic Modeling | 2017 |
| 13 | Bonet, Javier; Wood, Richard D. | Nonlinear Continuum Mechanics for Finite Element Analysis | 2008 |
| 14 | Borja, Ronaldo I. | Plasticity: Modeling & Computation | 2013 |
| 15 | Braides, Andrea | Γ-Convergence for Beginners | 2002 |
| 16 | Brázdová, Veronika; Bowler, David R. | Atomistic Computer Simulations; A Practical Guide | 2013 |
| 17 | Broberg, K. Bertram | Cracks and Fracture | 1999 |
| 18 | Bui, Huy Duong | Fracture Mechanics: Inverse Problems and Solutions | 2006 |
| 19 | Chadwick, Peter | Continuum Mechanics: Concise Theory and Problems | 1999 |
| 20 | Chakrabarty, Jagabanduhu | Theory of Plasticity | 2006 |
| 21 | Chatzigeorgiou, George; Charalambakis, Nicholas; Chemisky, Yves ; Meraghni, Fodil | Thermomechanical Behavior of Dissipative Composite Materials | 2018 |

| | Author | Title | Publishing Year |
|---|---|---|---|
| 22 | Chen, Wai-Fah; Han, Da-Jian | Plasticity for Structural Engineers | 2007 |
| 23 | Chipot, Michel; Quittner, Pavol (eds.) | Handbook of Differential Equations – Stationary Partial Differential Equations Vol. 3 | 2006 |
| 24 | Cho, Kwang Soo | Viscoelasticity of Polymers: Theory and Numerical Algorithms | 2016 |
| 25 | Christensen, Richard M. | Theory of Viscoelasticity | 2003 |
| 26 | Coussy, Olivier | Mechanics and Physics of Porous Solids | 2010 |
| 27 | Drozdov, Aleksey D. | Finite Elasticity and Viscoelasticity: A Course in the Nonlinear Mechanics of Solids | 1996 |
| 28 | Epstein, Marcelo | The Elements of Continuum Biomechanics | 2012 |
| 29 | Eringen, A. Cemal; Maugin, Gerard A. | Electrodynamics of Continua I: Foundations and Solid Media | 1990 |
| 30 | Eringen, A. Cemal; Maugin, Gerard A. | Electrodynamics of Continua II: Fluids and Complex Media | 1990 |
| 31 | Freeman, Eric; Robson, Elisabeth; Sierra, Kathy; Bates, Bert | Head First Design Patterns: Building Extensi-ble and Maintainable Object-Oriented Software | 2020 |
| 32 | Freund, Lambert B. | Dynamic Fracture Mechanics | 1990 |
| 33 | Goedecker, Stefan; Hoisie, Adolfy | Performance Optimization of Numerically Intensive Codes | 2001 |
| 34 | Goriely, Alain | The Mathematics and Mechanics of Biological Growth | 2017 |
| 35 | Green, Albert E.; Zerna, Wolfgang | Theoretical Elasticity | 2012 |
| 36 | Gross, Dietmar; Seelig, Thomas | Fracture Mechanics | 2018 |
| 37 | Gross, Dietmar; Seelig, Thomas | Fracture Mechanics | 2018 |
| 38 | Gurtin, Morton E. | Configurational Forces as Basic Concepts of Continuum Physics | 2000 |
| 39 | Han, Weimin; Reddy, B. Daya | Plasticity: Mathematical Theory and Numerical Analysis | 2013 |
| 40 | Hashiguchi, Koichi | Elastoplasticity Theory | 2014 |
| 41 | Haupt, Peter | Continuum Mechanics and Theory of Materials | 2002 |
| 42 | Herrmann, Hans J.; Roux, Stéphane (eds.) | Statistical Models for the Fracture of Disordered Media | 1990 |
| 43 | Holzapfel, Gerhard A. | Nonlinear Solid Mechanics | 2000 |
| 44 | Huilgol, Raja R. | Fluid Mechanics of Viscoplasticity | 2015 |
| 45 | Hutchinson, John W. | A Course of Nonlinear Fracture Mechanics | 1980 |
| 46 | Jirásek, Milan; Bažant, Zdeněk P. | Inelastic Analysis of Structures | 2001 |
| 47 | Kačanov, Lazar' Markovič | Fundamentals of the Theory of Plasticity | 2004 |

| | Author | Title | Publishing Year |
|---|---|---|---|
| 48 | Kanninen, Melvin F.; Popelar, Carl H. | Advanced Fracture Mechanics | 1985 |
| 49 | Kardar, Mehran | Statistical Physics of Particles | 2007 |
| 50 | Kardar, Mehran | Statistical Physics of Fields | 2007 |
| 51 | Kinloch, Anthony James; Young, Robert J. | Fracture Behaviour of Polymers | 1995 |
| 52 | Krenk, Stehen | Non-linear Modeling and Analysis of Solids and Structures | 2009 |
| 53 | Kuna, Meinhard | Finite Elements in Fracture Mechanics - Theory - Numerics – Applications | 2013 |
| 54 | Lai, W. Michael; Rubin, David; Krempl, Erhard | Introduction to Continuum Mechanics | 2009 |
| 55 | Leach, Andrew R. | Molecular Modelling; Principles and Applications | 2001 |
| 56 | Lemaitre, Jean; Chaboche, Jean-Louis | Mechanics of Solid Materials | 1994 |
| 57 | Lubliner, Jacob | Plasticity Theory | 2008 |
| 58 | Madenci, Erdogan; Oterkus, Erkan | Peridynamic Theory and Its Applications | 2014 |
| 59 | Madenci, Erdogan; Roy, Pranesh; Behera, Deepak | Advances in Peridynamics | 2022 |
| 60 | Marsden, Jerrold E.; Hughes, Thomas J. R. | Mathematical Foundations of Elasticity | 1994 |
| 61 | Mate, C. Mathew; Carpick, Robert W. | Tribology on the Small Scale; A Modern Textbook on Friction, Lubrication, and Wear | 2019 |
| 62 | Maugin, Gérard A. | Configurational Forces: Thermomechanics, Physics, Mathematics, and Numerics | 2011 |
| 63 | Maugin, Gérard A. | The Thermomechanics of Plasticity and Fracture | 1992 |
| 64 | Maugin, Gérard A. | Material Inhomogeneities in Elasticity | 1993 |
| 65 | Meyers, Marc André and Chawla, Krishan Kumar | Mechanical Behavior of Materials | 2009 |
| 66 | Murdoch, A. Ian | Physical Foundations of Continuum Mechanics | 2012 |
| 67 | Oden, John T.; Reddy, Junuthula N. | Variational Methods in Theoretical Mechanics | 1983 |
| 68 | Oden, John Tinsley | Finite Elements of Nonlinear Continua | 2006 |
| 69 | Ogden, Raymond William | Non-Linear Elastic Deformations | 1997 |
| 70 | Oterkus, Erkan; Oterkus, Selda; Madenci, Erdogan | Peridynamic Modeling, Numerical Techniques, and Applications | 2021 |
| 71 | Phan-Thien, Nhan; Mai-Duy, Nam | Understanding Viscoelasticity: An Introduction to Rheology | 2017 |

| | Author | Title | Publishing Year |
|---|---|---|---|
| 72 | Pikus, Fedor G. | Hands-On Design Patterns with C++ | 2019 |
| 73 | Reddy, Junuthula N. | An Introduction to Continuum Mechanics | 2013 |
| 74 | Saramäki, Jari | How to Write a Scientific Paper: An Academic Self-Help Guide for PhD Students | 2018 |
| 75 | Schimel, Joshua | Writing Science: How to Write Papers That Get Cited and Proposals That Get Funded | 2011 |
| 76 | Shabana, Ahmed A. | Computational Continuum Mechanics | 2018 |
| 77 | Souza Neto, E. A. de; Perić, D.; Owen, D. R. J. | Computational Methods for Plasticity: Theory and Applications | 2008 |
| 78 | Spencer, Anthony James Merrill | Continuum Mechanics | 2004 |
| 79 | Steinmann, Paul | Geometrical Foundations of Continuum Mechanics | 2015 |
| 80 | Steinmann, Paul | Spatial and Material Forces in Nonlinear Continuum Mechanics - A Dissipation-Consistent Approach | 2022 |
| 81 | Steinmann, Paul; Runesson, Kenneth | The Catalogue of Computational Material Models | 2021 |
| 82 | Sun, Chin-Teh; Jin, Zhihe | Fracture Mechanics | 2012 |
| 83 | Szabo, Attila; Ostlund, Neil S. | Modern Quantum Chemistry; Introduction to Advanced Electronic Structure Theory | 1996 |
| 84 | Tadmor, Ellad B.; Miller, Ronald E. | Modeling Materials: Continuum, Atomistic and Multiscale Techniques | 2011 |
| 85 | Tadmor, Ellad B.; Miller, Ronald E.; Elliott, Ryan S. | Continuum mechanics and thermodynamics: From fundamental concepts to governing equations | 2016 |
| 86 | Torquato, Salvatore | Random Heterogeneous Materials | 2002 |
| 87 | Truesdell, Clifford; Noll, Walter | The Non-Linear Field Theories of Mechanics | 2004 |
| 88 | Voyiadjis, George Z. (Ed.) | Handbook of Nonlocal Continuum Mechanics for Materials and Structures, Volume 1 | 2019 |
| 89 | Voyiadjis, George Z. (Ed.) | Handbook of Nonlocal Continuum Mechanics for Materials and Structures, Volume 2 | 2019 |
| 90 | Ward, Ian M.; Sweeney, John | Mechanical Properties of Solid Polymers | 2013 |
| 91 | Weinberger, Christopher R.; Tucker, Garritt J. (Ed.) | Multiscale Materials Modeling for Nanomechanics | 2016 |
| 92 | Wick, Thomas | Multiphysics Phase-Field Fracture; Modeling, Adaptive Discretizations, and Solvers | 2020 |
| 93 | Wu, Han-Chin | Continuum Mechanics and Plasticity | 2004 |
| 94 | Yvonnet, Julien | Computational Homogenization of Heterogeneous Materials with Finite Elements | 2019 |