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Annual Report 2020

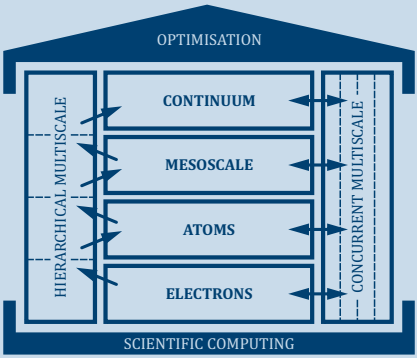
of the Research Training Group GRK 2423

FRASCAL

GRK 2423

Fracture across Scales:

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



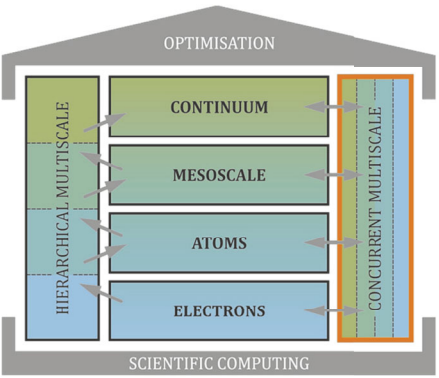
Annual Report
of the Research Training Group GRK 2423

FRASCAL
Fracture across Scales:

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

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

Prof. Dr.-Ing. Paul Steinmann (spokesperson)
Prof. Dr.-Ing. Erik Bitzek (co-spokesperson)



2020

www.frascal.fau.de

Impressum

Spokesperson:
Prof. Dr. Paul Steinmann
Chair 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
Central Institute for Scientific Computing ZISC
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.zisc.fau.de
www.frascal.fau.eu

Preface

FRASCAL started in January 2019 with its first cohort of doctoral researchers. Then, we were able to shape and use the first year largely as planned, i.e. onboarding the new doctoral researchers - preparing, scheduling and pursuing the qualification programme, in particular the multiple FRASCAL mini lectures – and developing initial success steps in the various research projects P1-P12. The past second year of FRASCAL, i.e. 2020, stood out, however, due to the restrictions imposed by the Corona pandemic. Our 2nd Visitors Workshop in the middle of March 2020 was the absolute last activity in attendance just a few days before the first lockdown. In summer 2020, the situation seemingly relaxed so that we were at least able to have the planned FRASCAL retreat in Waischenfeld, in attendance, of course, with all due hygiene measures in place. Unfortunately, in spring 2020 the pandemic tightened its viral grip again. As a result, other than the visitors workshop and the retreat, all further FRASCAL activities during 2020 took place online, e.g. FRASCAL seminars by guest researchers, FRASCAL mini lectures, and, of note, weekly FRASCAL online meetings. There, we also introduced FRASCAL TOPZ (Topical Overview Presentation Zoomposia) which, jointly with the ensuing and engaging discussions, helped review the amazing progress made in the various research projects P1-P12. At the end of the year 2020, we are still pursuing our research at home, however in the meantime with big hopes due to the recent release of new vaccines. FRASCAL's cohort of doctoral researchers will now enter into their third year, where they are thus approaching the home stretch by finishing their doctoral theses. There is no doubt that in a year from now we will see fantastic research work done. All FRASCAL members demonstrated great resilience and endurance even in view of the past and unfortunately still ongoing hardships. This annual report is testimony of FRASCAL's progress during the year 2020, which we will certainly look back to in the future as being historical in many regards.

Erlangen, December 2020

Paul Steinmann

Content

1 General Information

1.1 Title in German and English

Skalenübergreifende Bruchvorgänge:
Integration von Mechanik, Materialwissenschaften, Mathematik, Chemie und Physik

Fracture across Scales:
Integrating Mechanics, Materials Science, Mathematics, Chemistry, and Physics

1.2 Participating researchers

Spokesperson:

Prof. Dr.-Ing. Paul Steinmann

Co-spokesperson:

Prof. Dr. Ing. Erik Bitzek

Doctoral researchers' spokesperson:

Elmira Birang (until March 2020)

Jonas Ritter (from April 2020)

Doctoral researchers' gender representative:

Jonas Ritter (until March 2020)

Christof Bauer (from April 2020)

Table 1: Participating supervisors

Principal Advisors (PAs)	Chair, Department, Work Address	Contact Data (Tel / Fax, Email, Web)	Research Area
Bitzek, Erik, Prof. Dr.-Ing.	General Material Properties, Dep. of Mat. Science and Engineering, Martensstraße 5, 91058 Erlangen	+49 9131 85-27 507 / -504, erik.bitzek@fau.de, gmp.ww.uni-erlangen.de	Material Properties Simulation
Leyendecker Sigrid, Prof. Dr.-Ing.	Applied Dynamics, Dep. of Mechanical Engineering, Immerwahrstraße 1, 91058 Erlangen	+49 9131 85-61 001, sigrid.leyendecker@fau.de, ltd.tf.uni-erlangen.de	Computational Dynamics
Mergheim, Julia, Prof. Dr.-Ing.	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-28 505 / -503, julia.mergheim@fau.de, www.ltm.tf.fau.eu	Computational Mechanics
Meyer, Bernd, Prof. Dr. rer. nat.	Computational Chemistry, Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen	+49 9131 85-20 403 / -404, bernd.meyer@fau.de, chemistry.nat.fau.eu/ccc/groups	Surface Science
Moretti, Paolo, Dr	Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65 071 / -066, paolo.moretti@fau.de, matsim.techfak.uni-erlangen.de	Complex Microstructures
Pfaller, Sebastian, Dr.-Ing.	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-28 507/ -503, sebastian.pfaller@fau.de, www.ltm.tf.fau.eu	Scale Coupling Methods
Pöschel, Thorsten, Prof. Dr. rer. nat.	Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraße 3, 91058 Erlangen	+49 9131 85-70 501, thorsten.poeschel@fau.de, mss.cbi.fau.de	Granular Media
Smith, Ana-Sunčana, Prof. Dr. rer. nat.	Theoretical Physics, Dep. of Physics, Cauerstraße 3, 91058 Erlangen	+49 9131 85 70 565 / -518, smith@physik.uni-erlangen.de, puls.physik.fau.de/	Soft Matter
Steinmann, Paul, Prof. Dr.-Ing.	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-28 501 / - 503, paul.steinmann@fau.de, www.ltm.tf.fau.eu	Continuum Mechanics

Stingl, Michael, Prof. Dr. rer. nat.	Mathematical Optimisation, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen	+49 9131 85-67 141 / -20785, michael.stingl@fau.de, mso.math.fau.de	Optimization
Zahn, Dirk, Prof. Dr. rer. nat.	Theoretical Chemistry, Computer-ChemistryCenter, Nägelsbachstr. 25, 91052 Erlangen	+49 9131 85-20 205 / 404, dirk.zahn@fau.de, chemistry.nat.fau.eu	Condensed Matter
Zaiser, Michael, Prof. Dr. rer. nat.	Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65 060 / -066, michael.zaiser@fau.de, matsim.techfak.uni-erlangen.de	Statistical Mechanics of Materials

Table 2: Postdoctoral researcher

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

Table 3: Doctoral researchers

Doctoral Researchers	Chair, Department, Work Address	Contact Data (Tel / Fax, Email, Web)	Research Area
Bauer, Christof	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-28 508/ -503, christof.bauer@fau.de www.ltm.tf.fau.eu	Fracture in Thermoplastics: Discrete-to-Continuum
Birang Oskouei, Seyedeh Elmira	Central Institute for Scientific Computing, ZISC, Martensstraße 5a, 91058 Erlangen	+49 9131 85-20 783 / - 785, elmira.birang@fau.de, www.zisc.fau.de	Configurational Fracture/Surface Mechanics
Esfandiary, Nosaibeh	Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65 065 / -066, nosaibeh.esfandiary@fau.de, matsim.techfak.uni-erlangen.de	Collective Phenomena in Failure at Complex Interfaces
Konrad, Julian	Theoretical Chemistry, Computer-ChemistryCenter, Nägelsbachstr. 25, 91052 Erlangen	+49 9131 85-20 425 / -404, julian.konrad@fau.de chemistry.nat.fau.eu	Fracture in Polymer Composites: Nano to Meso
Kumar, Paras	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-20 323 / -503, paras.kumar@fau.de, www.ltm.tf.fau.eu	Fracture in Polymer Composites: Meso to Macro
Lakshmipathy, Tarakeshwar	General Material Properties, Dep. of Mat. Science and Engineering, Martensstraße 5, 91058 Erlangen	+49 9131 85-27 486 / -504, tara.ll.lakshmipathy@fau.de, gmp.ww.uni-erlangen.de	Atomistics of Crack-Heterogeneity Interactions
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
Singh, Sukhminder	Mathematical Optimisation, Dep. of Mathematics, Cauerstraße 11, 91058 Erlangen	+49 9131 85-67 048 / -20785, sukhminder.singh@fau.de, mso.math.fau.de	Fracture Control by Material Optimization
Velasco Sabogal, Ali Mauricio	Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraße 3, 91058 Erlangen	+49 9131 85-70 506, mauricio.as.velasco@fau.de, mss.cbi.fau.de	Fragmentation in Large Scale DEM Simulations

Table 4: Associated doctoral researchers

Associated Doctoral Researchers	Chair, Department, Work Address	Contact Data (Tel / Fax, Email, Web)	Research Area
Atila, Achraf	General Material Properties, Dep. of Mat. Science and Engineering, Martensstraße 5, 91058 Erlangen	+49 9131 85-27 468 / -504, achraf.atila@fau.de, gmp.ww.uni-erlangen.de	Crack nucleation and propagation in anisotropic oxide glasses
Becit, Bahanur	Theoretical Chemistry, Computer-ChemistryCenter, Nägelsbachstr. 25, 91052 Erlangen	+49 9131 85-20 422 / -404, bahanur.becit@fau.de chemistry.nat.fau.eu	MD simulation of meso-porous silica self-organization
Esfandiary, Samaneh	Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65 063 / -066, samaneh.esfandiary@fau.de, matsim.techfak.uni-erlangen.de	Robustness and failure of brain activity patterns
Hiemer, Stefan	Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65 062 / -066, stefan.hiemer@fau.de, matsim.techfak.uni-erlangen.de	Machine Learning of Failure of Disordered Materials
Hosseini, Seyyed Ahmad	Materials Simulation, Dep. of Mat. Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65 065 / -066, ahmad.hosseini@fau.de, matsim.techfak.uni-erlangen.de	Modelling Fracture of Hierarchically Structured Materials
Marzulli, Valentina	Multiscale Simulation, Dep. of Chem. & Biol. Engineering, Cauerstraße 3, 91058 Erlangen	+49 9131 85-70 498 / -518, valentina.marzulli@fau.de, mss.cbi.fau.de	Mechanical characterization of granular materials
Ries, Maximilian	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-67 619/ -503, maximilian.ries@fau.de, www.ltm.tf.fau.eu	Multiscale Simulation of Amorphous Polymers
Schmidt, Ina	Faculty of Mechanical Engineering Kesslerplatz 12 90489 Nürnberg	+49 911 5880-1327 ina.schmidt@th-nuernberg.de	Computational Bone Remodelling
Spannraft, Lucie	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-67 620 / - 503, lucie.spannraft@fau.de, www.ltm.tf.fau.eu	Grain Boundary Mechanics
Wullschläger, Florian	Computational Chemistry, Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen	+49 9131 85-20 424 / -404, flo.wullschlaeger@fau.de, chemistry.nat.fau.eu/ccc/groups	Atomistic Simulations of 2D Materials
Zhao, Wuyang	Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-28 511/ -503, lwuyang.zhao@fau.de www.ltm.tf.fau.eu	Small-Scale Informed Constitutive Modelling

Table 5: Student assistants

Students Assistants	Project, Supervisors	Course / Field of study	Member of RTG (from - to)
Dhamo, Kevin	P1, Meyer	Chemistry	Jan 2020 – Dec 2020
Elhaus, Nora	P4, Pöschel	Chemical Engineering	Apr 2020 – Sep 2020
Fahn, Max Joseph	P12, Smith	Physics	May 2020 – Aug 2020
Fuchs, Christian	P8, Mergheim	Mechanical Engineering	16 Aug 2020 – 15 Nov 2020
Gitizadeh, Mohammed	P6, Pfaller	Computational Engineering	Jan 2020 – Feb 2020
Gossler, Mattis	P1, Meyer	Chemistry	Sep 2020 – Dec 2020
Kashiri, Mani	P10, Steinmann	Mechanical Engineering	15 Jul 2020 – Dec 2020
Kirsan, Azad	P1, Meyer	Chemistry	Sep 2020 – Dec 2020
Livraghi, Mattia	P12, Smith	Integrated Life Sciences (ILS)	Jan 2020 – Apr 2020
Müller, Valentin	P3, Zahn	Molecular Science	March 2020 – Aug 2020
Müller-Hillebrand, Johannes	P3, Zahn	Chemistry	16 May 2020 – Dec 2020
Panda, Mahadev Prasad	P10, Steinmann	Mechanical Engineering	15 Jul 2020 – Aug 2020 16 Sep 2020 – Dec 2020
Pominov, Arkadii	P3, Zahn, Konrad	Materials Physics	Jan 2020 – Mar 2020
Rahman, Mijanur	P10, Steinmann	Petroleum and Mining Engineering	15 Jul 2020 – Aug 2020 16 Sep 2020 – Dec 2020
Raj, Ananya	P10, Steinmann	Physics	Aug 2020 – Oct 2020
Ritthaler, Marina	P6, Pfaller	Mechanical Engineering	Oct 2020 – Dec 2020
Rodrigues, Geovane de Jesus	P2, Bitzek	Materials Science and Engineering	Sep 2020 – Dec 2020
Rohracker, Maurice	P8, Mergheim, Kumar	Computational Engineering	Jan 2020 – Nov 2020
Tsankova, Svetoslava	P2, Bitzek	Materials Science and Engineering	Apr 2020 – Dec 2020
Weber, Felix	P10, Steinmann, Bauer	Mechanical Engineering	Jan 2020 – 10 Feb 2020
Wunder, Juliane	P9, Leyendecker	Medical Engineering	10 Aug 2020 – 09 Nov 2020

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

Figure 1: Members of FRASCAL at the 1st RTG-Retreat in Waischenfeld on September 15, 2020.

1.4 Reporting period

01 January 2020 to 31 December 2020

2 Research Programme

2.1 Research projects

FRASCAL comprises 11 doctoral projects (P1-P11), and an overarching postdoctoral project (P12), which reach from quantum mechanics (P1) via atomistic and particle-based methods (P1-P4) to the continuum scale (P8-P11). Several projects (P5-P7, P12) are dedicated to bridging between particle-based approaches (indicated in blue) and continuum-based techniques (indicated in green), whereby the postdoctoral project P12 integrates the results and the expertise developed in the doctoral projects in order to realise a concurrent multiscale modelling approach for fracture. The effect of heterogeneities on fracture behaviour is a common scientific question underlying all projects. Heterogeneities can exist at the atomic scale in the form of locally changed bonding (P1) or density (P2, P12), or at larger scales, where heterogeneities include second phases as in composites (P3, P6, P8, P11), and porous structures (P5), as well as interfaces and surfaces (P7, P10) or (micro) cracks (P4, P9).

P1: Chemistry at the Crack Tip

Tobias Müller and Bernd Meyer

Last year I had focused on setting up initial crack geometries by applying the "pacman" scripts of our project partners P2 and on performing first Car-Parrinello MD simulations with reactive molecules inside the crack. This year I refined the processes and had a closer look at the atomic structure at the crack tip and the boundaries connecting the atomic with the continuum level. It turned out that a large variety of crack surface patterns exist as local energy minima structures, see Figure 2 left.

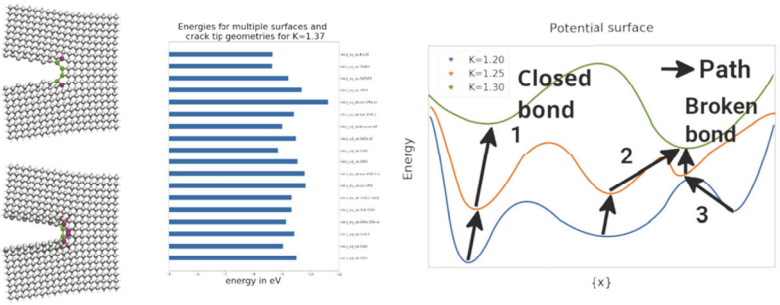


Figure 2: Left: two examples of stable crack tip structures. Middle: energy of different crack tip structures relative to the unrelaxed pacman at K=1.37. Right: illustration of kinetic trapping.

Figure 3 shows that the energetic order of the different crack tip structures strongly depends on the stress intensity factor *K*. In these calculations the initial structure for the geometry optimization at the next higher *K* value was obtained either by a linear rescaling of the old coordinates or by imprinting the displacement field of the specific tip structure to the new pacman. As can be seen, by this approach one tends to be trapped in the initial local energy minimum, while at higher *K* other crack tip structures may have become already more favourable (see Figure 2 right for a schematic illustration). This suggests that a multitude of reaction pathways for crack propagation exist and there is the risk of predicting a wrong path by only following the initial local minimum structure. Instead, one has to explore all local minima, the transition barriers between them and the probability that they can be crossed. In subcritical crack growth at finite temperatures it is reasonable that the reaction path follows the lowest energy minima. Finding this path, however, is a challenge.

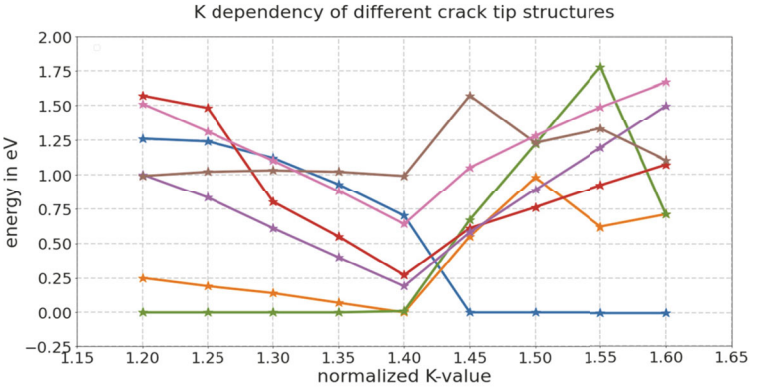


Figure 3: Each colour represents a different crack tip structure. The energetic order strongly depends on the stress intensity factor K.

Since we have to use rather small cutouts of the pacman structures due to the high computational cost of the DFT calculations, it is important to check for size consistency of the calculations before continuing to explore the crack propagation pathway. Increasing the size of the cutout should not lead to different relative energies of the local minima. Unfortunately, with our current approach, in which we generate pacman structures with a fixed, static centre of the strain field, we find a strong size dependency, see Figure 4 (the sizes of the cutouts are depicted in Figure 5 left).

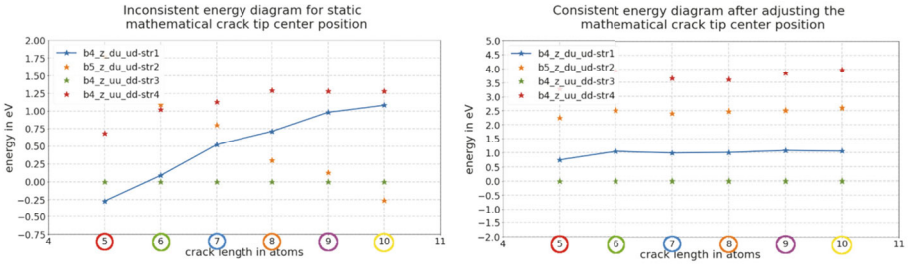


Figure 4: Left: relative energy of 4 different crack tip structures depending on the size of the pacman cutout for a static centre of the strain field. Right: same after alignment of the strain field centre.

The reason for this size inconsistency is the mismatch between the originally chosen “mathematical” centre of the strain field and the true “physical” crack tip centre after the structure optimization, as illustrated by the orange and red dot in Figure 5 right. In other words, the structure optimization was done with wrong boundary conditions (the fixed outer atoms of the pacman cutout), since they were derived from a pacman structure with a wrong strain field centre. Thus, the boundary conditions have to be adjusted until the true physical strain field aligns with the mathematical one (in the far field region where linear elasticity theory applies). To do this, an iterative correction scheme was implemented. A new mathematical crack tip centre was determined by a least square fit between the displacement fields of the relaxed structure and pacman structures with arbitrary strain field centres. With the new boundary conditions from the selected pacman, the next relaxation calculation is performed. This is repeated until no better match is found. The final result in Figure 4 right shows that this procedure completely removes the size inconsistency.

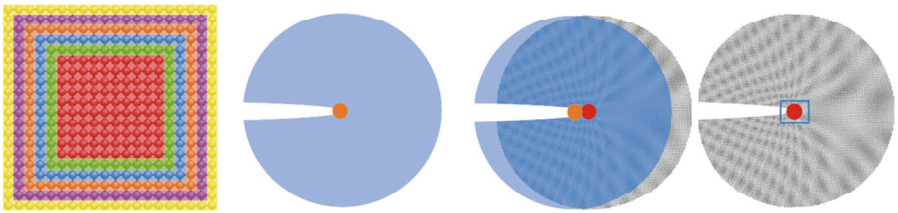


Figure 5: Left: sizes of the different pacman cutouts. Right: illustration of the mismatch between the true physical displacement field with orange centre and the mathematical displacement field with red origin (i.e., the pacman structure).

The results from Figure 4 are very promising for future calculations. Reliable energy difference between crack tip structures can be determined now with rather small pacman cutouts. This will allow me to explore the energy landscape for crack propagation pathways in more detail. The next challenge will be to establish a procedure that combines the iterative correction scheme for the boundary conditions with a molecular dynamics setup for the study of stress corrosion cracking.

P1: Physical Properties of Dislocations in Bilayer Graphene

Florian Wullschläger and Bernd Meyer

Dislocations, i.e. one-dimensional line defects, are the main carriers of plastic deformation in 3D crystalline solids. Furthermore, creation of dislocations and dislocation dynamics play an essential role in the fracture of ductile materials. A recent TEM study has shown that dislocations even exist in materials as thin as two graphene layers. In this ultrathin limit of a 2D material, their properties differ significantly from their 3D counterparts and one has to expect that 2D materials show a very different deformation and fracture behaviour than 3D materials.

I have started to explore the unique properties of dislocations in 2D by using atomistic simulations. Since unit cells for the description of line defects may contain up to a few million atoms, a proper force field for the atomic interaction within and between the layers is needed. The main challenge is to be able to capture simultaneously the interlayer cohesion energy and the corrugation of the energy profile when the layers are shifted with respect to each other. This is not possible with a simple Lennard-Jones potential. Instead, I rely here on our own implementation of the registry-dependent interlayer potential proposed by Kolmogorov and Crespi in LAMMPS.

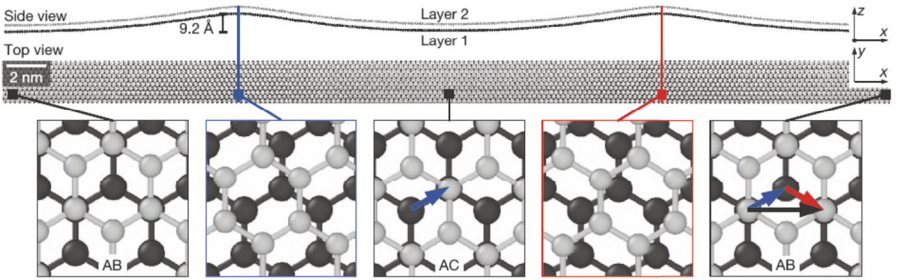


Figure 6: Structure of a graphene bilayer with two partial dislocations, which change the stacking from AB to BA (=AC) and back to AB. The Burgers vectors are shown in blue and red.

With this setup, I have performed first structural characterizations of dislocations in bilayer graphene (see Figure 6). The most important observations are that release of strain leads to a pronounced buckling of the bilayer, a mechanism that is not possible in 3D. Edge dislocations are therefore more favourable than screw dislocations. Furthermore, while in 3D the line energy of a dislocation shows a logarithmic divergence with increasing radius R of an enclosing cylinder, in 2D the line energy converges with $1/R^2$.

In 2D, dislocations also have a huge impact on the electronic structure of a material. Here, minimally twisted bilayer graphene is of special interest, which relaxes to a highly regular hexagonal network of partial screw dislocations. For this material, exotic electronic states have been postulated, leading, for example, to superconductivity at special “magic” twist angles. In a collaboration, Sam Shallcross from the Physics Department performed electronic structure calculations on our relaxed dislocation geometries in twisted bilayer graphene [1,2]. He could show that in an external electric field a very robust and perfect Fermi surface nesting exists [1]. Furthermore, areas with different stacking, separated by a partial dislocation, can possess different Chern numbers, which leads to topologically protected one-dimensional electronic states in the domain boundary (see Figure 7) [2], thus making the dislocation network of twisted bilayer graphene an ideal playground for studying properties of topological materials.

After the structural analysis of dislocations in bilayer graphene, I have started to simulate the dynamics of dislocations, with the aim to study their interaction with obstacles. Up to now, I have tested different settings for the MD simulations of dislocations, including the variation of the force field for the description of the atomic interaction within a graphene layer and different thermostats and temperature ramps to establish the simulation temperature.

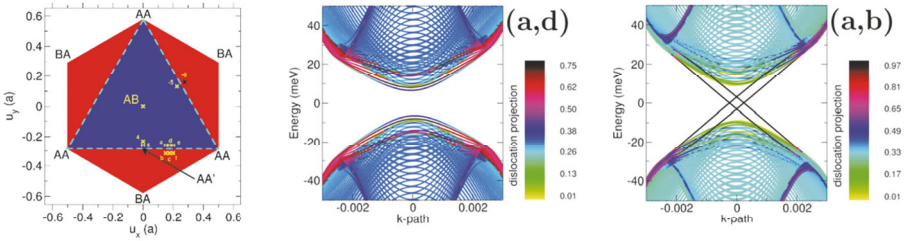


Figure 7: Left: Chern index phase diagram of bilayer graphene as function of the relative shift of the two layers (u_x,u_y). Blue area: Chern index 0, red area: Chern index 2. Middle and right: electronic band structures of a graphene bilayer with two domain boundaries separating two areas with different stacking with same (middle) and different (right) Chern index. The change of the Chern index leads to topologically protected states crossing the Fermi energy at 0 meV (right). These states are exclusively located at the domain boundary, which becomes metallic and behaves like a 1D metallic wire embedded in an insulating matrix. If changes in stacking do not alter the Chern index, the band gap of bilayer graphene is preserved (middle).

In summary, dislocations in 2D possess a wealth of fascinating properties: their unique energy density distributions and strain fields, which are qualitatively different from 3D dislocations, give rise to the expectation that the plastic deformation and fracture behaviour of 2D materials is distinctly different than in 3D. Furthermore, they have a pronounced impact on the electronic properties of 2D materials as demonstrated by the perfect Fermi nesting [1] and appearance of 1D metallic states [2] in an otherwise insulating material. Unfortunately, up to now no reliable setup for the simulation of dislocation dynamics could be established. This will be the topic of future work.

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P2: Influence of Crack Tip Radius on Fracture Toughness: An Atomistic Study

Tarakeshwar Lakshmipathy and Erik Bitzek

Objectives and status

A parameter study of the dependence of fracture reinitiation toughness (K_{Ic}) on the blunting radius (r_0) of a pre-existing crack was done using atomistic simulations under quasistatic loading. Starting from an atomically sharp configuration (r_0*), cracks were blunted up-to radii of 50 Å. A harmonic potential with a cut-off was used to ensure that the interatomic interactions were linear and local. In addition to being appropriate for the framework of linear elastic fracture mechanics (LEFM), the potential had the benefit of not displaying surface related phenomena. The calculations were performed using the open source code LAMMPS for different crack systems denoted by (crack plane)[crack front].

In crack system (100)[011] where the fracture behaviour was brittle, displacements due to relaxation were analysed at a load at which the sharp crack was stable at the centre of the simulation setup (K_{in}). The displacements were calculated with respect to the atomic positions prescribed by anisotropic linear elasticity. In the case of the atomically sharp crack, it was found that the displacements were negligible (see Figure 8(a)), showing that LEFM was valid. However, in the case of blunted cracks, large displacements were observed during relaxation (see Figure 8(b)), indicating deviations from LEFM. It was hypothesized that the deviations were a result of LEFM inadequately addressing the boundary value problem posed by blunted cracks (see schematics in Figure 8).

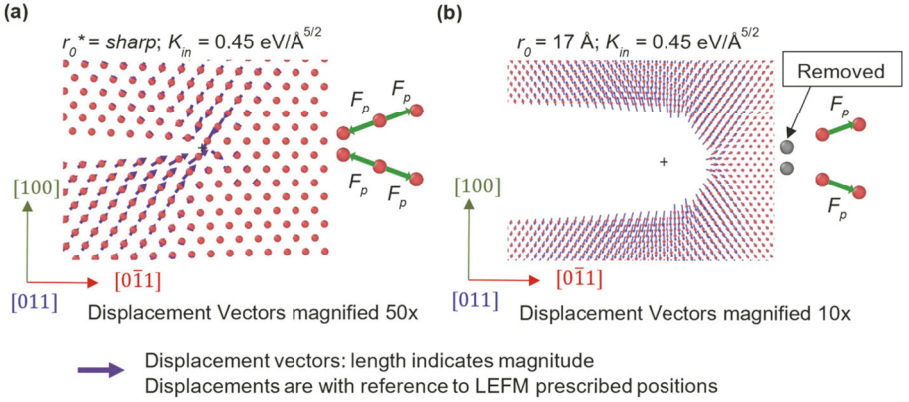

Figure 8: (a) Displacements during relaxation in the sharp crack configuration at K_{in}. (b) Example of displacements during relaxation in a blunted crack configuration at K_{in}. The schematics on the left of each figure illustrate the boundary value problem posed by the respective configurations (green arrows indicate pairwise force).

The consequences of the deviations on the stresses were analysed at K_{in} by considering atoms in a line ahead of the crack tip (see Figure 9(a)). The atomic stresses were calculated following the method described in [1]. Figure 9(b) plots the stresses as a function of distance from the mathematical centre of the crack tip. The stresses closely followed a square-root decay in the case of the atomically sharp crack, which is consistent with LEFM. In the case of the blunted cracks, the stresses peaked a few layers away from the crack tip surface. In addition, the values of the atomic stresses were much higher than on the corresponding atoms in the sharp crack configuration. It should be noted that these deviations were observed, not just at K_{in}, but at every iteration of the subsequent loading process. In Figure 10(a), it can be seen that the consequences of the deviations from LEFM are also reflected in the values of K_{Ic}, with the increased atomic stresses in the blunted cracks leading to significantly lower fracture toughness compared to LEFM predictions.

The (100)[001] crack system was also studied, where the displacements at K_{in} in blunted cracks were qualitatively similar. Hence, the values of K_{Ic} also deviated from the predictions of LEFM (see

Figure 10(b)). However, the results for blunted cracks displayed brittle precursors which could lead to energy dissipation before sharp crack reinitiation. Hence, quantitative analyses were not performed for this crack system. Furthermore, the presence of brittle precursors resulted in an offset in blunted cracks towards slightly higher fracture toughness values than would have otherwise been observed.

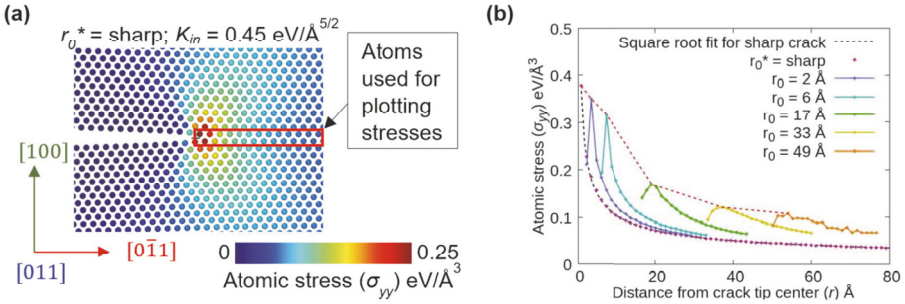

Figure 9: (a) Atoms used for stress analysis at K_{in} showing the example of the atomically sharp crack. (b) Stresses on atoms ahead of the crack tip in various configurations as a function of distance from mathematical crack tip centre.

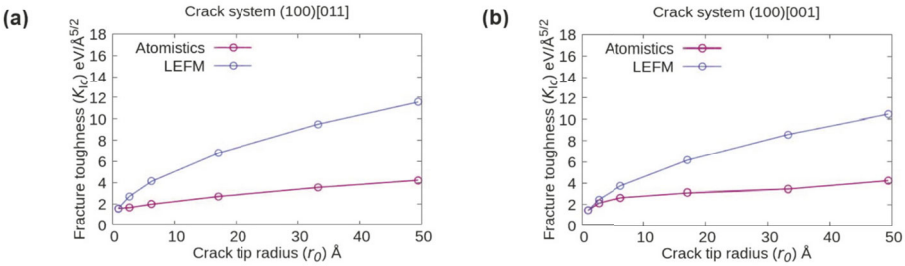

Figure 10: Fracture toughness (K_{Ic}) as a function of blunting radius in crack systems (a) (100)[011] and (b) (100)[001].

Conclusions, main achievements and outlook

An earlier study [2] had hypothesized that deviations from LEFM in blunted cracks were mainly due to non-linearities in interatomic interactions. However, this work has shown that the deviations could rather be due to an inadequacy in the mathematical framework of LEFM. A more recent phenomenological study of blunt notches [3] established a scaling relation based on physical quantities such as tensile stress. Preliminary analysis has shown that, while the relation itself can be fitted with the results of this work, the resultant parameters lose their physical significance. It is planned to study this in more detail, and possibly, propose a novel semi-empirical scaling relation based on the results of this work.

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P2: Atomistic Simulations of Crack-Heterogeneity Interactions

Achraf Atila and Erik Bitzek

Oxide glasses are archetypal brittle solids. They show excellent optical properties, which made them ubiquitous in many applications, including screens for mobile devices and optical fibres [1]. However, their application range is limited by their brittleness and low resistance to damage [2]. The strength of oxide glasses is strongly affected by microscopic flaws. The disordered structure of the glasses makes it difficult to analyse how these flaws lead to macroscopic fracture, in particular, how mechanical load influences the initial flaws. To understand the deformation behaviour and fracture of oxide glasses it is crucial to understand the atomic scale mechanisms of how defects are affecting glass strength. In particular, plastic deformation (e.g. under compression or shear) leads to flaws and how they influence the mechanical behaviour of glass?

We performed a series of molecular dynamics simulations of silica glass to address these questions using an empirical force field. A silica glass was produced through the conventional melt-quenching technique. Then, deforming it either by tension, compression or shear (both, at constant volume or pressure) and subsequently unloading it to 0 MPa from different maximum strain values. The pre-deformed glasses were then subjected to uniaxial tensile tests in X, Y, and Z directions.

Macroscopic mechanical properties such as Young's modulus showed an anisotropy, in the case of the pre-deformation in compression, while they stayed isotropic in the case of tensile and shear pre-deformations. Additionally, plasticity was observed in the glasses pre-deformed by compression and shear, with maximum plastic strain for the pre-compressed glasses (see Figure 11(b)). The increase in the glass plasticity was found to be related to the increase of the density. Simultaneously, the atomistic view of the glass structure showed us that the deformation behaviour of the glasses is related to the defect density, which was determined by analysing changes in the bond configurations (see Fig. 2 for an example of the bond switching mechanisms).

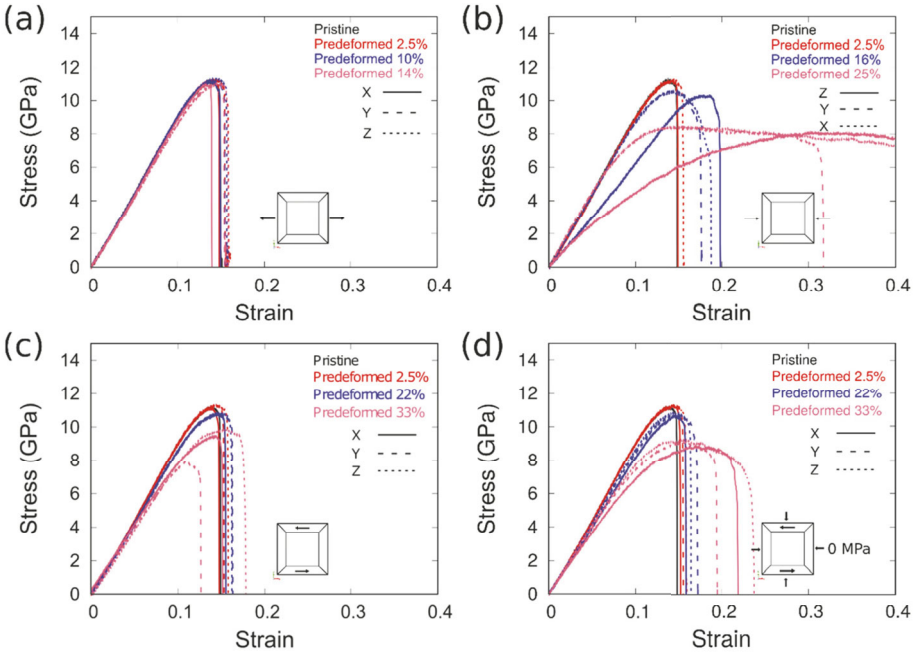

Figure 11: Tensile stress-strain curve of the pristine glass vs. the samples pre-deformed by (a) tension, (b) compression, (c) shear at a constant volume, and (d) shear while keeping the orthogonal stresses at 0 MPa. The insets on each plot show a schematic of the pre-deformation applied to the glass before the reloading.

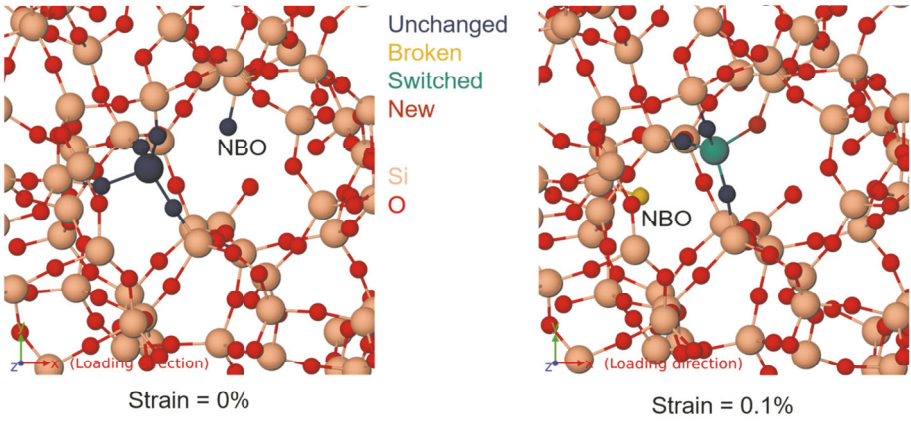

Figure 12: Example of bond-switching mechanism in the form of migration of nonbridging oxygen and a SiO4 tetrahedron rotation. Atoms are color-coded based on their bond status, as indicated in the legend.

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P3: Fracture Mechanics of Epoxy Resin with Dissociative Force Field

Julian Konrad and Dirk Zahn

Epoxy model development for fracture mechanics

Modelling an epoxy resin of EPON and DETDA for fracture mechanics demands understanding distinct atomic interactions. We used different methods to outline the critical processes as accurate as needed, whilst maintaining computational efficiency to enable large-scale simulation models. Describing a chemical bond cleavage or formation requires quantum mechanics (QM) calculations. However computing a whole polymer system on the quantum level is not feasible, so we captured primarily the energetics and dynamics of the crosslinking reaction and its dissociation with QM. On this basis, a reactive Force Field is created such that we now depict the complete system by (tailor-made) molecular mechanics models. This enables the modelling of >10 nm scale polymer networks whilst considering critical processes such as crosslinking and bond dissociation at reasonable accuracy.

QM

We identified the CN-bond between the EPON and DETDA compound as most important to be explored with quantum mechanics for the reason that it is formed at the curing reaction and is the weakest bond in the epoxy network backbone responding foremost with cleavage under stress. Calculations were performed to determine energy profiles as functions of the C-N-distance for bond dissociation with/without proton transfer and for a bi-radical based mechanism (see Figure 13).

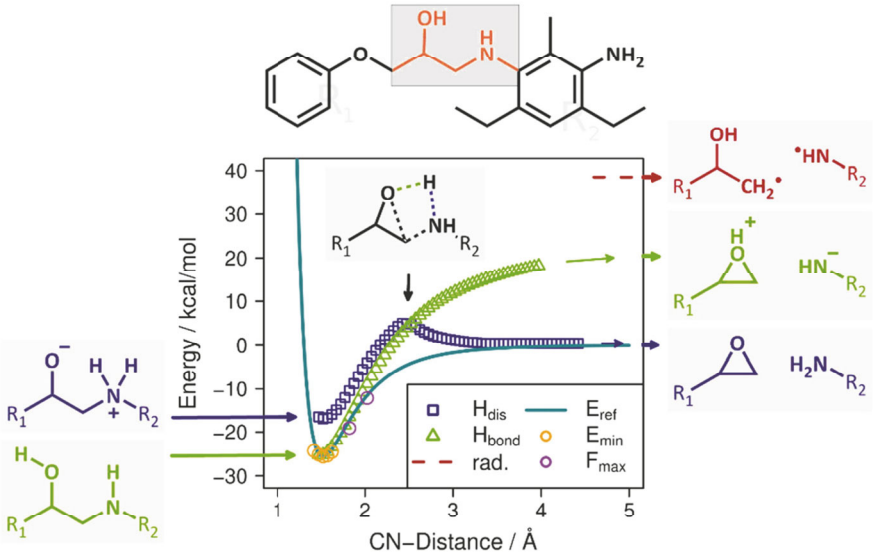

Figure 13: Mainly two QM calculations (blue & green) were sufficient to describe the PMF (turquoise) along the CN-distance with respect to the elastic properties (orange) around E_{min} and the toughness (purple) described by F_{max}.

While the bi-radical based C-N bond dissociation is energetically disfavoured, we created an effective minimum energy profile for C-N bond formation/dissociation along with H-transfer where needed. For this, the involved atomic moieties were coarsened and a newly created molecular mechanics potential is applied to the corresponding interaction sites. On this basis, a 'reactive force-field' is achieved that enables the study of both epoxy formation and fracture.

Curing

To perform calculations on greater length and time scales we had to transfer the QM CN-potential into a Force Field providing the results for molecular dynamics. To accomplish that transfer from QM to MM the topology of the system had to be changed. Inspired by the concept of forcing the reaction of a random pair of reactants [1], we adopted this procedure. Here our model contributes the advantage the topology transfer already implied in the Force Field, as well as covering the energetics of the reaction. The curing procedure we developed yields crosslinking degrees up to 98 %. Our model is satisfying the properties for this corresponding epoxy resin system in terms of thermodynamic and elastic properties.

Fracture

The reactive Force Field provides the possibility exploring manifold applications and, we give an example for a uniaxial tensile test until fracture. One great feature of the dissociability and reactivity is for instance the opportunity to response in terms of reorganization under stress, which we want to underline by examination of different tensile rates (see Figure 14). One can observe the slower the tensile rate the more time has the system to rearrange and reorganize broken bonds and thereby reducing the potential energy, which yields in less stress in the system and mechanical work that has to be invested for fracture.

With this model, we can move on investigating molecular mechanisms along deformation for different shapes and composites.

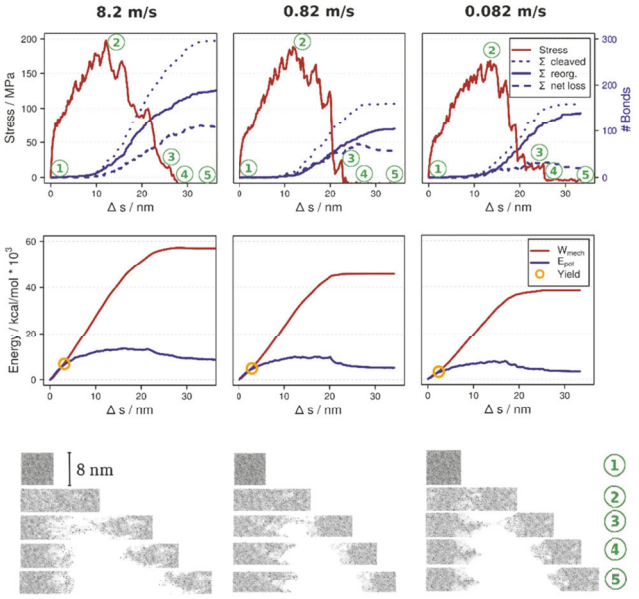

Figure 14: Tensile test at different rates shown with respect to stress (top) and mechanical work (mid) in red and degree of reorganization (top) and potential energy (mid). The associated snapshot provided at bottom marked in green for initial structure (1), ultimate stress (2), just before tearing up (3), after tearing up (4) and after potential energy relaxation (5). The yield point is here defined at 10 % differing of W_{mech} and E_{pot}. Stronger expression of reorganization and absolute number of bonds dissociated at faster tensile rates (left) due to the lag of time for rearrangements in comparison to slower tensile rates (right). Additionally, structures (3) depict a difference in the amount of damage at the material.

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P3: Modelling Silica Colloid as $SiO_ySi(OH)_x$ Core-Shell Particles Using Molecular Dynamics Simulations

Bahanur Becit and Dirk Zahn

Motivation and objective

In the past few decades, silica particles in colloidal form are used in many technological applications such as catalysis, coatings, reinforced plastics and composites, astrophysics.[1,2,3,4] Therefore, demand of colloidal silica in diverse applications renders understanding underlying physicochemical properties and thermodynamics of colloidal silica very appealing.

Synthesis, functionalizing and customizing properties of the silica nanoparticles for engineering in desired applications require broad knowledge of the behaviours of silica nanoparticles in aqueous solution. In terms of utilizing the knowledge on interfacial interactions with other particles/molecules, control of chemical and colloidal stability, coarse dispersion is undoubtedly vital to be able to tailor the properties for goal-oriented usage of colloidal silica particles.[3] In recent years, numerous experimental and computational studies have been carried out using colloidal silica in terms of coagulation[5], aggregation, adsorption[6], self-assembly[7]. Molecular modelling studies in atomistic scale of silica colloids can promote wide perspective of silica nanoparticles in aqueous solutions for optimizing stability and can assist empirical studies by overcoming experimental difficulties[8]. And optimized colloidal silica particles can be used for further aimed applications, for example, to model silica-epoxy nanocomposites.

Modelling wetted amorphous silica particle and molecular dynamic simulation details

Alpha-quartz unit cell is replicated to create a crystalline cube with the size of 38.5x38.5x38.5 Å, consisting of 1369 silicon (Si) atoms and 2972 oxygen (O_B) atoms. To obtain a wetted surface, 468 dangling oxygen atoms in outer surface were converted to silanol oxygens (O_H) and saturated by adding hydrogen (H) atoms. All MD simulations in this study were performed with LAMMPS simulation software using a time step of 1 femtosecond (fs)[9]. For intramolecular pairwise interactions of particle, CMAS94 model from Matsui *et al.* was chosen[10]. Parameters of CMAS94 model was converted for Buckingham potential, which is implemented in LAMMPS. Simulations in vacuum were run using canonical ensemble with Nose-Hoover thermostat with damping time unit of 0.1 ps. Melt and quench procedure was used to create amorphous silica nanoparticle from quartz silica. The cube was melted by applying vacuum in all directions of the box by increasing the temperature to 2300 K and then instantaneously but stepwise cooled down to room temperature, 300 K. Obtained spherical structure from crystalline cube, with the average diameter 49.5 Å, was equilibrated further at 300 K. After long equilibration run using canonical ensemble in vacuum, obtained particle was solvated in water. Potentials from Ciacchi L. *et. al.*[11] combined with TIP3Pm water model of Mark *et. al.* was used to model silica-water interface interactions.[11,12] To calculate long-range Coulomb interactions, damped shifted force model was applied.[30] All simulations with the system in solution were carried out within the isothermal-isobaric ensemble at 300 K and 1 atmosphere (atm) and under periodic box conditions. The Nose/Hoover thermostat and barostat were introduced with damping time of 0.1 ps and 1 ps, respectively.

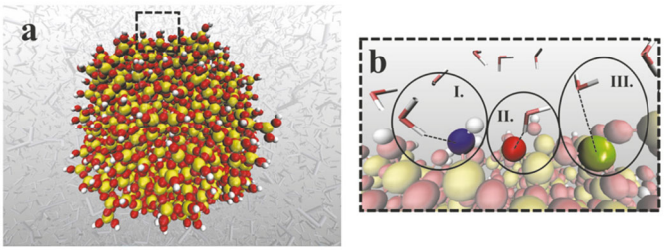

Figure 15: Wetted amorphous silica nanoparticle. (a) Perspective view of our solvated model of silica nanoparticle. (b) Three main paths for interactions of surface ions and water molecules with a magnified image of a region, which is indicated with, dashed square in (a). Each interaction indicated with dashed lines. Path I exemplifies hydrogen bond (H-bond) between water hydrogen (H_W) and oxygen of surface hydroxyl group (O_H, blue) in our model. Path II indicates H-bond formed by H_W and surface bulk oxygen (O_B, red). Path III shows salt bridging between surface silicon and water oxygen.

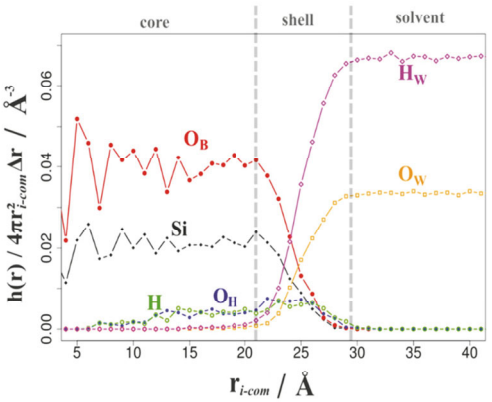

Figure 16: Normalized radial density profiles as functions of the distance from the colloid centre, indicating a SiO2 core zone, a SiOx(OH)4-2x shell area and the solvent interface, respectively. We note that there is a small, yet non-zero density of hydroxide ions in the particle interior. While this feature is indeed also observed from experiments[1], a quantitative assessment would call for more rigorous configuration sampling.

The silica colloid model was subjected to a structural analysis to ensure stable and reasonable colloidal silica for further use in applications. Upon melting and re-solidification of the core-shell quartz nanocube, we obtained spherical silica colloids of amorphous inner SiO_2 core, whilst the surface comprises of silanol groups. The distribution of Si^{4+},O^{2-} and OH^- ions as functions of the distance from the centre-of-mass is shown in Figure 16. We find the corresponding density profiles in line with the comparable simulation studies of Wendland[13] and Singer[14]. This also holds for the interactions with water molecules, once the colloid is immersed into aqueous solution. Interfacial water molecules form O(water)••Si salt-bridges and H(water)••O (OH^- and O^{2-}) hydrogen bonds (Figure 15) with the silica particle. While it is intuitive to expect such strong electrostatic interactions to provoke well-defined solvation shells, the local roughness of the particle (as reflected by the overlap of water).

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P4: Fragmentation in Large Scale DEM Simulations

Ali Mauricio Velasco Sabogal and Thorsten Pöschel

Once the multisphere representation algorithm was developed and tested for virtually any irregular shape, the next step, and the current state of this project is focused on three main points. The first is the geometrical description and computation of the grain fracture, the second is the implementation of the developed models in a third party DEM software to simulate ca. 10^5 grains, and the third is the application of these models and software to study interesting physical and industrial systems.

a. The design and implementation of an algorithm to subdivide the grains after a fracture.

As described in the previous report, the shape, mass, and inertia of the grains are computed and tracked through a triangulated mesh, while the possible contact points of each grain are computed from the multi-sphere representation. Driven by these concepts, a natural way to describe grain fragmentation is describing it directly on the triangulated shape. The proposed procedure is the following: when a fracture occurs, the triangulated mesh is subdivided, and the triangulation is reconstructed (see Figure 17 A, B, C), afterwards, a new multi-sphere representation of each new fragment is computed. This method assures that the number of spheres per fragment stays constant, and therefore, the fragmentation of a grain is not limited by its original multi-sphere representation. Figure 17 D shows the multi-sphere representation of five fragments. The phenomenological description of the fragmentation probability, the fracture criteria and the fragment size distribution are work in progress.

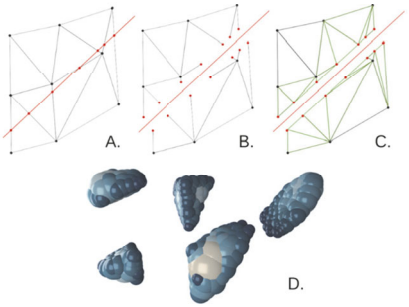

Figure 17: Particle plane subdivision.

b. Implementation of breakable multi-spherical particles using Mercury DPM. The possibility to simulate a huge number of particles with this method thanks to optimization algorithms.

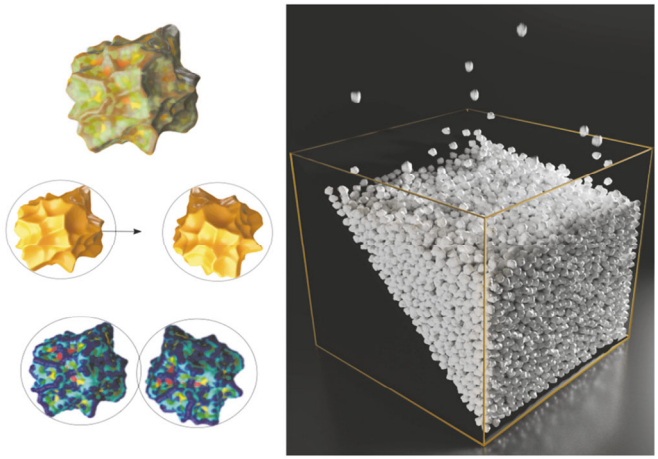

Figure 18: Schematic representation of a two-particle collision (left). Prismatic container with 8000 multi-sphere particles, simulated with MercuryDPM (right).

The simulation of granular materials by the Discrete Element Method (DEM) requires the individual dynamic tracking of each grain and the computation of the particle-particle and particle-wall contacts. In our case, each real particle is composed by the triangulated shape and a clump of around 10 spheres, in contrast with the single sphere grains of a typical MercuryDPM simulation. Therefore, the computational costs of simulating a granular system composed by realistic particles (see Figure 18) is expected to be

much higher. To solve this, our differentiation between the particle triangulated shape and multi-sphere representation is useful again: if a particle is not in contact with other particles or walls, the translation and rotation of the particle is updated only by considering the triangulated shape and its inertia. The boundaries of the particle are modelled as a spherical envelope (Figure 18 left middle). If an object of the system (particle or wall) overcomes the particle spherical boundary (Figure 18 left bottom), we transform the positions of the spheres of the multi-sphere representation from particle-fixed to lab-fixed coordinate systems taking into account both the translation and rotation of the particle. In this way, we can find the nearest spheres between the two particles (or between the particle and the wall) and compute the contact between them and the computation of the dynamics of each sphere is not necessary. The upper bound of the grey region of Figure 19 is the time needed to make a simulation if the all-sphere dynamics are computed each time step. The fat lines are obtained by searching for the closest spheres only between the ones that are in the direction of the vector that links the two particles. The described procedure allows us to simulate granular materials with ca. 10^5 three-dimensional irregular particles, one of the main objectives of the project (see Figure 18 right).

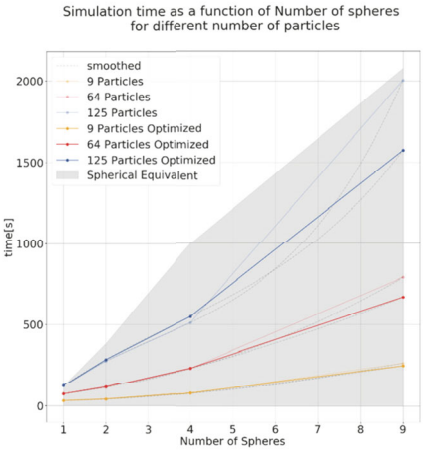

Figure 19: Computational time as a function of the number of spheres for systems with different particles, compared with the computational time of simulating the same number of spheres as independent particles.

c. Utilization of the model in the study of interesting physical and industrial systems.

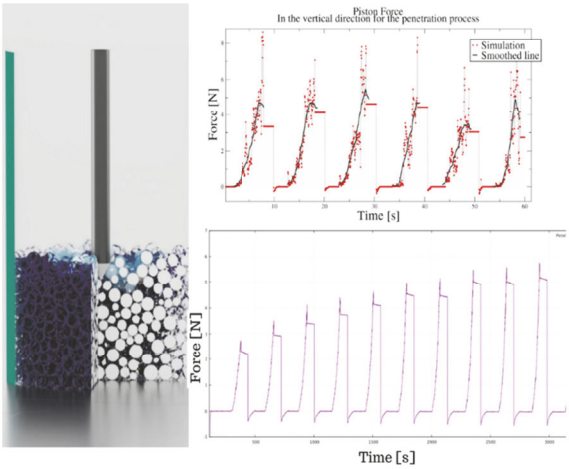

Figure 20: Snapshot of the simulation of the penetration process (left). Preliminary results of the simulations for the force exerted on the piston as a function of time (right top) compared with the obtained in the experiments (right bottom).

In search of interesting applications to our model we start a collaboration with Valentina Marzulli for the simulation of the perforation process in granular material confined in a cylindrical container. The force felt by the penetrating piston and the distribution of pressure along the cylinder walls are quantities of great importance, since they give account of the mechanical response of the granular material to the perforation and the evolution of the system after several penetrations. In this process, phenomena like compactification, particle cohesion and fracture are ubiquitous. Our aim to predict pressure and force values by numerical simulations. The predictions are needed for sensor calibration and a microscale understanding of the involved mechanisms. The preliminary results for spherical particles are in good agreement with the obtained experimentally and can be seen in Figure 20. The extension to irregular breakable grains is a work still in progress.

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

Valentina Marzulli and Thorsten Pöschel

My research project aims at measuring the stress regime during a quasi-static penetration process within a layer of granular material under different gravity levels. For this purpose, I have successfully submitted a proposal to the ground-based facilities programme of ESA-CORA-GBF in collaboration with other colleagues from different institutions. We have now the unique opportunity to get access to the Large Diameter Centrifuge of ESA and, thus, to perform our experiment in hyper-gravity conditions. The main objectives of this project can be divided in two different parts: a) understanding the physics behind a quasi-static penetration process in granular materials under different gravitational conditions and b) develop a reliable mechanical model capable of simulating a wide range of processes that will take place on the Moon (e.g. building of lunar structures, in-situ tests, modelling of wheel-soil interaction for rovers operating on the lunar surface, and so on). Unfortunately, it is not possible to directly carry out this experiment under Moon gravity conditions. In fact, in a parabolic flight it is possible to maintain Moon gravity conditions for just few seconds, while this experiment takes place in few minutes. Therefore, to overcome this problem we decided to perform such experiment under hyper-gravity conditions (up to 20g) and to extrapolate the results to the low gravity conditions. To achieve our goal, we first needed to design and build the experimental setup. In the past months, I have been involved in the design of this innovative setup (Figure 21) and on the modelling via DEM simulations of the penetration process. In parallel, I have also carried out preliminary tests to calibrate each component (i.e. piezoresistive sensors, electric piston, force sensor). It has been designed taking into account all the restrictions and requirements provided by the LDC user's guidelines.

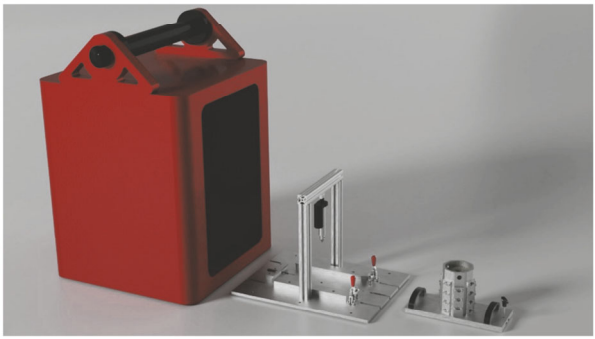

Figure 21: 3D model of experimental setup and gondola in which it will be placed (in collaboration with Achim Sack, Mauricio Velasco Sabogal, Walter Pucheanu).

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

Once the setup is mounted in the gondola, the experimental procedure is designed as follows:

1) Preparation of the sample: fill the cylinder with granular material following a standardised procedure.
2) Positioning of the cylinder into the setup.
3) Starting the test: the centrifuge starts to spin up to a certain desired gravity level. Once it is reached, the acceleration is kept constant for the whole duration of our experiment.
4) Relaxation time: we let the system relax before starting the penetration process.

5) Penetration process: the penetration velocity is kept constant during the test and once the piston reaches the maximum depth it is held in place for a few seconds until a static regime is reached again.

6) Extraction of the piston: the piston is pulled out at the same velocity as during penetration.

7) The cylinder is pulled out from the gondola and a new sample of granulate can be prepared.

I have tested three different granular materials with different grain size distribution and properties (particle shape, roughness, stiffness), using different preliminary setups and varying the velocity of the piston (Figure 22; Ottawa sand, glass beads and Lunar simulant DNA-1A).

Figure 22: Preliminary setup (a) and tested materials: DNA-1A (b), glass beads (c), Ottawa sand (d).

The main features of a penetration process are shown in Figure 23. In particular, we observed that for each cycle we reach a maximum force value (Fa, activation force) when the piston reach the maximum depth and that it suddenly decrease while the piston is held in place. When the piston is pulled out the penetration force reaches a minimum value (Fh, holding force) which represents the ability of the material to hold the piston. The holding force increases while increasing the number of penetrations up to a constant value for each material except for the lunar simulant. This is due to the cohesive properties of this material (Figure 23b). Finally, the activation force increases too up to a saturation value, which is characteristic for each material. Glass beads and Lunar simulant do not show significant variation in the activation force during the multiple penetration test rather than Ottawa sand.

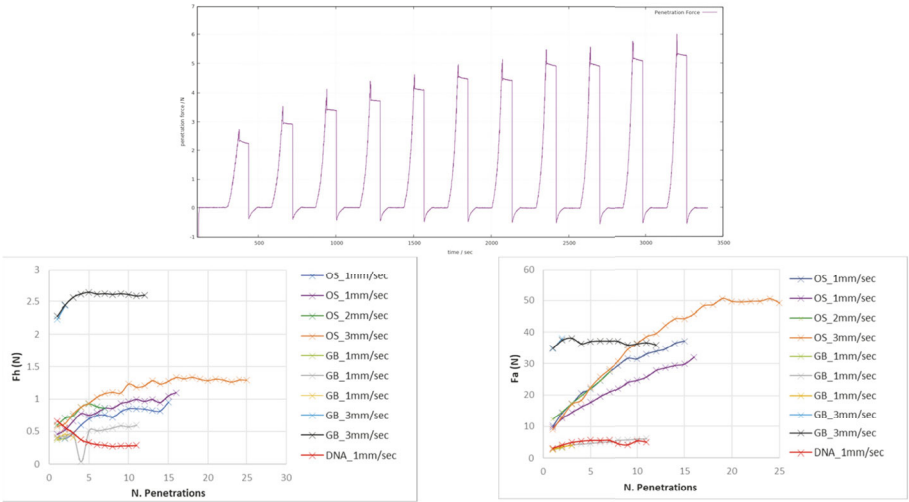

Figure 23: Preliminary results: penetration force vs time (a), holding force vs number of penetrations (b), activation force vs number of penetrations (c).

P5: Progress in Peridynamic Simulations of Porous Microstructures

Jonas Ritter and Michael Zaiser

Objectives and status

In projects second year phase it was mainly worked on a reliable setup for the simulation of porous structures compression within a peridynamic simulation environment. Initial geometries in terms of micro-computed tomography images of snow are provided by our cooperation partner SLF, which were already investigated with respect to the elastic regime by measurements and FE simulations [1]. Moreover, successful peridynamic simulations of ice fracture were among others already done by [2]. As stated in the last project report [3] as productive peridynamics simulation code Sandia's Peridigm research code is utilized [4]. For the simulations data management a Python environment based on the signac framework was written and is under continuous development [5]. It defines a standard workflow, takes care of the related metadata and the simulation runs. In combination with self written extensions it provides help for a more robust simulation process. Furthermore, the automatic management helps to keep track of metadata to ensure long-time reliable results. Currently, the integration of simulation runs on the RRZE Emmy cluster in combination with the job scheduler is under development. The Peridigm code is already migrated to work on the Emmy cluster.

To justify the applicability of a pure elastic material model and the LEFM to simulate ice fracture in the brittle regime with loading rates greater than 10^{-3} s^{-1} simulations of the uniaxial tests performed in [6] and CT-tests by Liu and Miller [7] were conducted. Results showed elastic waves travelling through the specimen after pulling apart which highlights the need of a dissipative mechanism in the simulation setup. Figure 24 (a) shows the discretized CT-specimen and Figure 24 (b) its related force-displacement curve with its periodic fluctuations of the pin forces.

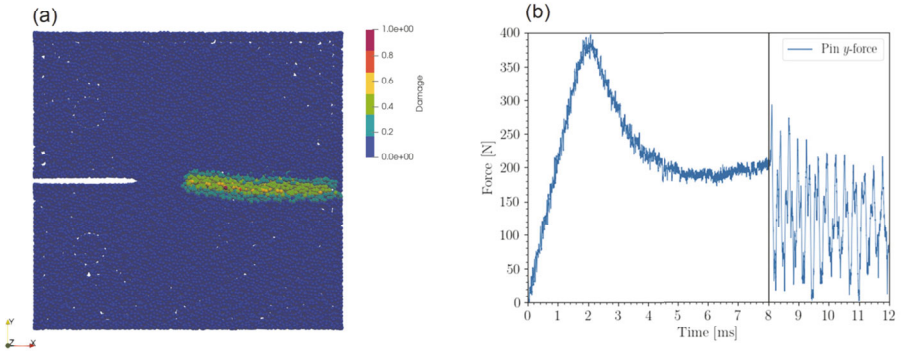

Figure 24: Simulated CT test of an ice specimen according to [7]. (a) Damage pattern of the pre-notched CT-specimen after t = 7.99892 ms. (b) Time-force graph for a loading rate of 9.6667 mm/s. The point in time of the snapshot in Figure 24 (a) is marked by a black vertical line.

Additionally, align structures in an unstructured mesh led to a local disturbed discretization and subsequent to pre-defined “weak spots” were the specimens preferentially failed. Due to the mentioned issues those calculation should potentially be rerun in a modified setup, which provide dissipative mechanism such material or numerical damping. If the experimental results cannot be reproduced a more sophisticated material model must be used.

First peridynamic simulation of the porous snow microstructures showed similar difficulties as the validation simulations. The initial geometries are voxel discretized with a resolution of 10 µm. This leads to an approximate voxel mass of around 9 x 10^{-16} kg in case of ice. As a consequence, for 1 s of simulation time around 740 million time steps would be required. In a first attempt, it was planed to bridge the elastic regime by an implicit time integration scheme or a quasi-static solver, both provided by the Peridigm code. Despite all efforts, it was not possible to obtain a solution.

To overcome the issues of transient explicit simulations and required small time steps an adaptive dynamic relaxation scheme can be used. The idea is to assume a quasi-static loading case while computing the solution by an explicit scheme with large time steps but an adapted damping to ensure stability of the integration [8]. This is implemented in Peridigm and is based on the work of Kilic and Madenci [9] and Underwood [10]. Currently, the implemented version is not stable for complex geometries such as porous structures. This might be due to the complex stiffness matrix, which is partially required to determine the artificial masses.

In addition to the simulations, it is planned to work on compression experiments of 3d-printed snow microstructures. A proof-of-concept print was done by selective laser sintering of PA12 polymer powder (Figure 25).

Figure 25: Upscaled and 3d-printed snow microstructure with an original edge length of 2 mm.

For that reason, the microstructure edge length of 200 voxels per edge (corresponds to a real edge length of 2 mm) was upscaled to 60 mm, i.e. the microstructure was scaled by a factor of 30. Due to the increase of the specimen size the time step is of the order of 10^{-8} s. Simulations with an overall time of 0.01 s are possible in almost 1 day on the Emmy cluster. Material parameters of PA12 can be estimated from the published data, e.g. by [11].

Beside this work, several bugs in the Peridigm code were fixed, improvements implemented, including the possibility to periodically dump restart files during a simulation and an update to Python 3. Those were also provided to the maintainers of the code.

Conclusions, main achievements and outlook

In last few months, several important experiences with peridynamics and its intricacies were gained. Simulations of ice fracture in the millimetre scale showed current limitations of the approach, due to very small masses after discretization. Nevertheless, compression simulations with the assumption of quasi-static loading should be feasible. For that reason, further investigations and effort must be invest to gain a more robust stimulation framework that can be used for a variety of structures and boundary conditions to study systematically the influence of the geometry and the load on the fracture behaviour of porous structures under a quasi-static assumption. In combination with the planned experiments, this provides a comprehensive framework for systematic investigations.

References

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P5 Modelling Failure and Flaw Tolerance of Hierarchically Structured Materials

Seyyed Ahmad Hosseini and Michael Zaiser

Objectives and status

We developed a Beam Network Model (BNM) to study fracture and flaw tolerance of hierarchically structured materials and randomized variants thereof (see Figure 26). We used our model to analyse the process of damage accumulation (characterized by the locations and timings of beam breakage avalanches prior to global failure) and of global failure.

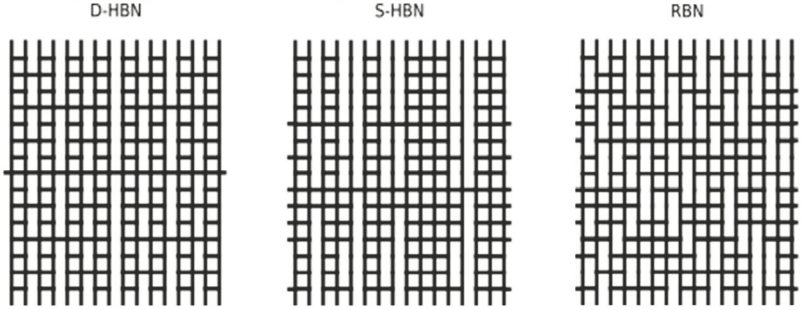

Figure 26: Examples of deterministic and stochastic hierarchical beam networks with n = 4 hierarchical levels (DHBN, SHBN), and non hierarchical reference structures of the same size (RBN); loading is in all cases in tension along the vertical directio n, all structures have the same number and length of load carrying fibres and RBN, DHBN and SHBN have equal numbers of lateral connectors; the dangling beams on the left and right boundary of the networks mutually connect, thus implementing periodic boundary conditions perpendicular to the loading direction.

Conclusions, main achievements and outlook

We demonstrate that load-parallel gaps in hierarchical materials have the effect of confining damage by preventing concentrated local load transfer from among the longitudinally aligned beam failures that otherwise would create a crack-like stress-concentration. Instead the load redistribution becomes more 'diffuse' among broken and many intact beam elements in the neighbourhood of an emergent cluster, thus causing large up-and-down jumps in growth of clusters (see Figure 27) that grow in a 'stop-and-go' manner to the point that the material is not 'crack-sensitive' and brittle and the unloading as damage progresses is more gradual. As a result, the material has much higher toughness than under eventual crack instability and catastrophic brittle crack growth.

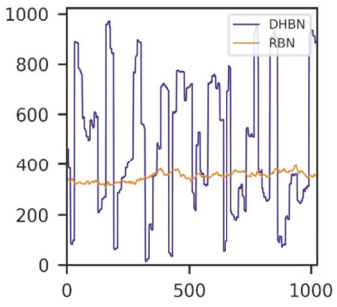

Figure 27: Typical crack shapes of different network variants, with L = 1024 and Weibull-distributed beam thresholds with shape parameter β = 4.

The differences in failure modes of hierarchical and non-hierarchical materials are apparent at low and intermediate degrees of material disorder but disappear in very strongly disordered materials where the local failure strengths exhibit extreme scatter. We furthermore demonstrate that, independent of material disorder, the different modes of failure lead to significant differences in fracture surface morphology.

From a point of view of strength, however, hierarchical organization is not inherently favourable. Our simulations indicate that hierarchical and non-hierarchical samples consisting of the same number of beams with the same statistical properties have identical peak stresses. The main benefit of hierarchical organization may thus not be enhancement of absolute strength, but rather toughening and mitigation against propagation of large flaws.

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

Stefan Hiemer and Michael Zaiser

Objectives and status

The objective of this project is to study failure in disordered systems (e.g. glasses) using machine learning approaches and thus to identify the variables leading to failure across scales. Data sources are atomistic simulations of glasses with the open-source molecular dynamics code LAMMPS, an in-house fuse network code, a Deal II based stochastic mesoscale model and at later stages experimental data stemming from acoustic emission. The fuse network captures characteristics of brittle fracture and serves as a cheap model for the feasibility of different machine learning applications. The mesoscale model serves as the next step closer to experiments ideally to complement and reduce the number of experimental samples. While molecular dynamics simulation is unable to describe subcritical failure due to time constraints, we aim to identify and predict local plastic rearrangements and the formation of shear bands as these events form the basis of models working at larger time scales.

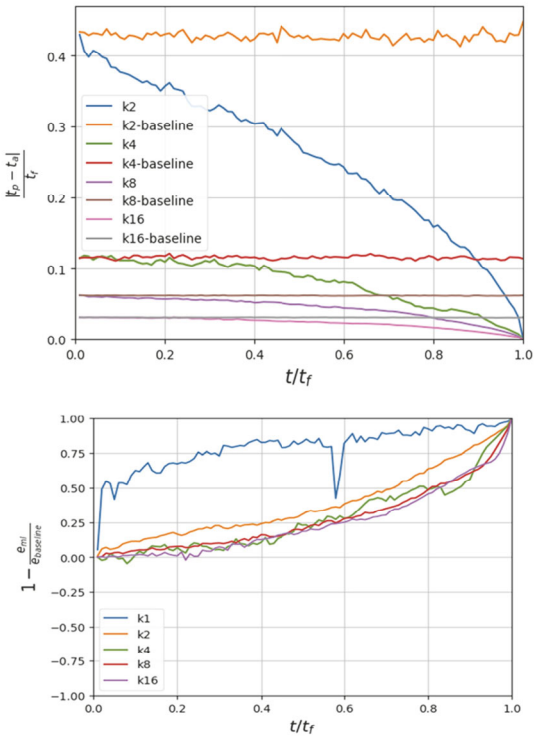

Figure 28: a (top): Prediction error of the random forest forecast t_p and the true value t_a of the remaining time to failure normalized by the total time to failure t_f for systems of different disorder. The higher k, the more ordered the system. The baseline is a prediction based on the average life; b (bottom): Comparison of the lifetime prediction of the random forest by the ratio of the error of the forest e_{ml} and the average prediction baseline $e_{baseline}$.

Binary fuse networks consisting of edges with identical work of failure but different stiffness-yield strength ratios have been generated (~ 2 million samples). Our current attempt is to predict the work of failure for randomly generated fuse models and use this for further topology optimization. For the mesoscale model, we have recovered a dataset of creep simulations used in a previously published study. We successfully reproduced predictions with a random forest of the remaining time to failure based on the time and handcrafted features. Hyperparameter optimizations did not show any improvements. The random forest clearly outperforms an average lifetime prediction (Figure 28a und b). For the prediction of plastic events in molecular dynamics simulations, a dataset of the Kob-Andersen glass shear tests has been acquired (~ 3 million particles). A quench scheme to generate silica glass with reasonable density and radial distribution function (Figure 29a and b) with the BKS potential was found, but not yet used as basis for the predictions. Two machine learning approaches have been tested: A graph neural network published earlier this year and a support vector machine approach with Behler-Parinello symmetry functions as features. The first approach did not prove to work while the second is still work in progress.

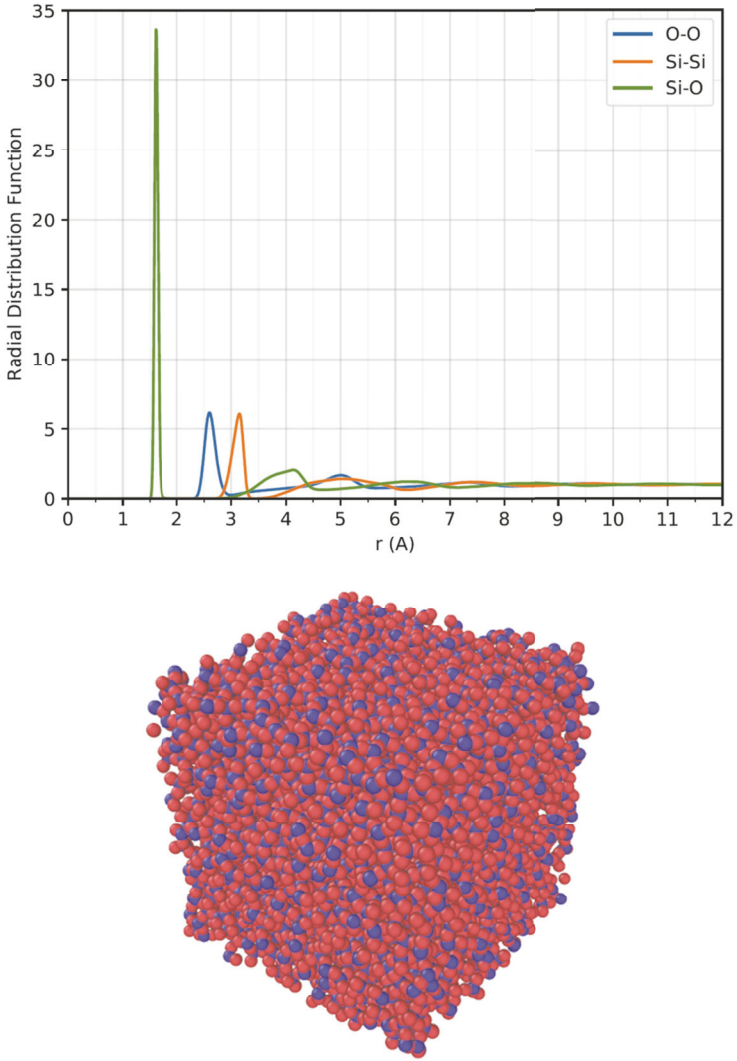

Figure 29: a (top): Radial distribution function of SiO_2 generated with the BKS potential at a density of $\sim 2.21 \frac{g}{cm^3}$.); b (bottom): Snapshot of the final SiO_2 system at 300 K.

Conclusions, main achievements and outlook

Binary fuse networks in large number have been generated and training of neural networks to predict the work of failure currently takes place. As next step optimization of the fuse networks with respect to the work of failure is planned. For the mesoscale model we will have to either subsample the creep time series or employ dimensionality reduction techniques as feeding the full time series and spatial damage information is not feasible. To predict the plastic events, we will proceed on the Behler-Parinello symmetry functions and test if they generalize from Kob-Andersen to models of silica glass.

P6: Deriving Properties of Polymeric Interphases in Nanocomposites via Coupled MD-FE Pseudo-Experiments

Maximilian Ries, Gunnar Possart, Paul Steinmann and Sebastian Pfaller

The properties of polymer composites can usually be determined using classical mixing rules. However, this does not work with nano-sized filler particles, as the comparatively large surface-to- volume ratio of the particles is crucial here. These effects can be modelled by so-called interphases representing the polymer matrix regions whose properties are influenced by the filler particles and deviate from the bulk polymer properties. The determination of the corresponding property gradients within the interphases is challenging and costly since the nano-scale is hardly accessible by experiments. To this end, we present a pseudo-experimental approach based on FE-MD simulations to identify elastic and inelastic property gradients in polymeric interphases around nanoparticles. Since it is specially designed for amorphous polymers, we employ the Capriccio method, a concurrent multiscale method, to couple the continuum and particle descriptions.

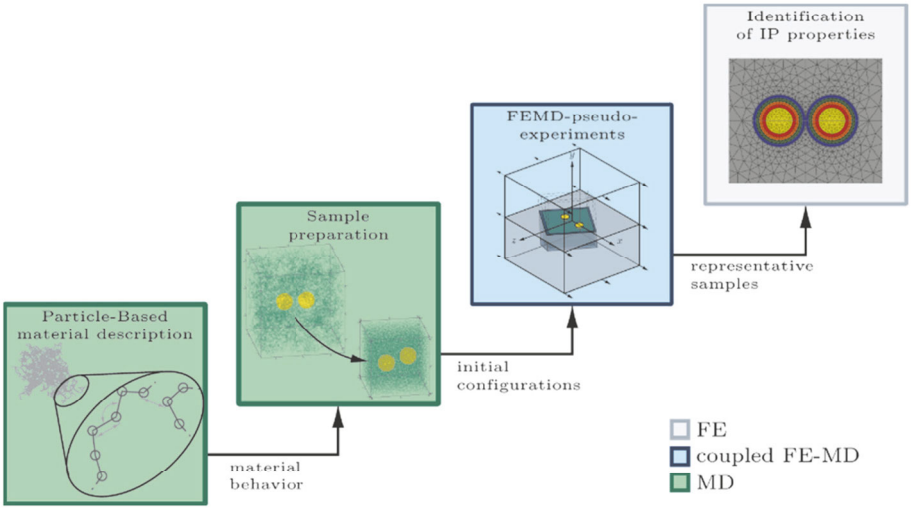

Figure 30: The behaviour of the investigated polymer is prescribed via a particle-based material description enabling the sample preparation. The resulting initial configurations are used in subsequent, coupled MD-FE pseudo-experiments. Representative samples are chosen to identify interphase properties in an FE framework [1].

Following the methodology visualized in Figure 30, we rely on coarse-grained force fields for the MD part since they are well-established and computationally efficient. A constitutive law derived from this is used to describe the continuum. MD samples, consisting of two silica-nanoparticles with varying initial distances surrounded by a polystyrene matrix, are equilibrated before being embedded into a larger continuum cuboid. We perform uniaxial tension tests by applying Dirichlet boundary conditions to the continuum to identify the polystyrene-silica volume elements' deformation behaviour. The resulting interparticle strain has been proven to be a suitable measure to capture the influence of the particles' distance. An FE-based inverse parameter identification revealed that interphases are indeed needed to model the observed deformation behaviour. Furthermore, the interphases are required to be elastoplastic despite the overall elastic force-deformation relation. The best fit of the pseudo-experimental data, shown in Figure 31, is achieved using exponential profiles for the interphase properties.

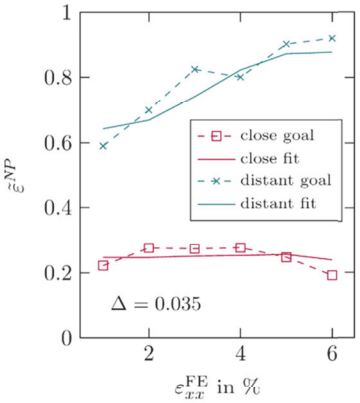

Figure 31: Best fit of normalized interparticle strain for close and distant cases with optimized exponential saturation profiles of the elasto-plastic interphases [1].

These results, which are presented in more detail in [1], are of significant importance for the engineering of nanocomposites and corresponding adhesive formulations.

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P6: Towards Adaptivity of the Capriccio Method: Relating Particle Kinematics and Continuum Mechanics

Christof Bauer and Sebastian Pfaller

The Capriccio method developed b Pfaller et al. [1] has been continuously improved in recent years. Our project aims at extending this multiscale, partitioned-domain approach to an adaptive discrete-to-continuum coupling scheme. For this purpose, we first investigate how to move the particle-based region within the continuum (Figure 32).

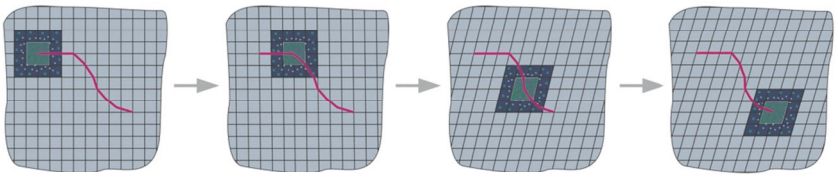

Figure 32: A particle-based region coupled to FE using the Capriccio method. The fine-scale region moves within the continuum, which deforms due to given loads.

A main challenge is the change from FE to MD and vice versa. This requires a deeper understanding of particle kinematics driven by molecular dynamics (MD) compared to those of a continuum.

Based on recent investigations, a hybrid approach has been developed, which partly substitutes MD simulations by continuum mechanical computations. With such a scheme at hand, the computational time required to obtain particle configurations under specific loading conditions may be reduced significantly. This provides the basis for an adaptive switching from a continuum treatment to a particle-based description of a specific region. Figure 33a shows the strain applied in a tensile simulation for the pure MD system compared to that applied in the hybrid scheme. The corresponding stress-strain responses of both systems are given in Figure 33b. As the results indicate, the hybrid MD-CM method appropriately reproduces the overall system stress-strain behaviour. In addition, the local system behavior in terms of the particle displacements is also considered in our research. Furthermore, approaches to perform FE calculations using data from MD simulations are currently being investigated in order to implement the switching back from the particle-based treatment to the continuum.

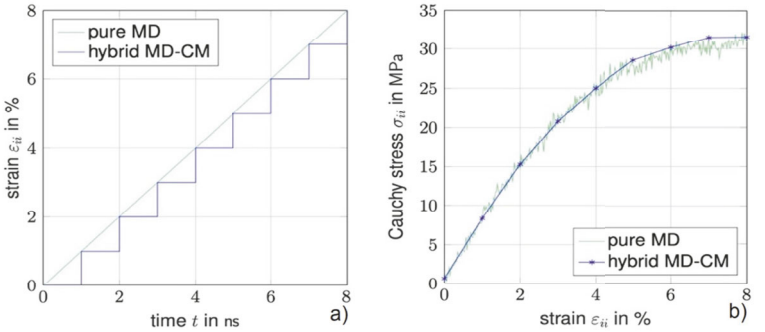

Figure 33: a) Strain ε_{ii} applied in small steps to the MD reference system mimicking a continuous load application in contrast to comparatively large load steps used in the hybrid MD-CM method b) Stress-strain response of the pure MD system in comparison to the results of the hybrid scheme.

Reference

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P6: Extension of the Capriccio Method for Inelastic MD-FE Coupling Simulations of Amorphous Polymers

Wuyang Zhao, Paul Steinmann and Sebastian Pfaller

The initial Capriccio method in [1] was designed for MD-FE coupling simulations of polymers, which employs an elastic constitutive model in the FE domain. However, under larger deformation, the viscoelastic and viscoplastic behavior of polymers have to be taken into account, which requires a corresponding constitutive model in the continuum region. To this end, we extended the Capriccio method to inelasticity by employing a viscoelastic-viscoplastic (VE-VP) constitutive model [2] in the FE domain. This model has been developed by fitting the coarse-grained molecular dynamics (CGMD) simulations of polymers in [3]. The inelastic Capriccio method is compared with the purely elastic set-up to pure MD simulations under uniaxial tension at constant strain rate. As shown in Figure 34, the inelastic extension of the Capriccio method is able to capture the material behavior of larger deformation, which is not possible by the elastic version.

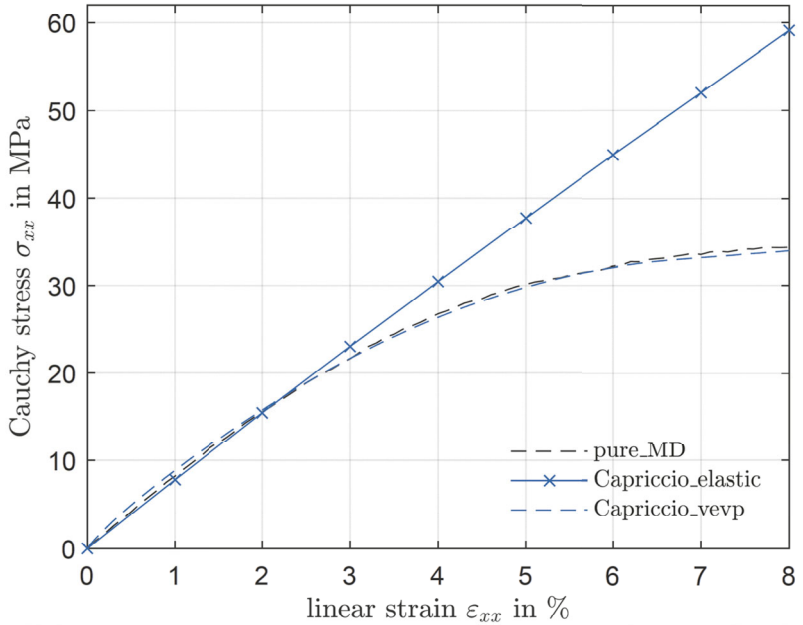

Figure 34: Averaged Cauchy stress of the nodes at the Dirichlet boundaries of the coupled system with the linear elastic and the VE-VP constitutive model in the FE domain compared to the pure MD system under uniaxial deformation with a constant strain rate of 1%/ns.

References

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P7: Modelling of Interface Failure of Hierarchical Material

Nosaibeh Esfandiary and Paolo Moretti

Our research in the second year of the project funding period has focused on the performance aspects of hierarchical network systems in problems of adhesion, in comparison with reference heterogeneous systems displaying no hierarchical organization, and as a function of the strength of quenched disorder. As in the previous year, we model elasticity using scalar models and we describe failure adopting a von-Mises type criterion, according to which a link (or element) breaks as soon as it carries a load above its fixed threshold. We consider the case of thresholds extracted from a Weibull distribution of shape parameter k, which becomes an effective measure of the disorder in the system.

Our findings show that while hierarchical systems always display scale invariant fracture surfaces (regardless of the disorder strength), when monitoring the work of failure, i.e., the area below the force-displacement curve, an interesting transition is found as disorder increases (or as k decreases). While for unrealistically low disorder, the performance of hierarchical systems is nearly indistinguishable from that of reference systems, at high disorder hierarchical systems show significantly higher work of failure (see Figure 35). This allows us to conclude that under the realistic assumption of load carrying elements of broadly varying strengths (as relevant for biosystems), the hierarchical organization provides a significant advantage in terms of fault tolerance. These results are included in a manuscript, currently in preparation.

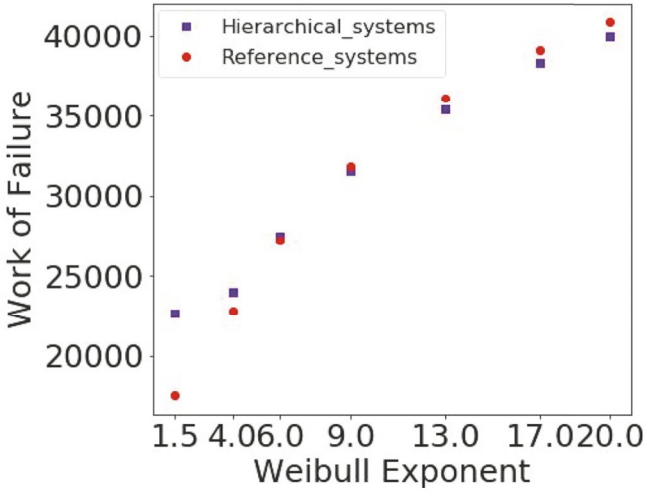


Figure 35: Work of failure. The work of failure of hierarchical systems is compared to that of reference non-hierarchical systems, showing a significant advantage in high-disorder configurations (low Weibull exponent).

Our current work is concentrating on a number of extensions of our findings, namely:

- Computation of work of failure for ensembles of configurations with pre-existing cracks, of variable areas A, as a way to measure the fracture toughness of hierarchical systems in the problem of adhesion (in conjunction with P5, which has conducted the same research, but for bulk failure)
- Study of subcritical failure, where links break well below their local threshold as a result of thermally activated local failures. We are implementing a Kinetic Monte Carlo failure criterion, in which failure rates for each link depend on the local load, the local threshold and an effective temperature.
- Study of crack morphologies and load profiles using the spectral graph methods devised by the P7 associate doctoral researcher.

P7: Robustness of Neural Activity Patterns in Hierarchical Models of Brain Connectivity

Samaneh Esfandiary and Paolo Moretti

During the second year of the Ph.D. project, we focused on the emergence of slow dynamics and localization in bio-systems with a hierarchical microstructure and on the robustness of these dynamic patterns against failure. While our model system is the brain, with its hierarchical connectivity patterns, similar microstructures are found in biological materials, such as those studies within the main P7 research project. In brain activity models, slow dynamics and localization are instrumental to parallel neural computation. In materials, the ability to localize and confine stresses/cracks provides functional advantages, such as increased work of failure and fault tolerance, as currently investigated within P7 (main project).

Our results regarding brain activity modeling, recently published in Physical Review Research, show that the emergence of large time scales in neural activity can be traced back to a specific property of the Laplacian spectrum of hierarchical network models of brain connectivity, namely an excess of low eigenvalues which we call Lifshitz tail (see Figure 36), borrowing the term from the analogous quantum problem of localization in disorder low-dimensional systems.

We use a combination of analytic calculations and very-large-scale parallel simulations, run at the Regionales Rechenzentrum Erlangen (RRZE). We are able to provide the first exhaustive proof of Lifshitz tails in models of brain connectivity and to relate their standard parametrization (the Lifshitz dimension) to the emergent properties of dynamic slowing down in models of activity described by the Laplace operator (such as neural oscillation and synchronization).

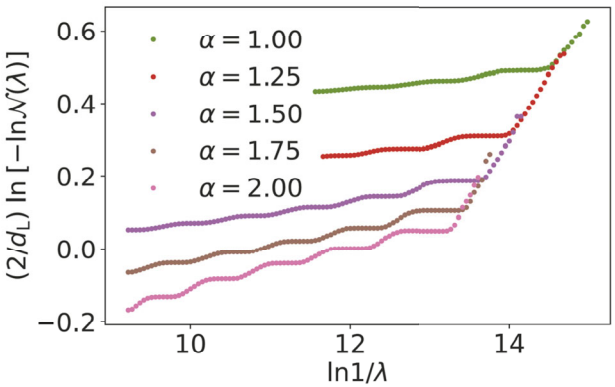


Figure 36: Lifshitz tails in hierarchical models of brain connectivity. The integrated density of states is plotted for different strengths of hierarchical connectivity. Smaller eigenvalues are shown on the right.

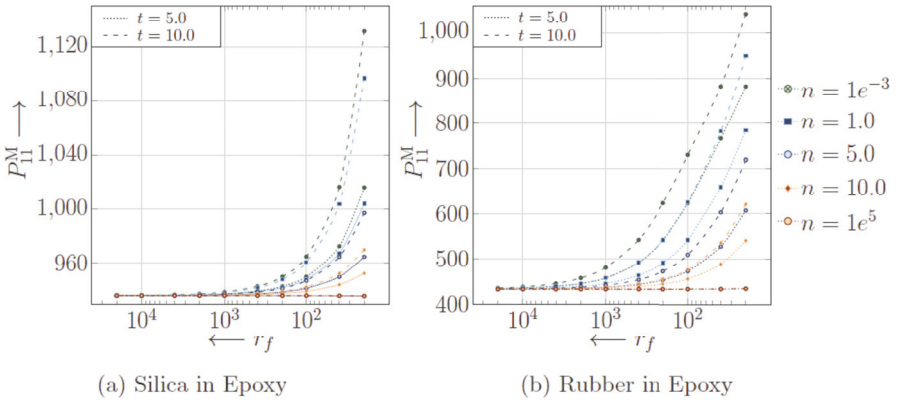
Our current work is devoted to the following extensions of our results:

- Exploration of the robustness of our results in systems exiting failure, i.e. alterations/suppression of the hierarchical structure due to pathological states.
- Validation of our results using real brain connectivity data and real brain functional time series, provided to us though our ongoing collaboration with J. Cortes (Biocruces Bizkaia Health Center, Spain)
- Extension of our spectral analysis tools, to the study of fracture patterns and load profiles in model materials with hierarchical microstructures (P7, main project)

P8: A Comparison of Interface Energetics and Graded Interphase Based Techniques for Modelling Size-Effects in Polymer Nano-Composites

Paras Kumar and Julia Mergheim

Extensive experimental investigations re-affirm the supremacy of nano-sized reinforcements over their micro-sized counter-parts, with regards to their effectiveness in improving the mechanical behaviour of otherwise brittle polymer materials [1,2]. Inspired by these experimental findings, the subproject P8 focuses on development a multiscale simulation framework for *continuum mechanics* based modelling of fracture in polymer nano-composites. A first step towards such a simulation framework is the enhancement of the standard two-phase continuum model in order to model the *smaller is stronger* size-effect [3].



(a) Silica in Epoxy (b) Rubber in Epoxy

Figure 37: Size-effect scaling graphs for (a) silica and (b) rubber inclusions in epoxy matrix for the volumetric loading scenario. The parameter n denotes the exponent of the interpolation function employed for modelling the continuous variation of properties within the interphase region. Since, the rubber particles are much weaker than the epoxy matrix, the interphase stiffness at the filler particle end has been scaled by a suitable scaling factor $\alpha = 20000$.

In line with this objective, two such enhancements of the standard computational homogenization scheme, namely Interface-Energetics-Enhanced Computational Homogenization (IECH) and Graded Interphase-Enhanced Computational Homogenization (GICH), have been explored in detailed and the findings have been collected in [4]. The IECH approach is based on the idea of *interface energetics*, whereas GICH involves a *continuously graded interphase* model. Extensive numerical studies reveal the appropriateness of the GICH technique for modelling size-effects in composite materials with different matrix-filler stiffness ratio extremes under generic loading conditions. This however, comes at the additional computational cost stemming out of the high-resolution finite element meshes required for the interphase region. Figure-1 illustrates the variation of the macroscopic Piola stress with filler particle radius for the two filler-matrix stiffness ratio extremes considered in this work, i.e. the case of stiff (silica) filler particles in weak (epoxy) matrix, cf. Figure 37a, and the case of weak (rubber) filler particles in stiff (epoxy) matrix, cf. Figure 37b. Further, the influence of interphase thickness on the size-effect scaling is depicted by means of the two thickness values considered. The IECH approach, based on elastic interfaces, on the other hand is only suitable for modelling nano-composites when the filler particles are much weaker than the matrix material, and under limited compressive loads.

The next step towards the aforementioned simulation framework is the development of an approach for modelling micro-cracking in heterogeneous materials. In order to circumvent the problems associated with explicit modelling of the cracks by means of *discontinuous modelling approaches* such as XFEM, especially in 3D, a *smeared approach,* based on the variational principles is being considered [5]. Herein, an additional crack phase-field variable is employed for tracking the propagation of cracks within the body.

As described in the previous annual report, all implementations, with regards to the modelling techniques developed in this sub-project, have been carried out in a modular software framework written in C++. This framework aims at providing the necessary building blocks for solving generic problems in finite deformation solid mechanics in a dimension independent manner by *employing template metaprogramming*. Particular emphasis has been laid on ensuring easy extensibility of the source-code and consequently many of the modern C++ software design practices, including *design patterns* have been taken into consideration. Presently, the implementation of the phase-field fracture model is underway.

Asides, RVEGen: a PYTHON based RVE generation tool, also introduced in the previous report, is being developed in order to generate the finite elements meshes for random heterogeneous microstructures being considered in this work.

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P9: Spatially Varying Regularisation Variable in Quasi-Static Phase-Field Model for Brittle Fractures

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

Broadly, there are two computational modelling methodologies in fracture mechanics, namely discrete and diffusive crack approaches. In many cases, the discrete crack approaches are algorithmically complex, computationally expensive or both. In contrast, the diffusive crack approach, is quite simple to implement in the existing finite element libraries. Over the last decade, this method has been extensively developed for various material models and complex applications. However, there are a few issues associated with this method. It is known to suffer from convergence issues with the Newton method for monolithic approaches [1]. This approach is reliant on a regularisation parameter ϵ, under the requirement that $h \ll \epsilon$, where h is the mesh size parameter. Therefore, at lower ϵ the necessity of finer meshes can make it computationally expensive. Moreover, the actual solution of the numerical problem can be dependent on h itself. Our work strives to develop a formulation with spatially varying ϵ to alleviate mesh dependency, lowering the cost of this approach and making it more accessible.

The total energy in the system given by the standard phase field model is

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

where $\mathbf{u}$, c and $\boldsymbol{\varepsilon}$ are the displacement, phase field and strain respectively, ϵ is a constant regularisation parameter, and $\mathcal{G}_c$, λ and μ are material parameters. It has been shown that in the limit $\epsilon \to 0$ the standard phase field energy functional E approaches to the discrete brittle fracture energy functional in the sense of Γ-Convergence [2]. This implies increasingly smaller values of ϵ should be chosen, which is ultimately computationally expensive. To circumvent this issue, we interpret ϵ as a field variable, consequently argument of the energy function E. Furthermore, a regularization term $\beta\epsilon$ is added to the energy functional of the standard phase field model resulting in

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

now ϵ is spatially varying variable, and β and η are a penalty and model parameter respectively. Minimizing the energy functional (2) with respect to $\mathbf{u}$, c and ϵ we obtain the following Euler-Lagrange equations

$$\begin{aligned} \nabla \cdot \boldsymbol{\sigma} &= \mathbf{0} && \text{in } \Omega \\ \frac{c\mathcal{G}_c}{\epsilon} - 2[1-c]\psi(\boldsymbol{\varepsilon}) - \mathcal{G}_c \nabla \cdot [\epsilon \nabla c] &= 0 && \text{in } \Omega \\ \epsilon &= \sqrt{\frac{c^2 + \eta}{|\nabla c|^2 + \frac{2\beta}{\mathcal{G}_c}}} && \text{in } \Omega \end{aligned} \tag{3}$$

In addition to these equations of motion (3), the typical boundary conditions for phase-field problems are $\mathbf{u} = \mathbf{u_0}$ on $\partial\Omega_{\mathrm{d}}$, $c = c_0$ on $\partial\Omega_{\mathrm{p}}$ and $\nabla c \cdot \mathbf{n} = 0$ on $\partial\Omega \backslash \partial\Omega_{\mathrm{p}}$. As these are nonlinear PDEs the choice of η and β is not straight forward and very sensitive. It is chosen such that the ϵ is smaller at the crack-tip or in the region of larger stress and large everywhere else. The domain is discretized using linear and quadratic finite elements for $\mathbf{u}$ and c respectively. The discrete problem is solved using a staggered approach. We have implemented this for a Single Edge Notch Tension (SENT) specimen as seen in Figure 38 for $\eta = 421.87$ and $\beta = 3.125$.

[1] Division of Engineering and Applied Sciences, California Institute of Technology, California, USA

[2] Lehrstuhl für Festkörpermechanik, Universität Siegen, 57076 Siegen, Germany

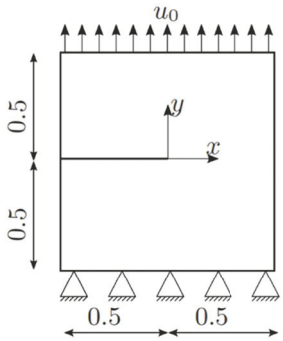

Figure 38: 2D problem set-up.

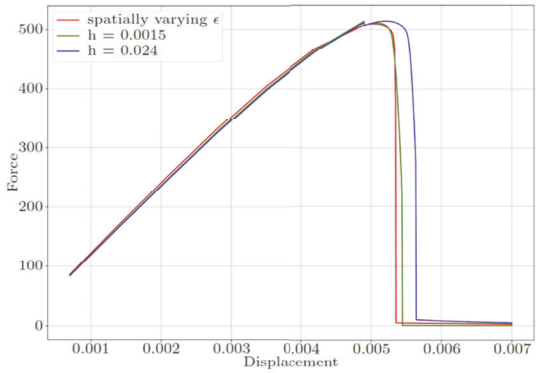

Figure 39: Force vs. displacement plot.

The force vs displacement plots are largely comparable with that of the standard phase field model of constant $\epsilon = 0.1$ as in the Figure 39. Evolution of ϵ w.r.t. displacement can be seen in Figure 40 and it illustrates ϵ is indeed smaller at the crack tip. The next step is to develop robust mesh refinement strategy utilizing this spatially varying ϵ.

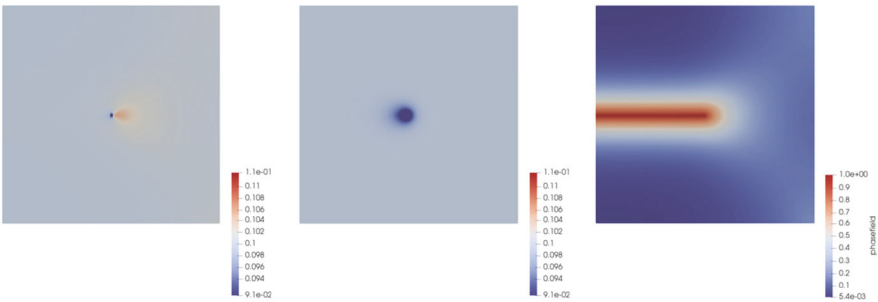

Figure 40: Evolution of ϵ with displacement $u_0^y = 0.0007, 0.005047$ and phase field at $u_0^y = 0.005047$.

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P10: Configurational Fracture Mechanics

Elmira Birang, Ana-Sunčana Smith and Paul Steinmann

In this project based on Discrete Configurational Mechanics [1], we present a theoretical and computational framework for deformational and configurational mechanics of three-body potentials. The breaking of bonds at the crack tip is the sole source of energy release. In line with this physical phenomenon and according to the second law of Thermodynamics, discrete configurational forces render the magnitude and direction of energy release. Considering this property, we study the propagation of a pre-defined pre-crack into the diamond lattice of Silicon under static process based on Stillinger-Weber Potential [2]. Configurational bond and triplet forces at the material configuration identify the location of the pre-defined crack and free surfaces. Moreover, as depicted in Figure 41, the configurational forces trace the crack propagation into the lattice, whereby they appear on the atoms undergoing extreme bond stretches and variations in their triplet angle. We will utilize configurational mechanics of Stillinger-Weber potential to study irreversible crack propagation based on Configurational-Force-Criterion introduced in our prior work [3].

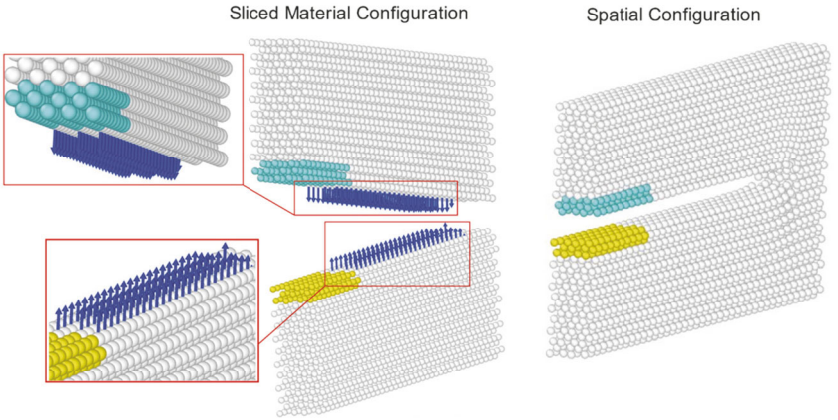

Figure 41: Material and spatial configuration of a bulk lattice of Silicon. Configurational forces appear at the crack surfaces belong to the atoms undergoing extreme material bond stretches and material triplet angle variations. Configurational forces at the material configuration corresponds with the crack morphology at the spatial configuration.

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P10: Extended Continuum Bone Remodelling

Ina Schmidt, Areti Papastavrou and Paul Steinmann

Motivation

Bone fractures are usually caused by an increased load, which the material cannot withstand. The difficulty in predicting fractures, their healing or implant integration is the variability of bone, as it is a living tissue. The so-called remodelling process involves the adaption of bone structure and thus of bone density through repetitive loads, resulting in changes in stiffness and load capacity. This effect is used in therapeutic measures and can also be observed in professional sports, for example on the dominant arm of a tennis player. On the other hand, factors such as advanced age, degenerative diseases, disuse or altered gravities, as in the case of an astronaut, lead to a reduction in bone density and thus to a significantly increased risk of fracture. The main goal of this project is to create a tool, which calculates the development of human bone under mechanical loading using finite element methods and therefore predicts fractures and their local origin.

Project status

A model including the essential process of bone density adaption due to mechanical loading was created based on a continuum approach and tested on different two- and three-dimensional models of the femur and humerus. With the aim of simulating real influences on bone density evolution, different age dependencies were investigated, as well as the availability of nutrients and hormones. In addition, an automatic time-step control was created to improve the performance of the calculation.

Recent work mainly focused on reformulating the model by introducing the initial volume fraction, which allows the distinction between cortical and cancellous bone and the interaction of both bone types. In contrast to previous research, which assumes a homogeneous initial state over the entire bone cross-section usually by neglecting cortical bone, an initial density distribution according to bone type as well as differences in their density evolution can be determined.

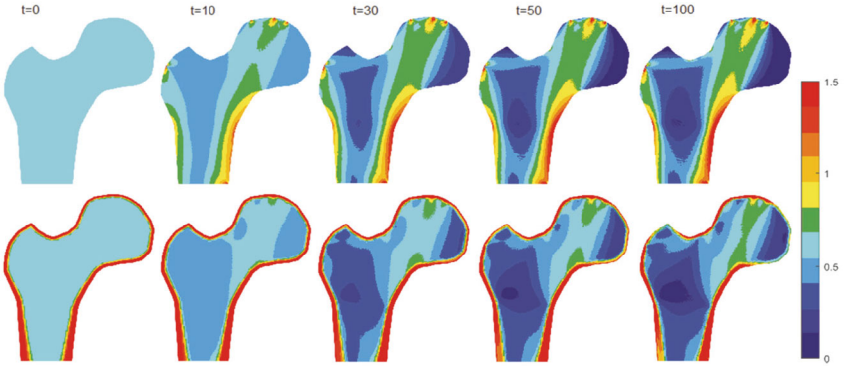

Figure 42: 2D femur example without (top row) and with (bottom row) consideration of cortical bone.

Figure 42 displays the density evolution without and under consideration of cortical bone at different points in time. The example clearly points out changes in density pattern and therefore underlines the importance of this investigation.

Conclusion and outlook

Using the mentioned model extensions improves continuum bone remodelling such that important real factors influencing bone density evolution can be considered in a simulation.

Current research focuses on structural optimisation of cancellous bone on a mesoscopic scale. A subsequent coupling with the macroscopic model based on the continuum approach allows a more precise consideration of bone tissue using daily loads on bone.

P10: Grain Boundary Mechanics

Lucie Spannraft and Paul Steinmann

The constitutive properties of a polycrystalline metal depend on the size and shape of the grains, as well as on the interaction along the grain boundaries. In [1], we characterize this interaction by means of a geometrically non-coherent grain boundary premised on gradient crystal inelasticity and decohesion. In an on going cooperation with international research partners Magnus Ekh, Fredrik Larsson and Kenneth Runesson from Chalmers University of Technology, Gothenburg, Sweden we introduced an energetic and dissipative microtractions model and a mixed-mode decohesion model. The microtractions and the decohesion model are coupled via a damage variable d_Γ. Thus, decohesion exerts not only an influence on the standard tractions but also on the microtractions along the grain boundaries, i.e. the grain interaction reduces with increasing cohesive damage. Furthermore, the crystallographic orientation of neighbouring grains has a major impact on intergranular fracture, more specifically on the damage initiation and the softening progression.

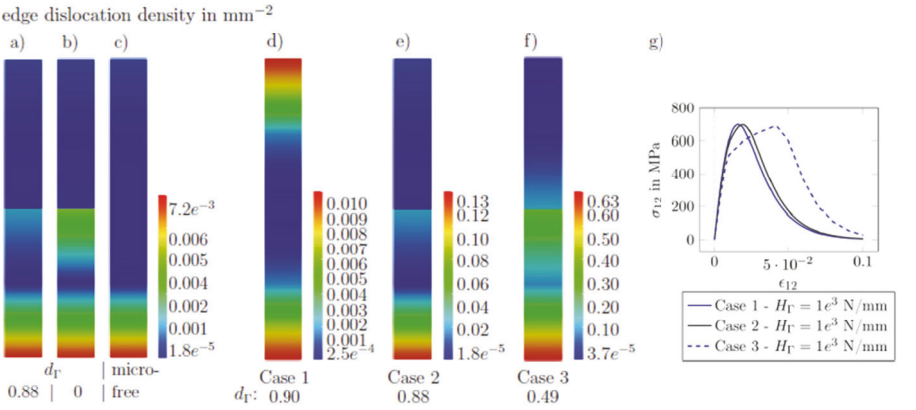

Figure 43: (a-f) Edge dislocation density (in mm^{-2}) for simple shear (u_x = 0.1mm) of a bicrystal. (a) Damage coupled to microtractions. (b) No coupling of damage to microtractions. (c) Microfree condition along grain boundary. (d-f) Different grain orientations with (case 1) no crystallographic misfit, (case 2-3) misfit at grain boundary. (g) Stress-strain. [1].

Figure 43 presents computational results for a bicrystal subjected to simple shear. Figure 43a-c visualize the numerically computed edge dislocation density in the bicrystal with crystallographic misfit at the grain boundary. Prior to damage initiation, the cohesive model has no impact onto the microtractions. With increasing decohesion, the edge dislocation density is lower as compared to the simulation without accounting for damage into microtractions model, cf. Figure 43a,b. For high damage, a microfree boundary is approached, since the microtractions eventually vanish at the boundary, see Figure 43c. Figure 43d-g visualize the effect of grain misorientation onto decohesion in terms of damage initiation and softening progression. Thereby, Figure 43d shows the case of no crystallographic misfit. In Figure 43e,f a misfit exists. The stress-strain curve of the simulation with case 3 significantly differs form case 1 and 2 with regard to the softening progression.

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P11: Material Optimization for Fracture Control

Sukhminder Singh, Lukas Pflug and Michael Stingl

In this work, we have developed a material optimization model to maximize the interfacial fracture resistance of composite structures under quasi-static conditions. The state problem, in its original form, is ill posed because of the non-unique solution, posing challenges in the application of gradient-based optimization methods. To overcome this issue, we have incorporated a small viscosity term [1] in the governing equation with an exponential cohesive law [2], rendering the state solution unique. As a result, the optimization objective/cost function becomes C^1 continuous. Additionally, an elastic approximation of the cohesive law is used at a given time step to efficiently solve the state problem. It is observed that this adds further regularization in the form of numerical damping, providing the time steps taken are sufficiently large.

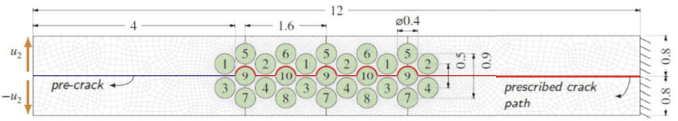

Figure 44: Structural setup of double-cantilever beam with orthotropic inclusions and a prescribed crack path. The orientations of the inclusions are optimized for maximum external mechanical work done by the applied boundary displacements with three different initial designs (I, II and III).

In response to the stabilization of inherently unstable crack states, which leads to exceptionally lower objective values and narrow troughs in the objective function landscape, we have limited the fracture problem to a single crack along a predefined path. The space domain is discretized using finite elements and the material optimization problem is then solved using a trust-region algorithm. The gradients of the objective w.r.t. the design are computed via an efficient discrete adjoint-sensitivity analysis.

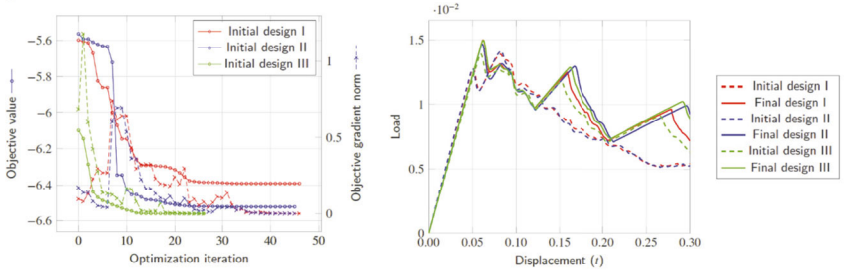

Figure 45: Objective value and its gradient norm w.r.t. optimization iteration (left) and the load-displacement curves for initial and final designs (right). Significant improvement is seen in the fracture resistance with the optimized designs.

Conclusion and outlook

In practice, the material optimization model with regularized fracture problem and prescribed crack path works robustly. Optimization problems where the crack paths are not confined to the material interfaces remain to be addressed in the future. Additionally, incorporation of irreversibility criteria for the crack growth into the optimization problem would be a possibility. Finally, more sophisticated structural setups and boundary conditions are required to faithfully reflect the material properties of a more general two- or three-dimensional composite structure.

References

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P12: Development of a Quantum-to-Continuum Multiscale Model for the Fracture of Thermosets

Christian Wick, Mattia Livraghi and Ana-Sunčana Smith

Objectives and status

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.

A priori, this includes the reliable generation of molecular models for cured amorphous epoxy-based thermosets. In the current reporting period, we investigated an example system based on the epoxy resin diglycidyl ether of bisphenol A (DGEBA) and the curing agent 4,4'-diamino diphenyl sulfone (DDS). While we delineated our general procedure for force field parameterization and model generation in the first annual report, our focus in this report is the validation of the cured models and the investigation of hybrid methodologies for mechanochemical investigations of fracture in epoxy networks. Former includes the analysis of our model systems before and after cure. Starting at a liquid, unreacted state, the increasing number of covalent crosslinks during the curing simulation leads to the formation of a highly crosslinked system, which forms a glass at a temperature below the glass-transition temperature T_g. The glass-transition temperature T_g is system dependent and a function of the curing state, as depicted in Figure 46 (left). The simulated T_g values were computed from temperature dependent changes of the density at 10 fixed curing states from 5% to 95 % cure and a hyperbolic fitting procedure[1]. A master hyperbolic fit was generated including all data points to encompass previously observed convergence problems for low T_g.[1] It is evident, that our developed force field and curing procedure give very reasonable results, which are in line with the experimental data depicted in Figure 46 (left).[2,3]

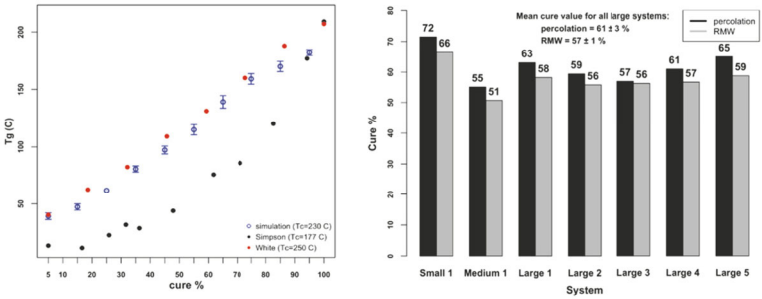

Figure 46: Preliminary determination of the gel point and the glass transition temperature. Left: Glass transition temperatures (T_g) determined by simulation and experimental methods[2,3] as a function of curing state. Right: Approximations to the gel-point obtained by the Reduced Molecular Weight (RMW) approximation and by percolation theory. The experimental gel point is at 57±2 %.[4]

Besides the computation of T_g as a function of curing state, we also investigated the gel point of our model systems based on two different approaches. The reduced molecular weight (RMW) method represents a crude approximation to the gel point,[5] while we also developed an algorithm to obtain the percolation point of our systems in three dimensions of a cubic box with periodic boundary conditions. Both methods compare well to the experimental gel point of 57±2%. We are currently preparing two manuscripts regarding our force field parameterization[6] and our algorithm to compute the percolation point of epoxy resins in a cubic box with periodic boundary conditions.[7]

To examine the quality of bond rupture by ONIOM type QM/MM methods with Harmonic potentials, we conducted COGEF (Constraint Geometries simulate External Force)[8] calculations for several model systems. Two examples are shown in Figure 47. Using harmonic potentials to describe the bonds in the MM part leads to reliably reproduction of the pure QM (DFT) curves (Figure 47, left). However, attention needs to be paid to the high level selection (Figure 47, right): Cutting polar bonds leads to large energy differences during the COGEF calculations with the typical ONIOM-EE link

atom approach. Nevertheless, we also identified systems, where a simple harmonic potential to describe the bonds in the MM region is not suitable to reproduce accurate energies. We were able to show that this discrepancy can be corrected by using accurately fitted morse potentials instead.

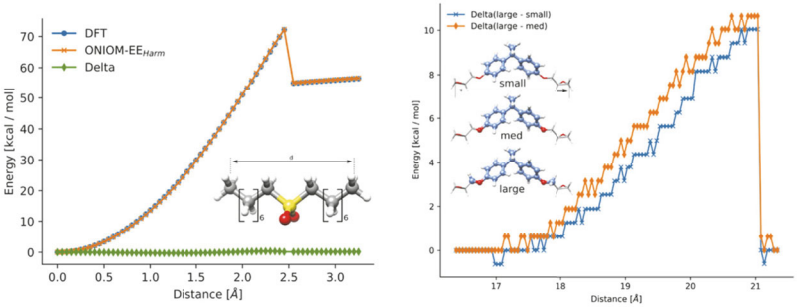

Figure 47: Left: Full-DFT vs. ONIOM-EE(DFT:AMBER$_H$) energies during COGEF simulations. QM calculations were conducted at the UTPSS-D3/cc-pvdz level of theory. The model system is shown as inset. The distance between the edge C atoms was increased in steps of 0.05Å. The ONIOM QM region includes all atoms less than 4 bonds away from the fractured bond. Right: influence of the high layer definition in COGEF simulations. QM atoms are shown as balls and sticks. SP energies were conducted with ONIOM-EE(UTPSS-D3/cc-pvdz:AMBER$_H$), while the structures were obtained with relaxed scans at the UTPSS/cc-pvdz level of theory and a step size of 0.05 Å.

Conclusions, main achievements and outlook

In the last period, we concentrated our studies to the validation of our force field in pure and hybrid calculations. Pure MM simulations included the calculation of the gel point and the glass transition temperature as function of the curing reaction. Furthermore, we showed that a harmonic approximation of interatomic bonds in the MM part of hybrid ONIOM-EE calculations is able to reproduce full QM COGEF calculations of bond fracture in linear polymers. In this regard, several model systems and high layer definitions have been investigated. This is the basis for our future work, which will utilize our force field in combination with the ONIOM method to study fracture of large epoxy networks in the scope of hybrid molecular dynamics simulations.

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2.2 Publications

(in alphabetical order)

Journal Articles

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

[2] **José Luis Colón Quintana, Stefan Hiemer, Nancy Granda Duarte, Tim Osswald**
Implementation of shear thinning behavior in the fused filament fabrication melting model: Analytical solution and experimental validation
Additive Manufacturing, 2020, 101687
DOI: 10.1016/j.addma.2020.101687

[3] **Denis Davydov, Martin Kronbichler**
Algorithms and Data Structures for Matrix-Free Finite Element Operators with MPI-Parallel Sparse Multi-Vectors
ACM Transactions on Parallel Computing, Vol. 7, No. 3 (2020) Article 20
DOI: 10.1145/3399736

[4] **Samaneh Esfandiary, Ali Safari, Jakob Renner, Paolo Moretti, Miguel A. Muñoz**
Anomalous Lifshitz dimension in hierarchical networks of brain connectivity
Physical Review Research 2, 043291 (2020)
DOI: 10.1103/PhysRevResearch.2.043291

[5] **Robert H. Meißner, Julian Konrad, Benjamin Boll, Bodo Fiedler, Dirk Zahn**
Molecular Simulation of Thermosetting Polymer Hardening: Reactive Events Enabled by Controlled Topology Transfer
Macromolecules 2020, 53, 22, 9698-9705
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[6] **Areti Papastavrou, Ina Schmidt, Kefu Deng, Paul Steinmann**
On age-dependent bone remodeling
Journal of Biomechanics (2020) 109701
DOI: 10.1016/j.jbiomech.2020.109701

[7] **Areti Papastavrou, Ina Schmidt, Paul Steinmann**
On biological availability dependent bone remodeling Computer Methods
Biomechanics and Biomedical Engineering (2020)
DOI: 10.1080/10255842.2020.1736050

[8] **Jonas Ritter, Henning Löwe, Johan Gaume**
Microstructural controls of anticrack nucleation in highly porous brittle solids
Scientific Reports 10 (2020) 12383
DOI: 10.1038/s41598-020-67926-2

[9] **Lucie Spannraft, Magnus Ekh, Fredrik Larsson, Kenneth Runesson, Paul Steinmann**
Grain boundary interaction based on gradient crystal inelasticity and decohesion
Computational Materials Science 178 (2020) 109604
DOI: 10.1016/j.commatsci.2020.109604

Conference papers

[10] **Maximilian Ries, Paul Steinmann, Sebastian Pfaller**
Characterization of Polystyrene Under Shear Deformation Using Molecular Dynamics
In: *Abali B., Giorgio I. (eds) Developments and Novel Approaches in Nonlinear Solid Body Mechanics. Advanced Structured Materials, vol 130. Springer, Cham (2020) pp 219-229*
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Discrete configurational mechanics for the computational study of atomistic fracture mechanics

S. Elmira Birang O.[a,b,*], Paul Steinmann[a,c]

[a] Institute of Applied Mechanics (LTM), Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), Erlangen, Germany
[b] Central Institute for Scientific Computing (ZISC), Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), Erlangen, Germany
[c] Glasgow Computational Engineering Centre, University of Glasgow, Glasgow, United Kingdom

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ABSTRACT

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

1. Introduction

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

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

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

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

* Corresponding author at: Institute of Applied Mechanics (LTM), Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), Erlangen, Germany.
E-mail address: elmira.birang@fau.de (S.E. Birang O.).

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Additive Manufacturing
Volume 37, January 2021, 101687

Research Paper

Implementation of shear thinning behavior in the fused filament fabrication melting model: Analytical solution and experimental validation

José Luis Colón Quintana [a], Stefan Hiemer [b], Nancy Granda Duarte [c], Tim Osswald [a]

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Abstract

Fused Filament Fabrication (FFF) has been on the forefront of Additive Manufacturing (AM) due to low costs, ability to manufacture complex geometries, and broad availability of AM machines in the market. Various theoretical models have been proposed to explain the melting behavior of the polymer filament in the FFF process. The most prevalent model involves the formation of a pool of polymer melt at the nozzle that is pushed out of the orifice by the solid filament acting as a piston (Bellini et al., 2004) [1]. An alternative model that suggests the formation of a melt film, with thickness varying as a function of the force exerted by the solid filament, is used as basis for this work. This model, known as the "Fused Filament Fabrication melting model", was proposed by Osswald et al. (2018) [2] and assumes a Newtonian fluid, which is a simplification of the real rheological behavior of polymeric melts. This work aims to improve this model by implementing the shear thinning behavior of the material into the equations. The analytical solution of the shear thinning model is compared to models found in literature using experimental data at different printing conditions. By comparing these models, it was shown that the implementation of shear thinning effects enhances the prediction of the melting behavior of the filament material at both low and high printing temperatures using the corresponding assumptions.

Algorithms and Data Structures for Matrix-Free Finite Element Operators with MPI-Parallel Sparse Multi-Vectors

DENIS DAVYDOV, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
MARTIN KRONBICHLER, Institute for Computational Mechanics, Technical University of Munich, Germany

Traditional solution approaches for problems in quantum mechanics scale as $O(M^3)$, where M is the number of electrons. Various methods have been proposed to address this issue and obtain a linear scaling $O(M)$. One promising formulation is the direct minimization of energy. Such methods take advantage of physical localization of the solution, allowing users to seek it in terms of non-orthogonal orbitals with local support.

This work proposes a numerically efficient implementation of sparse parallel vectors within the open-source finite element library `deal.II`. The main algorithmic ingredient is the matrix-free evaluation of the Hamiltonian operator by cell-wise quadrature. Based on an *a-priori* chosen support for each vector, we develop algorithms and data structures to perform (i) matrix-free sparse matrix multivector products (SpMM), (ii) the projection of an operator onto a sparse sub-space (inner products), and (iii) post-multiplication of a sparse multivector with a square matrix. The node-level performance is analyzed using a roofline model. Our matrix-free implementation of finite element operators with sparse multivectors achieves a performance of 157 GFlop/s on an Intel Cascade Lake processor with 20 cores. Strong and weak scaling results are reported for a representative benchmark problem using quadratic and quartic finite element bases.

CCS Concepts: • **Mathematics of computing → Partial differential equations**; *Mathematical software performance*;

Additional Key Words and Phrases: Finite element method, matrix-free method, density functional theory

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1 INTRODUCTION

In recent years there has been a growing interest in using finite element (FE) discretizations for problems in quantum mechanics [7, 16, 18, 19, 21, 25, 47, 52, 53, 56, 61, 63, 64, 67, 68], including an open-source production-ready FE-based implementation [46] of the Density Functional Theory (DFT) [33, 39]. An FE basis has the following advantages: (i) it is a locally adaptive basis with

Authors' addresses: D. Davydov, Chair of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 5, Erlangen, 91058, Germany; email: denis.davydov@fau.de; M. Kronbichler, Institute for Computational Mechanics, Technical University of Munich, Boltzmannstr. 15, Garching, 85748, Germany; email: kronbichler@lnm.mw.tum.de.

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Anomalous Lifshitz dimension in hierarchical networks of brain connectivity

Samaneh Esfandiary,[1] Ali Safari,[1] Jakob Renner,[1] Paolo Moretti,[1,*] and Miguel A. Muñoz[2]
[1]*Institute of Materials Simulation, FAU Universität Erlangen-Nürnberg, Dr.-Mack-Straße 77, 90762 Fürth, Germany*
[2]*Departamento de Electromagnetismo y Física de la Materia e Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, E-18071 Granada, Spain*

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The spectral dimension is a generalization of the Euclidean dimension and quantifies the propensity of a network to transmit and diffuse information. We show that in hierarchical-modular network models of the brain, dynamics are anomalously slow and the spectral dimension is not defined. Inspired by Anderson localization in quantum systems, we relate the localization of neural activity—essential to embed brain functionality—to the network spectrum and to the existence of an anomalous "Lifshitz dimension." In a broader context, our results help shed light on the relationship between structure and function in biological information-processing complex networks.

DOI: 10.1103/PhysRevResearch.2.043291

I. INTRODUCTION

Understanding the interplay between dynamical processes and the architecture of the networks embedding them is a fundamental problem in diverse fields including material science, genetic regulation, and neuroscience. Dynamical features and patterns of activity are often affected or controlled by key structural features of the underlying network, such as the degree distribution, degree correlations, modular organization, k-core structure, etc. [1–5]. However, given that such features are usually not independent, a more systematic way to tackle the problem of the interplay between structure and dynamics relies on the use of spectral-graph characterizations of the network architecture [6,7] and, importantly, the network dimension. Statistical mechanics teaches us that dynamical processes such as diffusion, vibrational excitations, and critical properties near second-order phase transitions exhibit universal behavior, which depends crucially on the lattice (Euclidean) dimension [1–3,8,9]. The case of heterogeneous networks is more complex, since multiple and diverse generalizations of the concept of dimension have been proposed [10–12]. Nevertheless, compelling pieces of evidence show that dimensionality measures are effective determinants of dynamics and activity in networked complex systems. The simplest example is provided by networks with the small-world property [13–15], which exhibit diameters that grow only logarithmically with the network size N and, consequently, with diverging Hausdorff dimension. We recall that the Hausdorff dimension $d_{\rm H}$, also called the "topological dimension" in the literature [16,17], can be computed easily starting from the number $u_i(r)$ of nodes within distance r from node i: if $\langle u_i(r)\rangle \sim r^d$ (where $\langle . \rangle$ stands for the average over all nodes in the network), implying $d_{\rm H} = d$. Diverging $d_{\rm H}$ typically implies enhanced transmission, signal propagation, and high synchronizability.

A somewhat more complex example of how dimensionality controls activity patterns in networks is provided by hierarchical-modular networks, as models, e.g., for brain connectivity [18,19]. It was first pointed out that the hierarchical-modular organization of brain regions results in network models of finite Hausdorff dimension $d_{\rm H}$ and, at odds with small-world graph topologies, with intrinsically *large* diameters [20]. The large-world property resulting from finite $d_{\rm H}$ in hierarchical-modular networks, a purely structural feature of the network, has been linked to signatures of anomalous activity patterns in brain network models, including, among others, sustained activity [21], subdiffusive dynamics [22], localization phenomena and stretched criticality in the form of Griffiths phases [17,23,24], broad avalanche distributions [17,25], states of localized and "frustrated" synchronization [26–30], rounding of first-order phase transitions [31], and ergodicity breakdown [32,33]. Importantly, some of these anomalous dynamical traits are, in fact, considered essential to the ability of brain networks and of brain-inspired hierarchical architectures to achieve an optimal balance between segregation and integration [18], allowing them to conduct multiple tasks simultaneously, entailing optimal computational capabilities [34]. Let us also note that a significant part of the above-mentioned phenomenology uses concepts, such as Griffiths phases, first introduced to study (Anderson) localization phenomena in quantum systems described, e.g., by a random tight-binding Hamiltonian [35], and later extended, for instance, to the Laplacian matrix of a graph [36,37].

In this paper, we aim at providing a theoretical foundation for the phenomenological observations of anomalous behavior and localization effects obtained so far in hierarchical-modular networks, establishing for the first time a clear link

*paolo.moretti@fau.de

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Molecular Simulation of Thermosetting Polymer Hardening: Reactive Events Enabled by Controlled Topology Transfer

Robert H. Meißner*, Julian Konrad, Benjamin Boll, Bodo Fiedler, and Dirk Zahn

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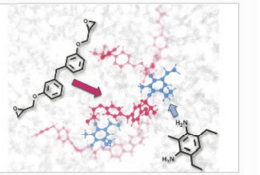
Macromolecules

Abstract

We present a nonhybrid quantum mechanical/molecular mechanics (QM/MM) type approach to tackle chemical reactions with substantial molecular reorganization. For this, molecular dynamics simulations with smoothly switched interaction models are used to suggest suitable product states, while a Monte Carlo algorithm is employed to assess the reaction likeliness subject to energetic feasibility. As a demonstrator, we study the cross-linking of bisphenol F diglycidyl ether (BFDGE) and 4,6-diethyl-2-methylbenzene-1,3-diamine (DETDA). The modeling of epoxy curing was supplemented by differential scanning calorimetry (DSC) measurements, which confirm the degrees of cross-linking as a function of curing temperature. Likewise, the heat of formation and the mechanical properties of the resulting thermosetting polymer are found to be in good agreement with previous experiments.



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On age-dependent bone remodeling

Areti Papastavrou [a,*], Ina Schmidt [a], Kefu Deng [b], Paul Steinmann [b]

[a] Faculty of Mechanical Engineering, Nuremberg Tech, Keßlerplatz 12, 90489 Nuremberg, Germany
[b] Chair of Applied Mechanics, University of Erlangen-Nuremberg, Egerlandstraße 5, 91058 Erlangen, Germany

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ABSTRACT

A number of previous studies have investigated the possibilities of modelling the change in density of bones. Remodeling can be formulated at the constitutive or the kinematic level. In this work we introduce a formulation for the density growth process which takes not only the mechanical stimulus into account but also the influence of age on the evolution of growth. We demonstrate the implementation in the context of the finite element method. This novel approach is illustrated for a simple uniaxial extension test and is verified against previous numerical results. Moreover, two further physiologically motivated examples are performed. The results of the proposed modified model show excellent agreement with comparable results from literature and are promising for the application to real-life problems.

1. Introduction

Against the background of an aging society the understanding of the diseases and aging of human bones becomes more and more important. The modeling, simulation and prediction of certain bone behaviour and failure is of growing interest scientifically and for medical doctors as well as for each subject affected. Bone is a living biomaterial with the ability to adapt not only its external shape to a certain extent but also mainly its internal microstructure. Depending on environmental changes, such as mechanical loading, hormonal metabolism and the availability of nutrition the density and trabecular orientation is altered. The first description of the functional adaption of hard tissues to changes in the mechanical loading situation was formulated by Wolff more than a century ago and is referred to as Wolffs law of bone remodeling, Wolff (1892). Some 80 years later Cowin and Hegedus presented the first continuum model of bone growth, which characterizes the isotropic functional adaptation of bone in response to mechanical loading, see Cowin and Hegedus (1976). During the last decades growth theory was incorporated into finite element based numerical simulations, and the first results in the area of computational bone remodeling were very encouraging, see e.g. Huiskes et al. (1987), Weinans et al. (1992), Harrigan and Hamilton (1993), even though numerical instabilities were observed by Jacobs et al. (1995). The bone density evolution is driven by the difference between the mechanical stimulus and a material specific optimal state, the so-called attractor state which is considered to be constant. In particular, our approach is to formulate an age-dependent function for the attractor state. The structure of the biomaterial is therein considered as an open system which is allowed to continuously exchange mass, momentum, energy and entropy with its environment, see Kuhl and Steinmann (2003). In addition several descriptions of growth phenomena in experimental examinations were published i.a. by Taber (1995) and Carter and Beaupré (2001).

In the present work, we focus on the age-dependence of the biomechanical growth processes in the context of the existing fully-nonlinear remodeling theory of Kuhl and Steinmann (2003), Kuhl et al. (2003). Even though the deformation of bone due to external loading (and/or remodeling) may be described by a geometrically linear approach, we choose to resort to a geometrically exact, i.e. nonlinear approach for the sake of generality and compatibility with earlier contributions to computational bone remodeling, e.g. Kuhl and Steinmann (2003), Kuhl et al. (2003).

It is widely accepted that bone density changes with age. Therefore, it is desirable to investigate parameters that determine bone remodeling as a function of age directly from experiments or clinical studies. It is currently not yet possible to determine the functional form of these changes over time. Fig. 1 showcases the changes in density of the human femoral bone for male and female as determined by Atkinson et al. (1962). The dots are taken from Atkinson et al. and the graphs are third-order polynomial regression curves to reflect the general trend in the dependence of density on age. Also other publications support the assumption that density depends on age, e.g. Ding et al. (1997), Emmert (2002).

In particular, two alternative formulations of the attractor stimulus as a function of age are suggested. The attractor stimulus can

* Corresponding author.
E-mail address: areti.papastavrou@th-nuernberg.de (A. Papastavrou).

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Articles

On biological availability dependent bone remodeling

Areti Papastavrou, Ina Schmidt & Paul Steinmann

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Abstract

Modeling the evolution of bone density is relevant for understanding, simulation and possible prediction of bone response to external and internal influences. In this work we present a formulation for the bone density evolution process that takes into account not only the commonly considered mechanical stimulus, but, as novelty, also the influence of the availability of nutrients and hormones, with its implementation pursued within the finite element method. A simple uni-axial extension test is used to illustrate and compare our novel model against the classical approach. The results of the proposed modified model are promising for application to real-life problems.

Keywords: Bone remodeling biological availability density change growth finite element method

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Microstructural controls of anticrack nucleation in highly porous brittle solids

Jonas Ritter[1], Henning Löwe[2] & Johan Gaume[2,3]✉

Porous brittle solids have the ability to collapse and fail even under compressive stresses. In fracture mechanics, this singular behavior, often referred to as anticrack, demands for appropriate continuum models to predict the catastrophic failure. To identify universal controls of anticracks, we link the microstructure of a porous solid with its yield surface at the onset of plastic flow. We utilize an assembly method for porous structures, which allows to independently vary microstructural properties (density and coordination number) and perform discrete element simulations under mixed-mode (shear-compression) loading. In rescaled stress coordinates, the concurrent influence of the microstructural properties can be cast into a universal, ellipsoidal form of the yield surface that reveals an associative plastic flow rule, as a common feature of these materials. Our results constitute a constructive approach for continuum modeling of anticrack nucleation and propagation in highly porous brittle, engineering and geo-materials.

The compression of porous brittle materials can lead to localization of compaction or compacting shear bands[1–3]. This singular behavior, referred to as anticrack, originates from microstructural failure processes and has been observed in the compression of porous sandstone[4,5], submarine landslides[6], firnquakes[7] or snow avalanches[8–10]. The latter is a particularly spectacular consequence of the nucleation of an anticrack under mixed mode loading: Snow as a highly porous material continuously changes its microstructure under thermodynamic forcing[11]. Under a high temperature gradient, a layer of small rounded crystals can turn into a weak layer of large faceted crystals[12]. Buried in a snowpack on a mountain slope, such a layer is always subjected to mixed-mode (shear-compressive) loading and the nucleation of an anticrack can lead to widespread anticrack propagation and dangerous slab avalanches[3,8]. To understand the generic mechanisms underlying these processes, irrespective of a particular material, it is necessary to decipher how the macroscopic behavior of mixed-mode anticrack nucleation originates from the microstructure.

From a continuum point of view, the nucleation of mixed-mode anticracks is controlled by the complex interplay between the yield surface, plastic flow rule and strain softening. It has been suggested that non-associated plasticity is necessary to reproduce anticracks in some porous sandstones[13]. In contrast, recent work on snow has demonstrated that anticrack nucleation and propagation in snow can be simulated using a continuum damage model with associated plasticity, if complemented by a modified strain softening law[3]. However, these question cannot be satisfactorily answered at the continuum level where involved assumptions cannot be traced back to and justified from the microstructure.

In the past decades, the extensive use of X-ray micro-computed tomography (XRCT) facilitated unprecedented insight into porous microstructures in all fields of material science[14]. Numerical simulations based on XRCT images allow to faithfully characterize and constrain the properties of the microstructural network (such as connectivity) on the mechanical behavior of different materials such as soils[15,16], lunar soils[17], snow[10–22], rocks[23,24] or concrete[25–27]. Simulations based on XRCT microstructure images are nowadays seen as complementary (numerical) experiments which can be repeatedly performed with different material properties, loading states and boundary conditions. This opens excellent opportunities in addition to (destructive) laboratory experiments which naturally lag behind in view of versatility and parameter variability. However, high resolution microstructure-based simulations still come with considerable computational requirements. Thus systematic

[1]Institute of Materials Simulation (WW8) and Central Institute for Scientific Computing (ZISC), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany. [2]WSL Institute for Snow and Avalanche Research SLF, Davos Dorf, Switzerland. [3]SLAB Snow and Avalanche Simulation Laboratory, EPFL Swiss Federal Institute of Technology, Lausanne, Switzerland. ✉email: johan.gaume@epfl.ch

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Grain boundary interaction based on gradient crystal inelasticity and decohesion

Lucie Spannraft [a], Magnus Ekh [b], Fredrik Larsson [b], Kenneth Runesson [b], Paul Steinmann [a]

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Abstract

This paper presents a model for geometrically non-coherent grain boundary interaction premised on gradient-extended crystal inelasticity. The appropriate kinematics, the constitutive relations and the balance equations are established for a polycrystal including grain interaction. More specifically, this contribution proposes a coupling of the microtraction and grain boundary decoheion, which is represented as damage. As a consequence, decohesion exerts an impact on the standard tractions as well as on the microtractions along the grain boundaries. The appropriate modeling framework is assessed in terms of numerical results for a bicrystal that is subjected to simple shear. A comparison with the situation without such coupling effect shows that the microtractions along the grain boundary reduce for increasing damage and a microfree boundary is approached when the damage approaches unity.

Chapter 14
Characterization of Polystyrene under Shear Deformation Using Molecular Dynamics

Maximilian Ries, Paul Steinmann, and Sebastian Pfaller

Abstract Nano-filled polymers are becoming more and more important to meet the continuously growing requirements of modern engineering problems. The investigation of these composite materials at the molecular level, however, is either prohibitively expensive or just impossible. Multiscale approaches offer an elegant way to analyze such nanocomposites by significantly reducing computational costs compared to fully molecular simulations. When coupling different time and length scales, however, it is in particular important to ensure that the same material description is applied at each level of resolution. The Capriccio method (Pfaller et al, 2012, 2013), for instance, couples a particle domain modeled with molecular dynamics (MD) with a finite element based continuum description and has been used i.a. to investigate the effects of nano-sized silica additives embedded in atactic polystyrene (PS), cf. Pfaller et al (2016); Liu et al (2017). However, a simple hyperelastic constitutive law is used so far for the continuum description which is not capable to fully match the behavior of the particle domain. To overcome this issue and to enable further optimization of the coupling scheme, the material model used for the continuum should be derived directly from pure MD simulations under thermodynamic conditions identical to those used by the Capriccio method. To this end, we analyze the material response of pure PS under uniaxial deformation using strain-controlled MD simulations (Ries et al, 2019). Analogously, we perform simulations under pure shear deformation to obtain a comprehensive understanding of the material behavior. As a result, the present PS shows viscoelastic characteristics for small strains, whereas viscoplasticity is observed for larger deformations. The insights gained and data generated are used to select a suitable material model whose parameters have to be identified in a subsequent parameter optimization.

Keywords: Molecular dynamics · Simulation of polymers · Mechanical properties of polymers · Material characterization

M. Ries, P. Steinmann, S. Pfaller
Chair of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg
e-mail: maximilian.ries@fau.de, paul.steinmann@fau.de, sebastian.pfaller@fau.de

B. E. Abali and I. Giorgio (eds.), *Developments and Novel Approaches in Nonlinear Solid Body Mechanics*, Advanced Structured Materials 130,
https://doi.org/10.1007/978-3-030-50460-1_14

Submitted / accepted / in press

Journal Articles

[1] **S. Elmira Birang O., Paul Steinmann**
Discrete Configurational Mechanics for the Computational Study of Atomistic Fracture Mechanics
Journal of Forces in Mechanics, accepted (Volume 2 (2021) 100009)

[2] **Seyyed Ahmad Hosseini, Paolo Moretti, Avraam Konstantinidis, Michael Zaiser**
Beam network model for fracture of materials with hierarchical microstructure
International Journal of Fracture, accepted

[3] **Maximilian Ries, Gunnar Possart, Paul Steinmann, Sebastian Pfaller**
A coupled MD-FE methodology to determine gradients of mechanical properties inside polymeric interphases in nanocomposites
International Journal of Mechanical Sciences, submitted

[4] **Ina Schmidt, Areti Papastavrou, Paul Steinmann**
Concurrent consideration of cortical and cancellous bone within continuum bone remodelling
Computer methods in biomechanics and biomedical engineering, accepted

[5] **Sukhminder Singh, Lukas Pflug, Michael Stingl**
Material optimization to control cohesive interfacial fracture using viscous regularization
Computer Methods in Applied Mechanics and Engineering, submitted

[6] **Simon Theil, Maximilian Fleischmann, Reena Gupta, Florian Wullschläger, Sangeeta Sharma, Bernd Meyer, Samuel Shallcross**
A general relation between stacking order and Chern index: a topological map of minimally twisted bilayer graphene
Phys. Rev. B 2020, submitted

[7] **Wuyang Zhao, Maximilian Ries, Paul Steinmann, Sebastian Pfaller**
A viscoelastic-viscoplastic constitutive model for polymers based on molecular dynamics simulation under uniaxial deformation
International Journal of Solids and Structures, submitted

[8] **Wuyang Zhao, Paul Steinmann, Sebastian Pfaller**
A particle-continuum coupling method for multiscale simulations of viscoelastic – viscoplastic amorphous glassy polymers
Computer Methods in Applied Mechanics and Engineering, submitted

Conference papers

[9] **Christof Bauer, Sebastian Pfaller**

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

Proceedings in Applied Mathematics and Mechanics, in press

[10] **Paras Kumar, Julia Mergheim**

Size Effects in Computational Homogenization of Polymer Nano-Composites

Proceedings in Applied Mathematics and Mechanics, in press

[11] **Sukhminder Singh, Michael Stingl**

Material optimization for controlling interfacial damage in composite structures

Proceedings in Applied Mathematics and Mechanics, in press

[12] **Wuyang Zhao, Sebastian Pfaller**

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

Proceedings in Applied Mathematics and Mechanics, in press

In preparation

Journal Articles

[1] **Achraf Atila, Erik Bitzek**

Atomistic origins of deformation-induced structural anisotropy in metaphosphate glasses

[2] **Christof Bauer, Sebastian Pfaller**

Investigation of particle movements under uniaxial loading using molecular dynamics and continuum mechanical approaches

[3] **Seyedeh Elmira Birang Oskouei et al.**

Configurational and Deformational Mechanics of Embedded-Atom Method

[4] **Seyedeh Elmira Birang Oskouei et al.**

Configurational and Deformational Mechanics of Three-Body Potentials

[5] **Seyedeh Elmira Birang Oskouei et al.**

Discrete Configurational Forces in Graphene: Structural Defects

[6] **Seyedeh Elmira Birang Oskouei et al.**

Discrete Configurational Forces in Graphene: Crack Mechanism

[7] **Samaneh Esfandiary, Paolo Moretti, Miguel A. Muñoz**

Localization and dynamic slowing down in hierarchical network models of the brain

[8] **Nosaibeh Esfandiary, Paolo Moretti, Michael Zaiser**

Adhesion and detachment properties of systems with hierarchical microstructures

[9] **Julian Konrad, Robert Meißner, Dirk Zahn**

A molecular simulation analysis of bond reorganization in epoxy resins: from curing to deformation and fracture

[10] **Paras Kumar, Julia Mergheim**

Enhanced Computational Homogenization Techniques for Modeling Size Effects in Polymer Composites

[11] **Tarakeshwar Lakshmipathy, Alexander Hartmaier, Erik Bitzek**

Influence of crack tip radius on fracture toughness: comparing atomistic simulations to LEFM

[12] **Mattia Livraghi*, Kevin Höllring*, Christian R. Wick, David M. Smith, Ana-S. Smith**

From Liquid to Gel: An Algorithm to Detect the Gel Point in Periodic Molecular Dynamic Simulations of Crosslinked Systems

**these authors contributed equally*

[13] **Mattia Livraghi, David M. Smith, Christian R. Wick*, Ana-S. Smith**

Towards a General AMBER Force Field to Model Amine Based Epoxy Resins: Liquid, Glassy, Fractured

**corresponding author*

[14] **Ali Mauricio Velasco Sabogal, Thorsten Pöschel**

Fast Method for Multi-sphere Filling of Complex Shapes

[15] **Ali Mauricio Velasco Sabogal, Thorsten Pöschel**

Fracture of Irregular Grains under Single Load Conditions

2.3 Participation in conferences and workshops

Achraf Atila

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
12.03.2020	2nd Visitors Workshop of the GRK 2423 FRASCAL	Marloffstein, Germany	Poster: *Atomic-scale Study of the Crack Nucleation and Fracture Behavior in Silica Glass*
16.06.2020 / 19.06.2020	USTV-DGG joint meeting (cancelled due to Covid-19 and shifted to 2021)	Orléans, France	Talk: *Atomistic Study of Mechanical and Structural Anisotropy of Metaphosphate glasses*

Christof Bauer

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
12.03.2020	2nd Visitors Workshop of the GRK 2423 FRASCAL	Marloffstein, Germany	Poster: *Describing particle movements using molecular dynamics and continuum mechanical approaches*
16.03.2020 / 20.03.2020	91st GAMM (cancelled due to Covid-19 and shifted to 2021)	Kassel, Germany	Talk: *Towards adaptive discrete-to-continuum modelling of thermoplastics*
19.07.2020 / 24.07.2020	WCCM-EC-COMAS 2020 (cancelled due to Covid-19 and shifted to 2021)	Paris, France	Talk: *Towards adaptive discrete-to-continuum modelling of thermoplastics*

Elmira Birang

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
12.03.2020	2nd Visitors Workshop of the GRK 2423 FRASCAL	Marloffstein, Germany	Poster: *Discrete Configurational Mechanics*
16.03.2020 / 20.03.2020	91st GAMM (cancelled due to Covid-19 and shifted to 2021)	Kassel, Germany	Talk: *Energy of Brittle Crack Propagation in Crystalline Lattices*
19.07.2020 / 24.07.2020	WCCM-EC-COMAS 2020 (cancelled due to Covid-19 and shifted to 2021)	Paris, France	Talk: *Atomistic Configurational Forces: Case Study of Britttle Crack Propagation*

Stefan Hiemer

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
12.03.2020	2nd Visitors Workshop of the GRK 2423 FRASCAL	Marloffstein, Germany	Participation only

Paras Kumar

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
10.02.2020 / 11.02.2020	7th GAMM Workshop on PHASE-FIELD Modelling	Kaiserslautern, Germany	Participation only
12.03.2020	2nd Visitors Workshop of the GRK 2423 FRASCAL	Marloffstein, Germany	Poster: *Modeling Size-Effects in Polymer Nano-Composites*
16.03.2020 / 20.03.2020	91st GAMM (cancelled due to Covid-19 and shifted to 2021)	Kassel, Germany	Talk: *Modeling Size Effect in Polymer Nanocomposites*
23.08.2020 / 28.08.2020	ICTAM 2020 (cancelled due to Covid-19 and shifted to 2021)	Milan, Italy	Talk: *Size Effects in Computational Homogenization of Polymer Nano-Composites*

Tarakeshwar Lakshmipathy

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
12.03.2020	2nd Visitors Workshop of the GRK 2423 FRASCAL	Marloffstein, Germany	Poster: *Influence of crack tip radius on fracture behaviour: an atomistic study*
27.06.2020 / 03.07.2020	ECF23, European Conference on Fracture 2020 (cancelled due to Covid-19 and shifted to 2022)	Funchal, Madeira, Portugal	Talk: *Influence of crack tip radius on fracture behaviour: an atomistic study*
15.09.2020 / 18.09.2020	ICSID 2020, 4th International Conference on Structural Integrity and Durability (participation cancelled due to Covid-19)	Dubrovnik, Croatia	Talk: *Influence of crack tip radius on fracture behaviour: an atomistic study*

Tobias Müller

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
12.03.2020	2nd Visitors Workshop of the GRK 2423 FRASCAL	Marloffstein, Germany	Poster: *Kinetic trapping in subcritical crack opening: How to find the true pathway*

Dhananjay Phansalkar

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
10.02.2020 / 11.02.2020	7th GAMM Workshop on PHASE-FIELD Modelling	Kaiserslautern, Germany	Talk: *On several challenges with a phase-field model for fracture*
12.03.2020	2nd Visitors Workshop of the GRK 2423 FRASCAL	Marloffstein, Germany	Poster: *Adaptivity in the Dynamic Simulation of Fracture Mechanics*
16.03.2020 / 20.03.2020	91st GAMM (cancelled due to Covid-19 and shifted to 2021)	Kassel, Germany	Talk: *Space dependent transition zone parameter for a phase-field model to fracture*

Maximilian Ries

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
12.03.2020	2nd Visitors Workshop of the GRK 2423 FRASCAL	Marloffstein, Germany	Poster: *Using coupled FE-MD simulations to derive interphase properties of polymer nanocomposites*
27.05.2020 / 29.05.2020	EMMC17 (cancelled due to Covid-19)	Madrid, Spain	Talk: *Investigation of interphase effects in polymer nanocomposites with FE-MD multiscale simulations using the Capriccio Method*
19.07.2020 / 24.07.2020	WCCM-ECCOMAS 2020 (cancelled due to Covid-19 and shifted to 2021)	Paris, France	Talk: *Multiscale FE-MD coupling: Rethinking the Capriccio Method*

Jonas Ritter

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
12.03.2020	2nd Visitors Workshop of the GRK 2423 FRASCAL	Marloffstein, Germany	Poster: *Compressive Failure of Highly Porous Materials*
04.05.2020 / 08.05.2020	EGU General Assembly 2020	Vienna, Austria (Web-based)	Talk: *Microstructural insights into the compressive failure of snow based on a peridynamic framework*

Ina Schmidt

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
12.03.2020	2nd Visitors Workshop of the GRK 2423 FRASCAL	Marloffstein, Germany	Poster: *Computational Bone Remodeling*
16.03.2020 / 20.03.2020	91st GAMM (cancelled due to Covid-19 and shifted to 2021)	Kassel, Germany	Talk: *On the influence of biological availability on bone remodelling*
12.07.2020 / 15.07.2020	ESB 2020 (cancelled due to Covid-19)	Milano, Italy	Talk: *Simulation of different influences on bone remodelling*

Sukhminder Singh

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
12.03.2020	2nd Visitors Workshop of the GRK 2423 FRASCAL	Marloffstein, Germany	Poster: *Gradient-based material optimization for fracture control*
16.03.2020 / 20.03.2020	91st GAMM (cancelled due to Covid-19 and shifted to 2021)	Kassel, Germany	Talk: *Material optimization for controlling interfacial damage in composite structures*

Lucie Spannraft

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
16.03.2020 / 20.03.2020	91st GAMM (cancelled due to Covid-19 and shifted to 2021)	Kassel, Germany	Talk: *Gradient-extended crystal inelasticity with a coupling of a microtractions and decohesion model*
12.03.2020	2nd Visitors Workshop of the GRK 2423 FRASCAL	Marloffstein, Germany	Poster: *Grain boundary interaction: Microtractions model coupled to decohesion model*
27.05.2020 / 29.05.2020	EMMC17 (cancelled due to Covid-19)	Madrid, Spain	Talk: *Grain boundary interaction including a mixed-mode cohesive zone model*
19.07.2020 / 24.07.2020	WCCM-EC-COMAS 2020 (cancelled due to Covid-19 and shifted to 2021)	Paris, France	Talk: *Grain boundary interaction: Energetic and dissipative microtractions model coupled to a mixed-mode cohesive zone model*

Christian Wick

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
17.02.2020 / 19.02.2020	34th MMWS 2020	Erlangen, Germany	Talk: *Modelling SILP catalysis: The Water-Gas Shift Reaction* Poster: (co-author; presenting author: Mattia Livraghi) *Highly cross-linked epoxy networks under mechanical strain*
02.11.2020 / 04.11.2020	16th GCC and SAMPL Satellite Workshop 2020	online, Germany	Flash Talk: *Modelling Epoxy Resins at the Molecular Scale: Liquid, Glassy and Fractured*

Florian Wullschläger

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
09.02.2020 / 14.02.2020	GSMS Winter School 2020	Kirchberg, Austria	Talk: *Atomistic Modelling of Twisted Bilayer Graphene and Surface-Assisted Cyclodehydrogenation*

Wuyang Zhao

From / to	Name of conference	Location	Title of own presentation / title of own poster presentation / participation only
12.03.2020	2nd Visitors Workshop of the GRK 2423 FRASCAL	Marloffstein, Germany	Poster: *Constitutive modelling of viscoelastic-viscoplastic glassy polymers based on MD simulations under uniaxial deformation*
27.05.2020 / 29.05.2020	EMMC17 (cancelled due to Covid-19)	Madrid, Spain	Talk: *Towards a particle-continuum coupling method for concurrent multiscale simulations of viscoelastic amorphous polymers bridging spatial and temporal scales.*
19.07.2020 / 24.07.2020	WCCM-EC-COMAS 2020 (cancelled due to Covid-19 and shifted to 2021)	Paris, France	Talk: *A particle-continuum coupling method for simulations of viscoelastic amorphous polymers and nanocomposites*

2.4 Collaborations with other research institutions

Christof Bauer

Partner institute	Researchers involved	Research topic
Theoretical Physical Chemistry Group, Technical University of Darmstadt, Germany	Florian Müller-Plathe, Yash Jain	MD-FE Coupling

Elmira Birang

Partner institute	Researchers involved	Research topic
Chair of Computer Science 10 (System Simulation), Friedrich-Alexander Universität Erlangen-Nürnberg, Germany	Rafael Ravedutti, Harald Koestler, Ulrich Rüde, Paul Steinmann	A High-Performance Computational Framework for Discrete Configurational Mechanics
Department of Mechanical Engineering, Boston University, USA	Harold S. Park	Fracture of Carbon-Based Atomistic Systems

Tarakeshwar Lakshmipathy

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

Valentina Marzulli

Partner institute	Researchers involved	Research topic
Polytechnic University of Bari, Italy	Francesco Cafaro, Annamaria di Lernia	Mechanical Characterization of Granular Materials/ Impact in granular matter
City University of Hong Kong, Hong Kong	Kostas Senetakis, Chitta Sai Sandeep	Micromechanical Characterization of Granular Materials
University of Birmingham, United Kingdom	Kit Windows-Yule	Impact in granular matter/Janssen effect in dynamic particulate systems

Maximilian Ries

Partner institute	Researchers involved	Research topic
Theoretical Physical Chemistry Group, Technical University of Darmstadt, Germany	Florian Müller-Plathe, Yash Jain	Multiscale modelling of amorphous polymers

Lucie Spannraft

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

Florian Wullschläger

Partner institute	Researchers involved	Research topic
Max-Born-Institute Berlin / Chair of Theoretical Solid State Physics, FAU Erlangen-Nuremberg, Germany	Samuel Shallcross, Reena Gupta, Maximilian Fleischmann	Electronic Structure of Twisted Bilayer Graphene
Chair of Organic Chemistry II, FAU Erlangen-Nuremberg, Germany	Norbert Jux, Helen Hoelzel, Dominik Lungerich	Surface-Assisted Cyclodehydrogenation
Chair of Experimental Physics, FAU Erlangen-Nuremberg, Germany	Sabine Maier	Surface-Assisted Cyclodehydrogenation
Chair of Organic Chemistry, Martin-Luther-University Halle-Wittenberg, Germany	Konstantin Amsharov, Arber Uka	Surface-Assisted Cyclodehydrogenation

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

3 Qualification Concept

3.1 Qualification programme

The qualification programme includes “qualification days”, “alumni and visitors workshops”, and “RTG retreats” as basic activities. These are accompanied by obligatory participations in international conferences and optional research stays abroad.

3.1.1 Qualification days

During each lecture period (typically from October to February and from April to July), one day per week is reserved for qualification days covering mini lectures, soft skills trainings, and RTG seminars.

Mini lectures

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

The mini lectures were hold by PAs, FRASCAL associated doctoral researchers*, guest lecturers** and FRASCAL doctoral researchers***.

Table 9: Mini lectures

	Date	Title	Lecturer
01	24 January 2020	Artificial Intelligence Methods in Materials Science (including failure forecasting)	M. Zaiser, P. Moretti, S. Hiemer*
02	31 January 2020	Introduction to Mesoscopic Modelling (IMEMO)	P. Moretti
03	21 February 2020	Introduction to Material Modelling (IMAMO)	J. Mergheim
04	24 July 2020	Introduction to Elastoplastic Fracture Mechanics (IPLAS)	R. Denzer**
05	31 July 2020	Introduction to Molecular Modelling of Polymer Materials (IMOPO)	D. Zahn, J. Konrad***
06	09 October 2020	Introduction to Concurrent Modelling (ICOMO)	S. Pfaller

Each lecture is also published as a printed script. This serves the doctoral students as a reference work after the lecture.

Figure 48: Impressions of some mini lectures and photo of the mini lecture notes (middle).

RTG seminars

In each lecture period, one qualification day is reserved for a RTG seminar mandatory for the doctoral researchers and associated doctoral researchers. Within the framework of this seminar, the current developments of each doctoral project is presented as talks of 15 min duration with 5 to 10 min subsequent discussion. Based on these seminars, the doctoral researcher and the mentoring team may evaluate the progress of the doctoral project also in comparison to the other projects.

Table 10: RTG seminars

	Date	Subject	Mode
01	20 February 2020	3. RTG Seminar	half doctoral researchers, half associated doctoral researchers and postdoctoral researcher
02	14-15 September 2020	4. RTG Seminar & 1. RTG Retreat	all doctoral researchers and postdoctoral researcher

Programmes see Appendix 1 and Appendix 3

3rd RTG Seminar

On February 20, 2020, the third RTG seminar of the Research Training Group GRK 2423 FRASCAL took place in the Seminar Room 00.044, LTM.

After a welcome and some introductory words, spokesperson of the RTG, Prof. Paul Steinmann, gave a preview of upcoming important events of the GRK 2423 FRASCAL.

Afterwards, seven doctoral researchers and four associated doctoral researchers presented the results they received in the first year of their scientific work. After each presentation, the already remarkable results were discussed. There were also very stimulating and detailed discussions, which were continued during the coffee breaks.

At the end of the official lecture program, a meeting between all doctoral researchers, post doctoral researcher and the spokesperson took place. There, GRK 2423 FRASCAL-relevant issues were discussed intensively and, among other things, the evaluation of the RTG by the doctoral researchers, which took place in October 2019, was discussed again in detail.

Figure 49: Impressions of the 3rd RTG Seminar.

4th RTG Seminar

Figure 50: Combined 1st RTG Retreat & 4th RTG Seminar at Forschungscampus Waischenfeld.

The fourth RTG seminar took place in a slightly different form than usual for the following reason:

Since the original date of the 1st RTG Retreat of the GRK 2423 FRASCAL (for each cohort, an RTG retreat is held after approximately 18 months) had to be postponed due to the COVID-19 pandemic, the new date of the retreat coincided with the fourth of the semi-annual RTG seminars. Thus, it was decided to hold a combined "1st RTG Retreat & 4th RTG Seminar" event.

For this event, all FRASCAL members met on the Fraunhofer Research Campus in the climatic spa Waischenfeld (Franconian Switzerland).

As usual at our RTG seminars, all FRASCAL doctoral researchers and the post doctoral researcher each gave a presentation on their latest research results.

A more detailed description of the event can be found in Section 3.1.3.

Special seminars

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

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

Table 11: Special seminars

	Date	Title	Lecturer
01	07 February 2020	**Physical and Mechanical Properties of Polymers** Part 1: Basic concepts of polymer physics and hierarchical coarse-graining: from particles to fields Part 2: Molecular mobility, physical aging, and mechanical rejuvenation in deformed (homo)polymer glasses Part 3: Nonlinear mechanical response of thermoplastic elastomers and semicrystalline polymers	Prof. Dr. Jörg Rottler, University of British Columbia, Vancouver, Canada
02	18 June 2020	**Phase-Field Modeling of Brittle Fracture: An Overview and a New Paradigm to Address Multiple Solutions** Part 1: Overview of the phase-field approach to fracture and of recent related research Part 2: Focus is placed on the issue of multiple solutions	Prof. Dr. Laura De Lorenzis, ETH Zürich, Switzerland
03	03 December 2020	**Simulating Long-Term Diffusive Heat and Mass Transport Phenomena in Nanoscale Systems** Presentation of a formulation and computational package to simulate long-term diffusive mass transport in systems with atomic scale resolution. The implemented framework is based on a non-equilibrium statistical thermo-chemo-mechanical formulation of atomic systems where effective transport rates are computed using a kinematic diffusion law	Dr. Mauricio Ponga de la Torre, University of British Columbia, Vancouver, Canada

Figure 51: Impressions of the Special seminars (M. Ponga (left), J. Rottler (middle), L. De Lorenzis (right)).

English language coaching

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

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

Attendance of English classes is optional.

Table 12: English coaching seminars

Date	Topic
Winter semester 2019/2020	English prosody: intonation & pausing; extemporaneous & spontaneous speech
	Practicing spontaneous speech; mock presentations
	Return to advanced pronunciation techniques & course review
Summer semester 2020	Individual language consultations
	Vocabulary acquisition through phraseological units (video)
Winter semester 2020/2021	Individual language consultations and group classes
	Varying linguistic expression in the written word, particularly as it pertains to scientific writing
	Logic in structure (linguistic complexity through structural simplicity)
	How an article differs from a dissertation and general structuring rules for smaller vs. larger texts
	Online reference tools for the writing process
	Presenting in a pre-recorded conference - how to make the video interactive and effective; tips on pronunciation, clarity of voice, transitions, introductions, accentuating point

Figure 52: English coaching with Paul Gahman (still from one of his learning videos).

3.1.2 Alumni and visitors workshops

In addition to the RTG seminars, the annual alumni and visitors workshop enables scientific exchange with external experts and shall thus stimulate intense discussions. The RTG's Mercator fellows and additional visiting researchers from the fields encountered in the RTG, but also from other related research fields, are invited to these workshops.

Each doctoral researcher has to attend at least two workshops, typically at the end of her/his first and second year.

Table 13: Alumni and visitors workshops

	Date	Subject	Location
01	12 March 2020	2nd Visitors Workshop	Schloss Atzelsberg, Marloffstein

Programme see Appendix 2

On March 12th, 2020 the 2nd Visitors Workshop of the GRK 2423 FRASCAL took place in the beautiful castle of Atzelsberg near Erlangen.

It should be emphasized that the planned programme of the workshop would have been two days long, with lectures by six internationally renowned scientists in the field of fracture behaviour. During the coffee breaks, two poster presentations of all FRASCAL doctoral researchers and associates were to take place. Due to the rapidly changing and unpredictable situation of the corona crisis at that time, the programme had to be constantly adapted and modified in the few days before the workshop began. Some speakers were unable to travel to the workshop because the flights were cancelled or stayed away due to health concerns. One and a half days before the workshop started, it was then decided to reduce the programme to just one day, with three guest speakers and one poster session.

The workshop started early Thursday afternoon with a welcome to all participants by the spokesperson of the GRK 2423 FRASCAL, Paul Steinmann, and a short presentation of the FRASCAL programme.

The first speaker was Gilles Francfort (Department of Mathematics, University 13, Paris, France and visiting professor at the Courant Institute, New York University, New York, USA). In his lecture entitled „Initiation and kinking: The fracture lines of fracture", he addressed in particular three major issues: crack initiation, crack path, and smoothness of the crack evolution.

James Kermode from the Warwick Centre for Predictive Modelling (University of Warwick, Coventry, UK) spoke in his lecture „Multiscale modelling of materials chemomechanics: Brittle fracture, dislocation glide and beyond" about the application of materials modelling algorithms to make quantitative predictions of chemomechanical materials failure processes where stress and chemistry are tightly coupled.

After these two stimulating lectures, all participants of the workshop gathered in front of the castle for a group photo in the fresh March weather.

The subsequent coffee break began with a so-called "Poster Blitz" session: Each doctoral researcher had the opportunity to draw attention to her or his poster in a one-minute oral presentation, thus arousing the audience's curiosity.

During the extended coffee break and parallel poster session, the posters offered the opportunity to discuss the FRASCAL projects and the latest results.

After the break, everybody was eagerly awaiting the presentation of Franz-Josef Ulm from MIT, Cambridge, MA, USA, who unfortunately had to cancel his participation only a few hours before the workshop started due to the shortly before changed travel conditions to the USA. Nevertheless, we managed to get him to join us live to the castle via a web conference, and he was able to share his ideas and new approaches about "Fracture mechanics in the „semi „grand-canonical ensemble" with us.

Finally, all participants were invited to a conference dinner, where, in addition to culinary delights, interesting technical discussions took place and even ideas and starting points for new collaborations were found.

Figure 53: Impressions of the 2nd Visitors Workshop.

3.1.3 RTG retreat

Table 14: RTG-retreat

	Date		Location
01	14-15 September 2020	1. RTG Retreat & 4. RTG Seminar	Fraunhofer Research Campus, Waischenfeld (Franconian Switzerland)

Programme see Appendix 3

On September 14 and 15, 2020, all members of GRK 2423 FRASCAL met for the first retreat of the Research Training Group (RTG) on the Fraunhofer Research Campus in the climatic spa Waischenfeld (Franconian Switzerland).

Since the original date of the retreat had to be postponed due to the COVID-19 pandemic, the new date coincided with the fourth of the semi-annual RTG seminars. Therefore it was decided to hold a combined event „1st RTG Retreat & 4th RTG Seminar".

As usual at our RTG seminars, all FRASCAL doctoral researchers and the post doctoral researcher each gave a presentation on their latest research results.

In addition, one session was reserved to discuss the important topic "Research Data Management (RDM)". The representatives of three so-called user groups of GRK 2423 FRASCAL presented a summary of the remarkable results of their meetings. These groups have been formed a few months ago from some members of the doctoral researchers to explore the possibilities of a comprehensive RDM system for this Research Training Group and to develop a concept that is as consistent and sustainable as possible.

Since the doctoral researchers of the RTG are already almost at the end of their second year and therefore (have to) think about their professional career after their doctorate, a further block was reserved at the retreat to present different career paths. In this session two aspects were considered:

On the first day, under the topic „Suddenly PhD, now what?", various options for the professional career of an academic were discussed. The various possibilities from staying as an academic at the university or going on as a scientist in institutions of applied sciences to an academic career in industry were presented. The Principal Advisors Bernd Meyer, Dirk Zahn and Thorsten Pöschel presented the different paths to a university professorship in a lively and entertaining way using the example of their own curriculum vitae. Ralf Meske, one of the four members of FRASCALs External Advisory Board, described very clearly how research and development in industry works and how it differs from research at universities or similar research institutions.

On the second day, Paul Steinmann gave a presentation titled „As there's no cash to splash, where should the funding come from?" on the various financing options for young researchers with doctorates.

It was a special pleasure that our Mercator Fellow, Laurent Ponson (Paris), despite the restrictions of Corona, joint FRASCAL's first retreat and enriched the many discussions with his constructive contributions. Not only during the retreat, but already since the beginning of his work as a Mercator Fellow in GRK 2423 FRASCAL, he brought invaluable additional expertise to the RTG. As a symbolic recognition and an expression of our gratitude, he was presented with a certificate at this event.

During a hike to the Burg Rabenstein and a guided tour through the Sophienhöhle, the discussions could be continued and deepened in small groups on Monday afternoon in a very informal way, but also the beautiful nature of Franconian Switzerland could be enjoyed. The day ended with a barbecue on the Fraunhofer Research Campus in still beautiful summer weather.

Our combined 1st RTG Retreat & 4th RTG Seminar in Waischenfeld was varied, informative and there was leisure time to discuss science and other important matters in life.

Figure 54: Impressions of the 1st RTG Retreat & 4th RTG Seminar.

3.2 Visiting researcher programme

Table 15: Visiting researchers

From / to	Guest	Research Subject
06.02.2020 / 07.02.2020	**Prof. Dr. Jörg Rottler** University of British Columbia Dept. of Physics and Astronomy and Quantum Matter Institute Vancouver, Canada	Special Seminar: Part 1: Basic concepts of polymer physics and hierarchical coarse-graining: from particles to fields Part 2: Molecular mobility, physical aging, and mechanical rejuvenation in deformed (homo)polymer glasses Part 3: Nonlinear mechanical response of thermoplastic elastomers and semicrystalline polymers **Host:** Prof. Erik Bitzek (WW1)
11.03.2020 / 13.03.2020	**Prof. Gilles A. Francfort** Paris University 13, Paris, France	Invited Lecture at the 2nd Visitors Workshop of FRASCAL: "Initiation and kinking: The fracture lines of fracture" and discussions with several FRASCAL doctoral researchers and PAs **Host:** Prof. Paul Steinmann (LTM)
12.03.2020 / 13.03.2020	**Prof. James Kermode** University of Warwick, Coventry, UK	Invited Lecture at the 2nd Visitors Workshop of FRASCAL: "Multiscale Modelling of Materials Chemomechanics: Brittle Fracture, Dislocation Glide and Beyond" and discussions with several FRASCAL doctoral researchers and PAs **Host:** Prof. Erik Bitzek (WW1)
12.03.2020	**Prof. Dr. Franz-Josef Ulm** Massachusetts Institute of Technology, Cambridge, MA, USA	Invited Lecture at the 2nd Visitors Workshop of FRASCAL: "Griffith's Conjecture: Fracture Mechanics in the Grand Canonical Ensemble" held via Webex video conference **Host:** Prof. Paul Steinmann (LTM)
18.06.2020	**Prof. Dr. Laura De Lorenzis** ETH Zürich, Zürich, Switzerland	Invited Lecture at the Joint GCEC and FRASCAL Special Seminar via Zoom: "Phase-field modeling of brittle fracture: an overview and a new paradigm to address multiple solutions" **Host:** Prof. Paul Steinmann (LTM)
24.07.2020	**Dr.-Ing. Ralf Denzer** Lund University/LTH, Division of Solid Mechanics, Lund, Sweden	Mini Lecture (via Zoom): "Introduction to Elasto-plastic Fracture Mechanics" **Host:** Prof. Paul Steinmann (LTM)
10.09.2020 / 16.09.2020	**Dr. Laurent Ponson** Pierre et Marie Curie University, Paris, France	Participation in the 1st RTG-Retreat & 4th RTG-Seminar of GRK 2423 FRASCAL Discussions with the FRASCAL doctoral researchers about their projects. The students benefited greatly from these fruitful discussions and constructive advice from the Mercator fellow. The new insights gained in their work certainly contribute to making rapid progress in further research. **Host:** Prof. Erik Bitzek (WW1)

09.11.2020 / 13.11.2020	**Prof. Michael Ortiz** California Institute of Technology, Pasadena, CA, USA	Invited Lecture: (hybrid) "Multiscale Modeling of Ductile Fracture in Metals" Collaboration with S. Leyendecker and D. Phansalkar, discussions about P9-relevant questions: 1. Discussion on mesh adaptivity approaches 2. Numerical implementation of different bcs. and irreversibility 3. Dynamic fracture mechanics Discussion with PA (S. Pfaller) and doctoral researchers (C. Bauer, M. Ries, W. Zhao) about: 1. the capriccio method in itself with current problems 2. the extension of the capriccio method to deal with questions concerning fracture processes **Host:** Prof. Sigrid Leyendecker (LTD)
03.12.2020	**Dr. Mauricio Ponga de la Torre** University of British Columbia Department of Mechanical Engineering Vancouver, Canada	Invited Lecture (via Zoom): "Simulating long-term diffusive heat and mass transport phenomena in nanoscale systems" **Host:** Prof. Paul Steinmann (LTM)

3.3 Additional qualification measures

3.3.1 Research stays or internships at other research institutions

Christof Bauer

From / to	Institute visited	Local supervisor (if applicable)	Research activities performed and skills acquired during stay
24.02.2020 / 29.02.2020	Department of Applied Mechanics, Indian Institute of Technology, Delhi, India	Ajeet Kumar	DAAD-DIP "Multiscale Modelling, Simulation and Optimization"

Paras Kumar

From / to	Institute visited	Local supervisor (if applicable)	Research activities performed and skills acquired during stay
24.02.2020 / 29.02.2020	Department of Applied Mechanics, Indian Institute of Technology, Delhi, India	Ajeet Kumar	Discussions on deal.II library, modelling of nano-structured objects

3.3.2 Summer / Winter schools

Florian Wullschläger

From / to	Name of summer school	Location
09.02.2020 / 14.02.2020	GSMS Winter School 2020	Kirchberg, Austria

3.3.3 Student projects and theses

Student work completed in 2020 that were supervised by FRASCAL doctoral researchers.

Bachelor theses

Student	Topic	Supervisor
Marcia Weigand	Expanding the Capriccio Method: Integration of Multiple Molecular Dynamics Regions	Maximilian Ries
Maximilian Striegel	Analysis of the molecular structure of polystyrene based on molecular dynamic deformation experiments	Maximilian Ries

Project theses

Student	Topic	Supervisor
Isabella Rank	Visualization of user-defined non-coherent inelastic elements in ABAQUS	Lucie Spannraft

Master theses

Student	Topic	Supervisor
Vinay Nagaraj	A literature review on fracture of graphene	Elmira Birang
Jatandeep Singh	Implementation and Analysis of a Phase-Field Model for Brittle Fracture	Paras Kumar

4 Equal Opportunity Measures

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

4.1 Workshops, seminars

In cooperation with the Office for Gender and Diversity at FAU and with the support of FAU's ARIADNE mentoring team, a completely new and comprehensive concept for a modular pilot seminar series "Gender Equality in Research" was developed exclusively for GRK 2423 FRASCAL, initially with three full-day seminars. Two trainers were recruited who are very renowned in this field throughout Germany and have excellent references. The individual modules were thematically linked, but did not build on each other and could therefore be attended individually and specifically according to interest (all three seminars had to be held in the form of webinars):

Table 16: Pilot seminar series: "Gender Equality in Research"

	Date	Title	Lecturer
01	30 April 2020	**Understanding Gender** This workshop provided a brief introduction to how gender plays a role in everyday life at the university. Gender stereotypes and sexism were discussed, as well as how gender affects us and our academic careers The workshop gave participants the opportunity to both reflect on the stereotypes that influence their own academic development and discuss how to deconstruct gender stereotypes to contribute to more gender equality in academia.	Dr. Susanne Frölich-Steffen (Zorneding)
02	30 October 2020	**Gender Competence Training** In this workshop, participants were introduced to "gender competence" in their research and teaching areas. The term "gender competence" and its different aspects (e.g. subcompetences) were outlined, contextualized and underpinned by the legal framework. Participants learned about tools for gender competent action and applied them to a practical case, e.g. planning a conference or a summer school.	Dr. Sabine Blackmore (Berlin)
03	20 November 2020	**Gender in Teaching and Learning** Gender and power relations are intrinsic to all social institutions, and this is particularly relevant for academic institutions. Gender constructions and relations begin at home, but stereotypes are also reinforced through teachers' behaviour, social interactions at university and the curriculum there. This workshop aimed to expand the gender perspective and skills of teachers at university. The methodology was participatory and included discussions, brainstorming and group work. It intended to increase gender responsiveness and sensitivity to teachers.	Dr. Susanne Frölich-Steffen (Zorneding)

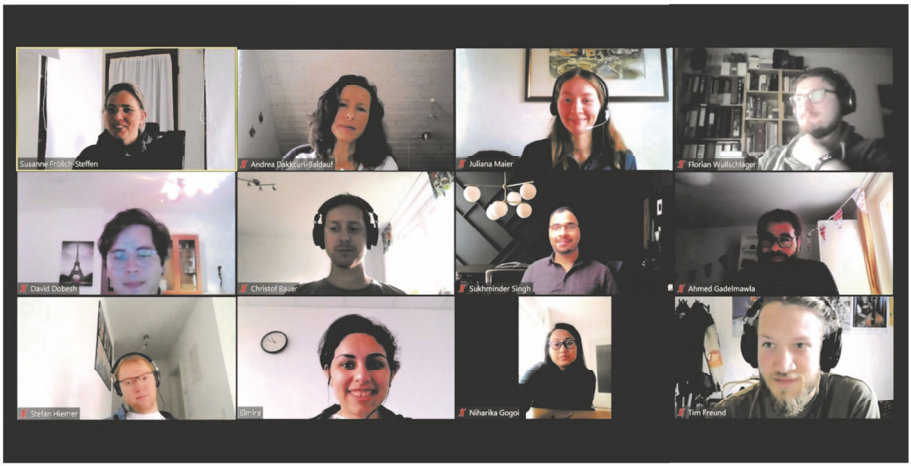

Figure 55: "Understanding Gender". Webinar with Dr. Susanne Frölich-Steffen on 30 April 2020.

The F³G network (Research Associations of Friedrich-Alexander-Universität Erlangen-Nürnberg for the promotion of equality) offers lectures and seminars on the topics of women's advancement, gender sensitization, etc., in addition to a variety of other gender equality measures, in which members of the affiliated research associations can participate. Thus, some FRASCAL members have also taken advantage of these training measures and participated in the following workshops:

Table 17: Workshops organized by F³G with participation of GRK 2423 FRASCAL members

	Date	Title	Lecturer
01	24 January 2020	Potential Analysis – Figuring Out Your Skills and Values	Dr. Silke Oehrlein-Karpi (Mainz)
02	18 May 2020	Self-Presentation	Julia Baumeister (Berlin)
03	29 May 2020	Time Management	Peter Kronenberg (Bonn)
04	01 October 2020	Career Paths and Academic Job Applications	Dr. Dunja Mohr (Erfurt)
05	29/30 October 2020	Conflict Management: Constructively Dealing With Conflict	Dr. Isabel Werle (Mainz)
06	23 October 2020	Publishing in Science, Technology, Engineering and Medicine	Petra Heermann, Stephanie Kolbe, Dr. Jürgen Rohrwild, Dr. Katrin Seyler (all Erlangen)

A further workshop, which dealt with the possibilities of a scientific career after the doctorate in general and the compatibility with family life in particular, took place at the end of the second year of this first GRK 2423 FRASCAL cohort. This workshop was developed especially for the GRK 2423 by Dr. Stefanie Herberger (Graduate Center of FAU) according to an expectation survey of the doctoral researchers.

Table 18: Further gender-related workshop

	Date	Title	Lecturer
01	04 December 2020	My Career in Academia: Conditions and Perspectives - Professional career, family building, and combining both	Dr. Stefanie Herberger (Erlangen)

The aim of the workshop was to clarify career paths in the science system - with a focus on Germany and with some experience reports from other countries. In addition, impulses for further career opportunities, also in research, will be given. Information and suggestions were given on how to develop further career options for oneself. Special attention was paid to the question "Can I have a scientific career and a family? How can I combine the two?" All relevant aspects were discussed.

4.2 Individual coaching

The F³G also organizes individual coaching sessions for young female scientists. The coaching offer aims to accompany the participants through the view from the outside in their reflections on the further development of a scientific career and includes individual counselling on questions of career and career planning issues.

Two of our female doctoral students have taken advantage of this offer and have been coached in two individual sessions each (so far).

The following points were covered in the coaching sessions:

Table 19: Individual coaching

	Date	Topic	Coach
01	24 August / 07 October 2020	Postdoc application process: writing proper emails, creating a short prototype, CV.	Dr. Susanne Frölich-Steffen (Zorneding)
02	21 September / 07 October 2020	Career planning and development: shaping the scientific career, preparation for the appointment process, job interviews, vocation training	Dr. Neela Enke (Berlin)

4.3 Vacation care

- Financial support for vacation care for the children of our FRASCAL members.
- Financial support of specific F³G projects in FAU holiday childcare programmes.

4.4 Further measures

- Pedagogic improvement of the infrastructure at FAU day care facilities for children
- Participation in F³G coordination costs

5 Selected Highlights

5.1 Presentation of the certificates to the Mercator Fellows

A particularly valuable aspect of the FRASCAL program is the possibility to involve Mercator Fellows, outstanding scientists from abroad, which enables an intensive and long-term scientific exchange with the young FRASCAL researchers.

Therefore, it was a great pleasure and honour that, despite the difficult pandemic-related circumstances, at least two of the three Mercator Fellows were able to visit GRK 2423 FRASCAL this year:

Dr. Laurent Ponson (Pierre et Marie Curie University, Paris, France) took the time to travel specially from Paris to Waischenfeld for the 1st RTG-Retreat of FRASCAL, and Prof. Michael Ortiz (California Institute of Technology, Pasadena, CA) was able to facilitate a 5-day research visit to the Chair of Applied Dynamics with Prof. Sigrid Leyendecker in November 2020. These on-site visits were used to officially present the two Mercator Fellows with a Mercator Fellowship Award certificate.

Prof. Elias Aifantis (Aristotle University of Thessaloniki, Greece) will hopefully be able to collect his certificate in person in 2021 under better travel conditions.


FRASCAL
GRK 2423

FAU

MERCATOR FELLOWSHIP
AWARD
(01/2019 – 09/2020)

to

Dr. Laurent Ponson

In appreciation of his contribution to the
Research Training Group
GRK 2423 FRASCAL

Fracture Across Scales: Integrating Mechanics, Materials Science, Mathematics, Chemistry, and Physics

Funded by the German Research Foundation (DFG).

Prof. Dr.-Ing. Paul Steinmann
Spokesperson
of the Research Training Group
GRK 2423 FRASCAL

Erlangen, 01 January 2019


FRASCAL
GRK 2423

FAU

MERCATOR FELLOWSHIP
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Professor Dr. Michael Ortiz

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Prof. Dr.-Ing. Paul Steinmann
Spokesperson
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GRK 2423 FRASCAL

Erlangen, 01 January 2019

Figure 56: Presentation of the certificates to the Mercator Fellows. Dr. Laurent Ponson (above); Prof. Dr. Michael Ortiz (below).

5.2 Weekly FRASCAL meetings

Usually, people met in person at the full-day events of the qualification programme and thus had the opportunity to exchange information about scientific, but also organizational, administrative and personal topics in a relaxed atmosphere before and after the events as well as during the breaks. Due to the pandemic-related conversion of the qualification programme from face-to-face to digital, these personal meetings suddenly fell away. Therefore, doctoral researchers' spokesperson Jonas Ritter initiated a weekly digital FRASCAL "coffee break". There, FRASCAL-internal social contacts were cultivated, but also technical topics were discussed.

User groups

At these regular digital FRASCAL meetings, the important topic of "Research Data Management (RDM)" was also discussed several times. Over time, three so-called user groups have emerged internally within FRASCAL (LAMMPS, Code Writing, FEM). These groups were formed by some of the doctoral researchers to explore the possibilities of a comprehensive RDM system for this RTG and to develop as consistent and sustainable a concept as possible. Representatives of these user groups presented the remarkable results of their meetings during the FRASCAL "coffee breaks".

TOPZ

At the end of July 2020, the FRASCAL "coffee break" was transformed into a so-called TOPZ. In this "**T**opical **O**verview **P**resentations **Z**oomposium", every week one or two FRASCAL doctoral researchers present their own latest research or current problems in five to ten minute talks and discuss them with the interested audience. After these usually very helpful and fruitful discussions, organizational or personal matters continue to be discussed informally.

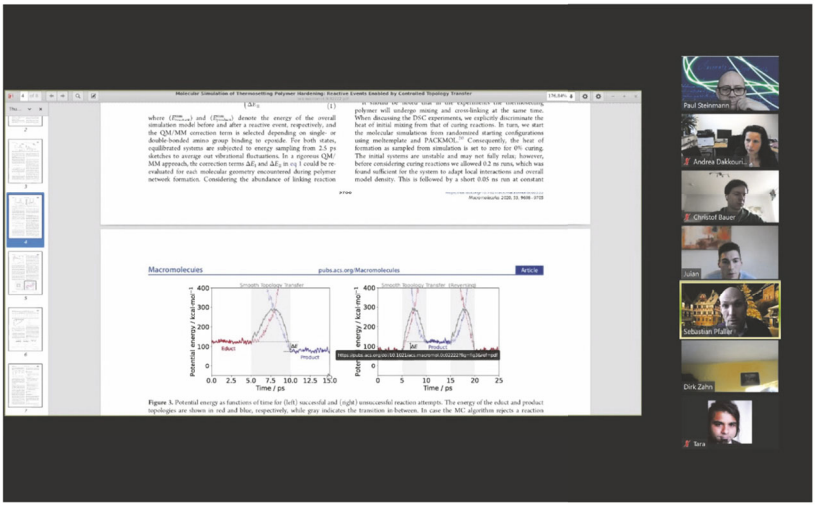

Figure 57: Topical Overview Presentations Zoomposium (TOPZ).

Open Sourcing Research Software

At one of these TOPZ, an expert on open sourcing of research software was also invited: Prof. Dirk Riehle (Department of Computer Science, FAU). He provided the FRASCAL members in advance with a presentation on "Open Sourcing Research Software", which was then discussed in detail at the TOPZ and Prof. Dirk Riehle patiently answered the many questions of the FRASCAL members.

5.3 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.

58 new books have already been acquired in the first two years of FRASCAL.

The library is very well received by FRASCAL members and usually at least one third of the books are borrowed.

Figure 58: FRASCAL library.

For a complete list, see Appendix 4.

6 Appendices

6.1 Appendix 1: Programme of the 3rd RTG Seminar

Programme of the 3rd RTG-Seminar			
Date	20 February 2020	Time	9:15 – 15:20
Venue	LTM, Seminar Room 00.044, Egerlandstraße 5, 91058 Erlangen		

Lectures: 15 min + 5 min discussion

Time	Name	Title of Presentation
9:15 – 9:30	WELCOME & INTRODUCTION	
9:30 – 9:50	Paras Kumar (P8)	*Modelling Size Effect in Polymer Nano-Composites*
9:50 – 10:10	Maximilian Ries (P6)	*Deriving Interphase Properties of Polymer Nanocomposites by Coupled FE-MD Simulations*
10:10 – 10:30	Elmira Birang (P10)	*Uncertainty of Energy Release Calculation in Molecular Mechanics; Can Configurational Forces Resolve It?*
10:30 – 10:50	COFFEE BREAK	
10:50 – 11:10	Nosaibeh Esfandiary (P7)	*Detachment Properties of Hierarchical Materials*
11:10 – 11:30	Samaneh Esfandiary (P7)	*Robustness and Failure of Brain Activity Patterns*
11:30 – 11:50	Wuyang Zhao (P6)	*A Viscoelastic-Viscoplastic Constitutive Model for Polymers Based on Molecular Dynamics Simulations under Uniaxial Deformation*
11:50 – 13:00	JOINT LUNCH	
13:00 – 13:20	Dhananjay Phansalkar (P9)	*On the Demanding Relation Between ε and h in a Numerical Phase-Field Model*
13:20 – 13:40	Christof Bauer (P6)	*Investigating the Relation of Particle Movements and the Continuum Displacement Field of Thermoplastics*
13:40 – 14:00	Ahmad Hosseini (P5)	*A Beam Network Model for Strength Optimization of Fibrous Materials*
14:00 – 14:20	COFFEE BREAK	
14:20 – 14:40	Jonas Ritter (P5)	*Designing a Confined Uniaxial Compression Test for Porous Materials within a Peridynamic Framework*
14:40 – 15:00	Ali Mauricio Velasco Sabogal (P4)	*Dynamics and Fractures of Real-Shaped DEM grains*
from 15:00	MEETING BOARD OF DOCTORAL RESEARCHERS and SPOKESPERSON	

6.2 Appendix 2: Programme of the 2nd Visitors Workshop

Programme of the 2nd Visitors Workshop			
Date	12 March 2020	Time	14:00 – 20:00
Venue	Schloss Atzelsberg, Atzelsberg 1, Marlottstein		

Lectures: 35 min + 10 min discussion

Time	Name	Title of Presentation
14:00 – 14:15	OPENING & WELCOME	
14:15 – 15:00	Gilles A. Francfort	*Initiation and Kinking: The Fracture Lines of Fracture*
15:00 – 15:45	James Kermode	*Multiscale Modelling of Materials Chemomechanics: Brittle Fracture, Dislocation Glide and Beyond*
15:45 – 17:00	COFFEE BREAK and POSTER SESSION (Posters with Poster Blitz)	
17:00 – 17:45	Franz-Josef Ulm	*Griffith's Conjecture: Fracture Mechanics in the Grand Canonical Ensemble* *via video conference*
18:00	DINNER	

6.3 Appendix 3: Programme of the 1st RTG Retreat & 4th RTG Seminar

Programme of the 1st RTG Retreat & 4th RTG Seminar			
Date	14 – 15 September 2020	Time	9:45 – 17:15
Venue	Forschungscampus Waischenfeld, Fraunhofer-Platz 1, 91344 Waischenfeld		

Lectures: 15 - 20 min + 10 – 15 min discussion

Time	Name	Title of Presentation
14 September 2020		
9:45 – 10:15	CHECK IN & COFFEE	
10:15 – 10:30	WELCOME & INTRODUCTION	
10:30 – 11:00	Ali Mauricio Velasco Sabogal (P4)	*Multi-Scale Fractures on Granular Materials*
11:00 – 11:30	Jonas Ritter (P5)	*Validation of a Peridynamic Model for Simulating Porous Materials*
11:30 – 11:45	COFFEE	
11:45 – 12:15	Christof Bauer (P6)	*Multiple Particle-Based Regions within a Continuum: Substituting FE with MD*
12:15 – 12:45	Nosaibeh Esfandiary (P7) (via Zoom)	*Failure and Crack Localization in Hierarchical Materials Adhesion*
12:45 – 14:15	LUNCH BREAK	
14:15 – 15:15	*"Suddenly PhD, now what?"* Ralf Meske, Bernd Meyer, Dirk Zahn, Thorsten Pöschel	*After the doctorate: academic career or in industry?* *CVs and experiences of Ralf Meske, Bernd Meyer, Dirk Zahn, Thorsten Pöschel*
15:30 – 18:45	HIKING & GUIDED CAVE TOUR	
19:00	BARBECUE	

Programme of the 1st RTG Retreat & 4th RTG Seminar			
Date	September 14-15, 2020	Time	9:45 – 17:30
Venue	Forschungscampus Waischenfeld, Fraunhofer-Platz 1, 91344 Waischenfeld		

Lectures: 15 - 20 min + 10 - 15 min discussion

Time	Name	Title of Presentation
15 September 2020		
8:00 – 9:00	BREAKFAST	
9:10 – 9:40	Paras Kumar (P8)	*Size-Effects in Nano-Composites: IECH vs. GICH*
9:40 – 10:10	Elmira Birang (P10)	*Configurational Mechanics of Crack Growth in Crystalline Lattice Structures*
10:10 – 10:40	*"As there's no cash to splash, where should the funding come from?"* Paul Steinmann	*What possibilities are there for acquiring funding directly after the doctoral thesis?*
10:40 – 11:00	COFFEE BREAK	
11:00 – 12:00	*User Groups / Data Management* Paras Kumar, Sebastian Pfaller, Stefan Hiemer	*Presentation of the results of the user group meetings with subsequent discussion*
12:00 – 13:30	LUNCH BREAK	
13:30 – 14:00	Sukhminder Singh (P11)	*Material Optimization for Controlling Interfacial Damage in Composite Structures*
14:00 – 14:30	Christian Wick (P12)	*Computational Modeling of Epoxy Networks*
14:30 – 15:00	Tobias Müller (P1)	*The Quest for the Correct Boundary Conditions*
15:00 – 15:30	COFFEE BREAK	
15:30 – 16:00	Tarakeshwar Lakshmipathy (P2)	*Influence of Crack Tip Radius on Fracture Toughness: An Atomistic Study*
16:00 – 16:30	Julian Konrad (P3)	*Polymer Fracture Mechanics Based on Dissociative Force Field*
16:30 – 17:15	OUTLOOK & CLOSING	

6.4 Appendix 4: List of book inventory

	Author	Title	Publishing Year
1	Anandarajah, Annalingam	*Computational Methods in Elasticity and Plasticity: Solids and Porous Media*	2010
2	Antman, Stuart S.	*Nonlinear Problems of Elasticity*	2005
3	Başar, Yavuz; Weichert, Dieter	*Nonlinear Continuum Mechanics of Solids: Fundamental Mathematical and Physical Concepts*	2010
4	Bertram, Albrecht	*Elasticity and Plasticity of Large Deformations*	2012
5	Bertram, Albrecht; Glüge, Rainer	*Solid Mechanics: Theory, Modeling, and Problems*	2015
6	Bland, David Russell	*The Theory of Linear Viscoelasticity*	2016
7	Bobaru, Florin; Foster, John T.; Geubelle, Philippe H.; Silling, Stewart A. (eds.)	*Handbook of Peridynamic Modeling*	2017
8	Bonet, Javier; Wood, Richard D.	*Nonlinear Continuum Mechanics for Finite Element Analysis*	2008
9	Borja, Ronaldo I.	*Plasticity: Modeling & Computation*	2013
10	Braides, Andrea	*Γ-Convergence for Beginners*	2002
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