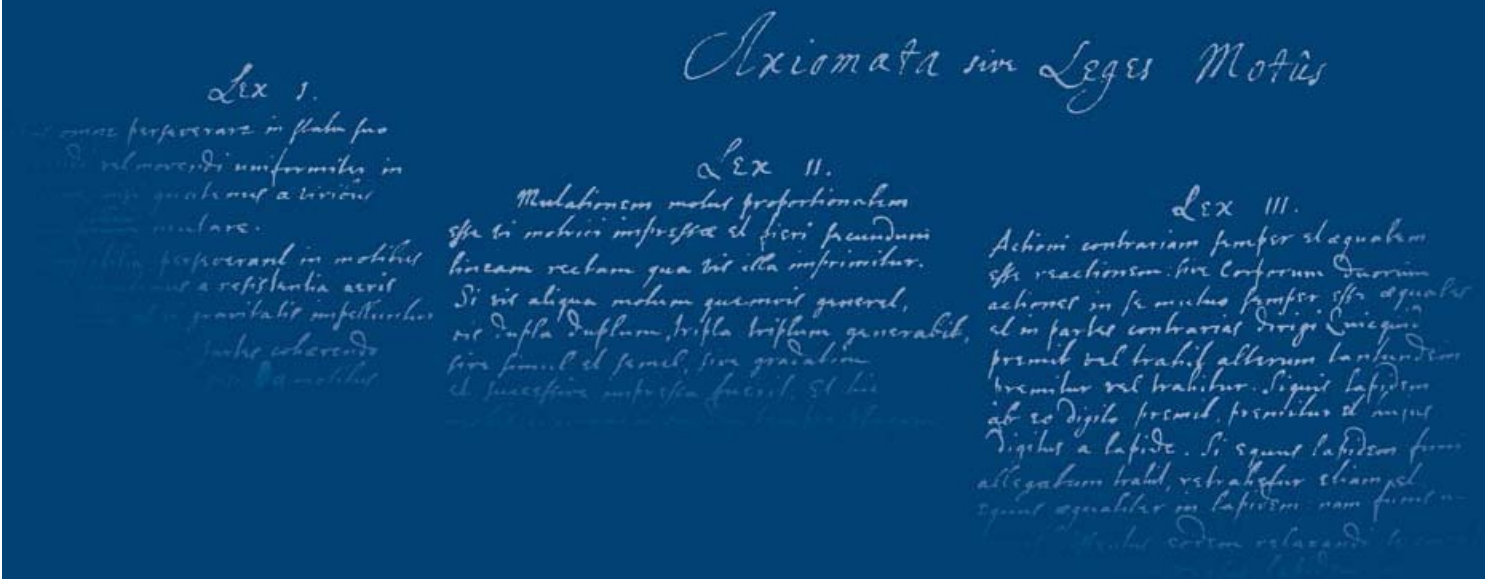
LTM LCM

Annual Report 2023



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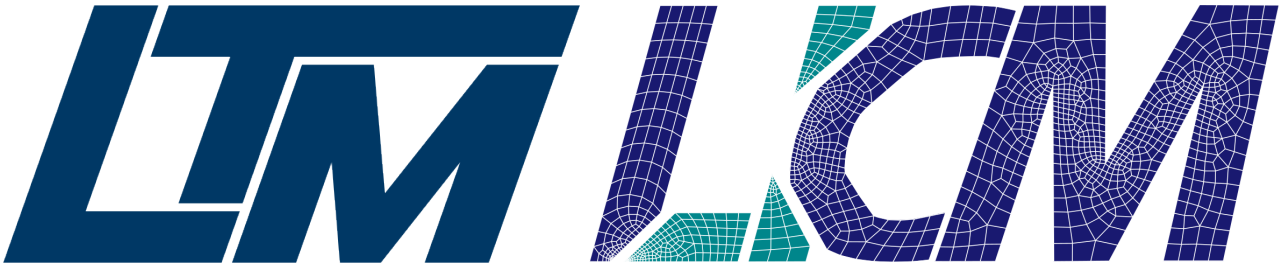

Annual Report 2023

Institute of Applied Mechanics
Prof. Paul Steinmann
Prof. Kai Willner
Prof. Julia Mergheim

—

Institute of Continuum Mechanics and Biomechanics
Prof. Silvia Budday

—

FAU Erlangen-Nürnberg

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Paul Steinmann, Kai Willner, Julia Mergheim; Silvia Budday
Institute of Applied Mechanics (https://www.ltm.tf.fau.de/);
Institute of Continuum Mechanics (https://www.lkm.tf.fau.eu/)
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Editor: Lucie Spannraft

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Preface

This annual report briefly documents the scientific, teaching, and social activities at the Institute of Applied Mechanics (LTM) and the Institute of Continuum Mechanics and Biomechancis (LKM) at the University of Erlangen-Nürnberg during 2023. At the scientific side the never ending enthusiasm of all members of the institutes did indeed result in exciting research and correspondingly in an internationally recognized output in terms of publications and conference contributions. Likewise the demanding teaching load, e.g. some several thousand written exams that require marking, could only be carried out due to the amazing level of dedication exhibited by all members of the institutes.
Of course all these efforts in turn fully justify team building activities in terms of excursions, barbecues, and various types of parties that characterize the social life at LTM and LKM. In summary we hope that this report convinces the reader of the level of academic achievements at the Institute of Applied Mechanics and the Institute of Continuum Mechanics and Biomechancis during the past year.

Erlangen, December 2023
Paul Steinmann, Kai Willner, Julia Mergheim
Silvia Budday

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1 Staff members

Professorship Continuum Mechanics
Prof. Dr.-Ing. habil. Paul Steinmann

Professorship Continuum Mechanics and Biomechanics
Prof. Dr.-Ing. Silvia Budday

Professorship Structural Mechanics
Prof. Dr.-Ing. habil. Kai Willner

Working group Computational Mechanics
Prof. Dr.-Ing. Julia Mergheim


P. Steinmann


S. Budday


K. Willner


J. Mergheim

Assistant and visiting lecturers
Dr.-Ing. Karsten Kolk, Siemens AG
Prof. Dr.-Ing. Ralf Meske, Federal-Mogul Nürnberg GmbH

Emeritus
Prof. Dr.-Ing. habil. Günther Kuhn

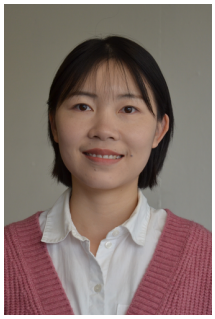
Technical and administrative staff
Christian Bänsch
Doris Bittner
Andrea Dakkouri-Baldauf (since 15/03)
Julia Deserno
Dr.-Ing. Xiaoling Luo (since 01/08)
Simone Schaetzlein (since 01/05)


C. Bänsch


D. Bittner


A. Dakkouri


J. Deserno


X. Luo


S. Schaetzlein

(Post-)doctoral researchers

Dr. Anahita Ahmadi Soufivand	
Dr.-Ing. Emma Griffiths	
Dr.-Ing. Markus Mehnert	
Dr. Stephen Melly	(since 19/04)
Dr. Miguel Ángel Moreno-Mateos	(since 01/04)
Dr.-Ing. Ina Schmidt	(until 31/03)
PD Dr.-Ing. habil. Sebastian Pfaller	
Dr.-Ing. Dmytro Pivovarov	
Dr.-Ing. Dipl.-Math. techn. Gunnar Possart	
Dr.-Ing. Maximilian Ries	
Nicole Tueni, Ph.D.	(since 15/09)
Daniel van Huyssteen, Ph.D.	
Dr.-Ing. Wuyang Zhao	
Özge Akar, M.Sc.	
Christof Bauer, M.Sc.	(until 30/06)
Christian Burkhardt, M.Sc.	(until 31/05)
Chaitanya Dev, M.Sc.	
Jessica Faber, M.Sc., M.Sc.	
Soheil Firooz. M.Sc.	
Johannes Friedlein, M.Sc.	
Alexander Greiner, M.Sc.	
Andreas Hegendörfer, M.Sc.	(until 30/06)
Ludwig Herrnböck, M.Sc.	(until 31/07)
Jan Hinrichsen, M.Sc.	
Paras Kumar, M.Sc.	
Sonja Kuth, M.Sc.	(since 01/08)
Jose Lara, M.Sc.	
Lukas Laubert, M.Sc.	(since 01/10)
Marie Laurien, M.Sc.	
Michael Lengger, M.Sc.	
Oskar Neumann, M.Sc.	(since 01/03)
Thomas Oberleiter, M.Sc.	
Nina Reiter, M.Sc.	
Maurice Rohracker, M.Sc.	
Laura Ruhland, M.Sc.	(since 01/04)
Emely Schaller, M.Sc.	
Lars Schmelzle, M.Sc.	
Michael Schwarz, M.Sc.	
Dominic Soldner, M.Sc.	
Andre Sommer, M.Sc.	(since 01/04)
Lucie Spannraft, M.Sc.	
Gabriel Stankiewicz, M.Sc.	(until 31/12)
Yashasvi Verma, M.Sc.	(since 01/04)
Felix Weber, M.Sc.	
Jana Wedel, M.Sc.	
Simon Wiesheier, M.Sc.	(since 01/01)
Mohammad Saeed Zarzor, M.Sc.	


A. Ahmadi Soufivand


Ö. Akar


C. Bauer


C. Burkhardt


C. Dev


J. Faber


S. Firooz


J. Friedlein


A. Greiner


E. Griffiths


A. Hegendörfer


L. Herrnböck


J. Hinrichsen


P. Kumar


S. Kuth


J. Lara


L. Laubert


M. Laurien


M. Lengger


M. Mehnert


S. Melly


M. Moreno-Mateos


O. Neumann


T. Oberleiter


S. Pfaller


D. Pivovarov


G. Possart


N. Reiter


M. Ries


M. Rohracker


L. Ruhland


E. Schaller



L. Schmelzle



I. Schmidt



M. Schwarz



D. Soldner



A. Sommer



L. Spannraft



G. Stankiewicz



N. Tueni



D. van Huyssteen



Y. Verma



F. Weber



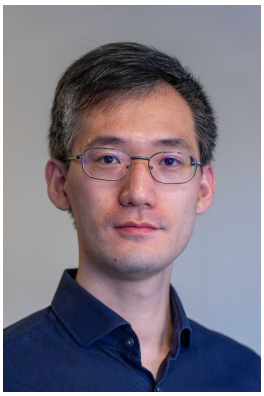
J. Wedel



S. Wiesheier



M.S. Zarzor



W. Zhao

Commissary

Industrial contact	G. Possart
Safety commissary	S. Pfaller
IT security commissary	C. Bänsch
IT administrator assistant	M. Ries
Editor of annual report	L. Spannraft
First Aid	Ö. Akar, C. Burkhardt, C. Dev, S. Firooz, M. Laurien, J. Mergheim, S. Pfaller, D. Pivovarov, E. Schaller, L. Schmelzle, D. Soldner, G. Stankiewicz, F. Weber

Academics

Exam organization	G. Possart
Teaching coordination	M. Ries
StudOn manager	M. Lengger
Teaching experiments contact	M. Ries, L. Spannraft, S. Pfaller
TM2 Excursion to FME	S. Pfaller, assisted by M. Ries, L. Spannraft
TM2 Ultimate Load Contest	M. Mehnert, P. Steinmann, assisted by M. Ries, L. Spannraft

Science communication

Girls' day/Schülertag	Ö. Akar
Mädchen/Schüler und Technik Praktikum	A. Greiner, M. Laurien, E. Schaller, M. Schwarz, L. Spannraft, F. Weber
Lange Nacht der Wissenschaften	FRASCAL and EBM members

Seminars (organization)

Advanced seminar on mechanics	G. Possart
LTM+LKM meeting	P. Steinmann
LTM+LKM TOPZ & Alumni TOPZ	Ö. Akar

Contributions to social life at LTM and LKM

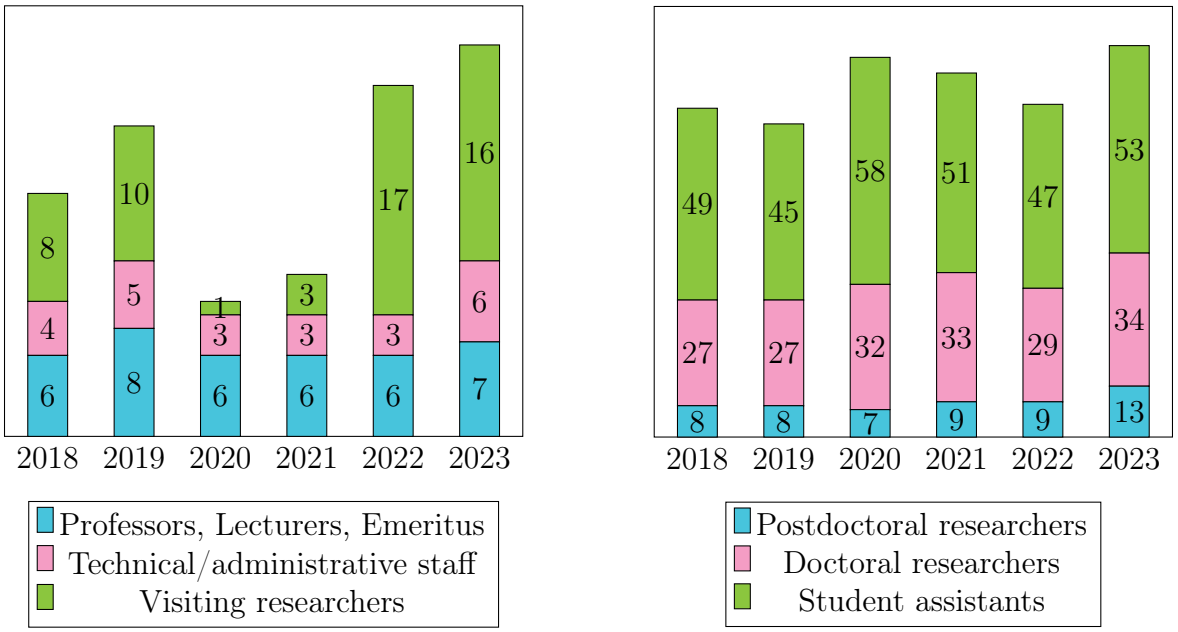
Beverages commissary	J. Faber
Chocolate commissary	L. Herrnböck, L. Schmelzle
Graduation hatter	Ö. Akar
Treasurer for graduation hats	C. Burkhardt, L. Ruhland
Organization of trip to Berg	L. Schmelzle
Organization of works outing	Ö. Akar, M. Ries
Organization of mid-year event	J. Hinrichsen, L. Schmelzle
Organization of year-end event	S. Melly, M. Moreno-Mateos, S. Kuth, L. Laubert, O. Neumann, L. Ruhland, A. Sommer, N. Tueni, Y. Verma, S. Wiesheier
LTM+LKM band	Ö. Akar, J. Deserno, S. Firooz, A. Greiner, L. Laubert, M. Ries, D. Soldner, L. Spannraft, G. Stankiewicz, F. Weber

Visiting researchers
Masoud Ahmadi, University of Glasgow, UK: 01/09–03/11/2023
Dr. Victor Borrell, CSIC-UMH, San Juan de Alicante, Spain: 23–25/10/2023
Dr. Ester Comellas, Universitat Politècnica de Catalunya, Spain: 12/07–05/08/2023
Dr. Anna De Villiers, Stellenbosch University, South Africa: 24–25/10/2023
Clément Ecker, ENS Paris-Saclay, France: 10/10/2022–31/07/2023
Carl Ferlay, École polytechnique, Palaiseau, Île-de-France: 27/03–14/07/2023
Prof. Matjaž Hriberšek, University of Maribor, Slovenia: 06–10/02, 03–07/07, 25–29/09/2023
Prof. Ali Javili, Bilkent University, Turkey: 15/06–14/12/2023
Prof. Ravnik Jure, University of Maribor, Slovenia: 06–10/02, 03–07/07, 25–29/09/2023
Prof. Ajeet Kumar, IIT Delhi, India: 15–31/05/2023
Prof. Andrew McBride, University of Glasgow, UK: 24–25/10/2023
Prof. Peter Pivonka, Queensland University, Australia: 20–24/03/2023
Prof. Kenta Seki, Nagoya Institute of Technology, Japan: 24–28/07/2023
Dr. Maxime Vassaux, Institute of Physics of Rennes, France: 02–06/10/2023
Vinayak, IIT Delhi, India: 01/04–31/05, 01/11/2023–02/01/2024
Ryota Yamamoto, Nagoya Institute of Technoloy, Japan: 05/03–30/06/2023

Student assistants
Charlotte Breitner
Kilian Brendel
Monika Buss
Cheuk Hang Chan
Vincent Dötschel
Lea Feiler
Johanna Fredrich
Taraswin Gottipati
Dominik Grützner
Nicole Häck
John Alejandro Hernandez Mora
Benedikt Hesche
Eluri Kashish Veda
Kaustubh Khanvilkar
Adrian Krämer
Mohamed Kriedy
Alexander Kulyabin
Lukas Laubert
Nils Leuthner
Paul Lindner
Maximilian Losert
Jonas Lotter
Sanskar Modi
Venkatesh Kumar Moorthy
Alexandre Nozadze
Arne Pietsch
Amin Ploner
Prateek Prateek
Nina Punger
Masoud Rahnama Esfahani
Alexander Rath
Jennifer Reitinger
Eva Richter
Florian Röhnert
Johannes Roksvaag
Sohini Roy
Behzad Safaei
Anne-Mareike Schäfer
Franziska Schön
Chiara Schoppe
Sumanthreddy Settipalli
Rutvi Shah
Amit Sharma
Aditi Sharma
Christian Strauss
Kalliana Raman Subramania Sharma
Harsh Vardhan Surana
Moritz Treschau
Ashish Vayangankar
Marcia Weigand
Sebastian Wittl
Kimia Zare
Zhao Zixuan

Student assistants are mainly active as tutors for young students in basic and advanced lectures within the bachelor and master programs located at the Technical Faculty of FAU.

Statistics of staff members, student assistants and guests 2018–2023



The statistics covering the staff over the last 6 years show a general increase in members because our many research projects. This year, Prof. Silvia Budday received her own institute (LKM), which was one contributing factor to the growth. Our institutes hosted a pronounced number of (inter)national guests except during the Covid pandemic.

Silvia Budday's appointment as Professor



This year, Silvia Budday was appointed Professor at FAU and became head of the new Institute of Continuum Mechanics and Biomechanics 'Lehrstuhl für Kontinuumsmechanik (Schwerpunkt Biomechanik)'. Her research focus lies on experiments, continuum mechanical modeling and simulations of the behavior of soft materials, such as the human brain. Previously, Silvia Budday was junior group leader in the Emmy-Noether program at the LTM.

2 Academic portfolio

2.1 Graduations

(Lucie Spannraft)

We are happy to announce six dissertation projects which were successfully finished or for which the defense is scheduled in the year 2023.

On Mai 23, **Dr. Thomas Hiller** earned a doctoral degree after defending his thesis titled 'Schwingungsverhalten von Abgasanlagen mit Entkoppelelementen' supervised by Professor Kai Willner in an external project.

On Mai 26, **Dr. Ludwig Herrnböck** defended his dissertation project by giving a talk on 'Numerische Methoden zur Modellierung elastoplastischer Balken und ihre Anwendung auf periodische Gitterstrukturen' supervised by Professor Paul Steinmann.





The – at this point luckily complete – committee announces Ludwig Herrnböck's success (left). Ludwig tries on the custom-made graduation hat capturing his most memorable moments at LTM (right).

On July 5, **Dr. Maximilian Ries** graduated after his talk on 'Characterization and modeling of polymer nanocomposites across the scales - A comprehensive approach covering the mechanical behavior of matrix, filler, and interphase'. The dissertation project has been supervised by Professor Paul Steinmann and PD Dr.-Ing. habil. Sebastian Pfaller.

On August 29, **Dr. Wuyang Zhao** received a doctoral degree after defending his thesis 'Multi-scale modeling of the fracture behavior of glassy polymers across the atomistic and continuum scale'. The dissertation project has been supervised by PD Dr.-Ing. habil. Sebastian Pfaller.



After the committee announces Wuyang Zhao's success (left), Wuyang receives his graduation hat reflecting on his time at LTM, including some of his witty and memorable remarks (right).

Andreas Hegendörfer submitted his doctoral thesis on 'System Simulations of Piezoelectric Energy Harvesters with the Finite Element Method'. The defense is scheduled for December 1, 2023. The dissertation project has been supervised by Professor Julia Mergheim.

Paras Kumar submitted his doctoral thesis on 'Enhanced Computational Homogenization and Phase-Field Fracture Approaches for Polymer Nano-Composites'. The defense is scheduled for December 8, 2023. The dissertation project has been supervised by Professor Julia Mergheim.

2.2 Teaching and student theses

The Institute of Applied Mechanics provides a wide variety of lectures, exercises and tutorials in German and English language to local and international students at the FAU. A large number of students writes their project papers and theses under the guidance of LTM staff members.

Lectures

Each year, several staff members dedicate their time to teach the huge number of students, who are interested in the applied mechanics, fundamental but also profound and specific knowledge. Only the help of the entire academic staff made the marking of the tremendous number of 1431 exams in 2023 possible.

Beyond FEM
Dr.-Ing. D. Pivovarov

Computational Dynamics
M. S. Zarzor, M.Sc.
Dr. M. A. Moreno-Mateos

Einführung in die Bruchmechanik
Dr.-Ing. K. Kolk

Höhere Festigkeitslehre
PD Dr.-Ing. habil. S. Pfaller

Introduction to the Finite Element Method
PD Dr.-Ing. habil. S. Pfaller

Linear Continuum Mechanics
Prof. Dr.-Ing. habil. P. Steinmann
D. Soldner, M.Sc.

Materialmodellierung und -simulation
Prof. Dr.-Ing. J. Mergheim
P. Kumar, M.Sc.

MATLAB Praktikum
E. Schaller, M.Sc.

Mikromechanik
Prof. Dr.-Ing. J. Mergheim
P. Kumar, M.Sc.

Methode der Finiten Elemente
Prof. Dr.-Ing. habil. K. Willner
M. Lengger, M.Sc.
Dr.-Ing. Dipl.-Math. techn. G. Possart

Nonlinear Finite Element Method
Prof. Dr.-Ing. J. Mergheim
D. Soldner, M.Sc.

Nonlinear Continuum Mechanics
Prof. Dr.-Ing. habil. P. Steinmann
D. Soldner, M.Sc.

Numerische und Experimentelle Modalanalyse
Prof. Dr.-Ing. habil. K. Willner
Ö. Akar, M.Sc.

Praktikum Technische Mechanik
E. Schaller, M.Sc.

Statik und Festigkeitslehre
Prof. Dr.-Ing. habil. K. Willner
Prof. Dr.-Ing. S. Budday
M. Lengger, M.Sc.
L. Spannraft, M.Sc.
Dr.-Ing. Dipl.-Math. techn. G. Possart

Strukturoptimierung in der virtuellen Produktentwicklung
Prof. Dr.-Ing. R. Meske

Technische Mechanik I+II (Statik, Elastostatik und Festigkeitslehre)
Prof. Dr.-Ing. habil. P. Steinmann
M. Ries, M.Sc.
L. Spannraft, M.Sc.

Technische Schwingungslehre
Prof. Dr.-Ing. habil. K. Willner
Ö. Akar, M.Sc.

Excursion to the Fränkische Museums-Eisenbahn e.V.

(LSp) As part of the module Applied Mechanics II, we offered our annual excursion to the 'Fränkische Museums-Eisenbahn e.V. (FME) Nürnberg' to interested students (https://www.fraenkische-museumseisenbahn.de/). The aim of this popular event is to demonstrate the application of the theoretical content of the lectures by means of traditional railway technology. The preparation and supervision was handled by Sebastian Pfaller supported by Maximilian Ries and Lucie Spannraft with regard to the coordination.



All participants in front of the 80 year old steam locomotive of class 52 8195 (top). Sebastian Pfaller acting as an external load on a spring (bottom left). The students figuring out the functions of certain elements by using the understanding of mechanics they gained during the semester (bottom right). Finally, the students (and Prof. Dr.-Ing. habil. Paul Steinmann) had fun trying out the train's braking system and could take a look into the driver's cab.

Ultimate Load Contest (Traglastwettbewerb)

(Markus Mehnert) Aiming at attracting the attention of students to challenging problems in mechanics, the Ultimate Load Contest was revived after 11 years of absence. On July 14th, 3 groups named 'Die 3,5 Muskeltiere', 'Die jungen Chef's und Max(i)' and 'Die Brüggenbauer' participated in the event. The objective of this contest is an optimization problem in applied mechanics: built a bridge structure consisting of medium-density fiberboard and commercial glue with a maximum weight of 2 kg. During the contest, the structure is supported at three points and is loaded vertically. The designs handed in by the students showed distinctly different approaches and interesting ideas to handle the applied force. While the slender designs by the first two groups were quickly destroyed, the behemoth build by 'Die Brüggenbauer' posed a fierce challenge to the testing device and consequently won the contest by a landslide. All contestants were rewarded with a custom-made trophy cup, an invaluable experience in the field of mechanics and an invitation to work as student tutors. Both the participants and the spectators truly enjoyed the event and it was decided unanimously that the next ultimate load contest will be held soon. As an exciting supplement to an engineering students curriculum, the Ultimate Load Contest deepens and enhances the understanding of Applied Mechanics and was considered as a complete success.



After 'Die jungen Chef's und Max(i)', who built their bridge in a kitchen, explain their concept, the load is applied and the participants discuss reasons for failure and possibilities to improve the structure (top). Professor Steinmann with the group 'Die 3,5 Muskeltiere', contestants of the ultimate load contest (bottom left). Everyone impressed by the amount of loading the last 'Brügge' could withstand (bottom right).

Student awards

This year student theses and master degrees from 2022 were awarded.



Photo: FAU | Erich Malter

Felix Weber (right), who now works on his doctoral project at LTM, received the 'Masterpreis der Diehl Stiftung & Co. KG' for his master degree in the Mechanical Engineering curriculum 2022. The award was received the Graduation ceremony of the Faculty of Engineering, FAU on July 21, 2023.

Student projects and theses

The following list of finished project papers and student theses for the academic year 2023 clearly reflects the broad range of ongoing research activities.

Bachelor theses

[1] A. Adams. *Advancing the Capriccio method: Parameter study with respect to load application.*

[2] S. Best. *Finite-Elemente Modellierung der Mechanotransduktion von Haarzellen.*

[3] L. Feiler. *Using Neural Networks to accelerate the Inverse Parameter Identification for Human Brain Tissue.*

[4] S. Frank. *Pattern formation in a Gray-Scott model.*

[5] A. Gill. *Experimental investigation of damage thresholds of porcine brain tissue under different loading modes.*

[6] A. Rath. *Development of a methodology for the vehicle dynamics set-up of a racing car with active suspension system.*

[7] F. Röhnert. *Vergleich und Implementierung verschiedener Substruktur-Reduktionsverfahren.*

Project theses

[1] V. Joschko. *Entwurf eines Versuchsaufbaus zur Identifizierung von Snap-Through-Instabilitäten.*

[2] L. Laubert. *Establishing a framework for conducting comparative one- and multidimensional studies on the coupling of the finite element method with particle-based techniques.*

[3] M. Rodschei. *Computational Modeling of Viscoelastic Polymer Nano-Composites.*

[4] M. Schmidt. *Computational Homogenization at Finite Strains using Neural Networks.*

Master theses

[1] L. Laubert. *Mechanical Analysis of Bio-Sourced Epoxy: Study of Elastic, Viscous, and Plastic Properties.*

[2] J. Lotter. *Simulation der Helmholtz-Bewegung einer Violinen-Saite mittels Finiter Elemente.*

[3] V. K. Moorthy. *Validation of FE-Analysis on e-Axle Housing Components Using Strain Correlation for Maximum Torque Load Condition.*

[4] D. Nguyen. *Bewertung des Vergleichs von Versuch und Simulation anhand objektiver Kurvenbewertungsmethoden.*

[5] A. Papadaki. *Topology Optimization via Convolutional Neural Networks: A Parameter Study.*

[6] S. Reber. *Entwicklung einer effizienten Volumen-Nebenbedingung für die Form- und Sickenoptimierung mit der Traction-Methode.*

[7] L. Ruhland. *Experimentelle und numerische Untersuchungen zum viskoelastischen Verhalten von Alginat-Gelatine.*

[8] P. Thiemann. *Dynamische Simulation der Befahrung eines Streckentrenners im Gesamtsystem Kettenwerk unter Berücksichtigung der Pantographendynamik.*

[9] D. Torres Huamani. *Gekoppelte MD-FE Simulationen für polymerbasierte Nanokomposite mit mehreren MD-Gebieten.*

[10] N. Vagga Chandramouli. *Advanced LS-Dyna User-Elements utilising AceGen's Automatic Linearisation and Code Generation.*

[11] J. Yu. *Optimization of Stiffness Simulation Methods based on Door Sinking and Overpressure Tests.*

2.3 Seminars

Advanced seminar on mechanics

Jointly with the Chair of Applied Dynamics, LTM and LKM organize a series of invited talks from researchers all around the world to present their current research projects and to stimulate discussion of their latest results among the staff members.

08/03/2023 Prof. Dr. Syn Schmitt, University of Stuttgart, Germany
Learning motion in muscle-driven systems - understanding biology and benefits for robotics.

22/03/2023 Prof. Prof. Peter Pivonka, QUT Brisbane, Australia
Computational simulation techniques for understanding bone remodeling.

15/05/2023 Prof. Ramona Hoffmann, HTW Saarland, Germany
Towards investigating gender differences in cycling motions using optimal control simulations.

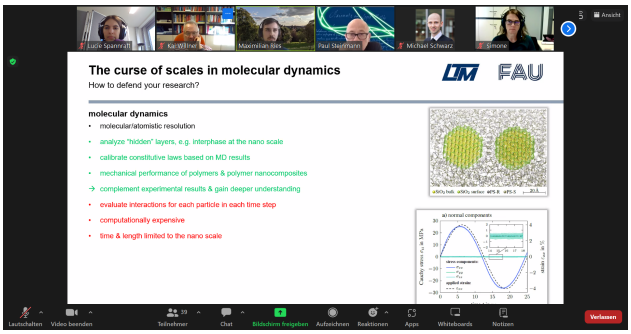
10/07/2023 Prof. Saulo Martelli, QUT Brisbane, Australia
Advances in multiscale experimental mechanics of bones.

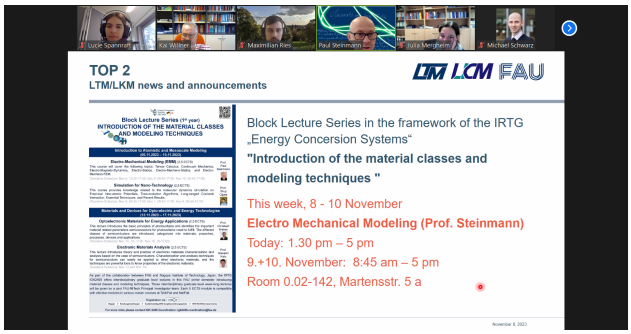
18/10/2023 M.Sc. Timo Ströhle, KIT Karlsruhe, Germany
Controlling nonlinear elastic systems governed by hyperbolic PDEs.

07/11/2023 Dr. Maxence Lavaill, QUT Brisbane, Australia
Assessment of shoulder musculoskeletal modelling procedures for clinical applications.

LTM+LKM Meeting and Alumni TOPZ

(LSp) Regular LTM+LKM meetings provide an opportunity for scientific and organizational exchange among all colleagues. Each week, either a (post-)doctoral researcher or an alumni gives a short presentation within the scope of the 'LTM+LKM/Alumni TOPZ' – short for 'Topical Overview Presentation *Zoom*posium' – coordinated by Özge Akar. Those presentations comprise, on the one hand, recent advances in research, interesting software, projects, or new formalities to follow. On the other hand, former colleagues provides short overviews on their curricula after leaving our institutes, on their current work in academia or industry, or on general topics, such as academic systems abroad. The wide variety of alumni speakers from all over the world working in various fields enrich the presentations and provide great insights in different career path. In addition, everyone is excited to regularly see former colleagues and old friends by means of this format. Afterwards, the latest LTM+LKM related news are announced, and important organizational issues are discussed.





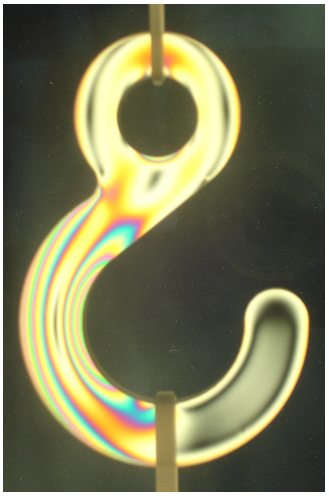
A LTM TOPZ presentation (left). The announcement of a block lecture series (right).

2.4 Science communication and gender equality

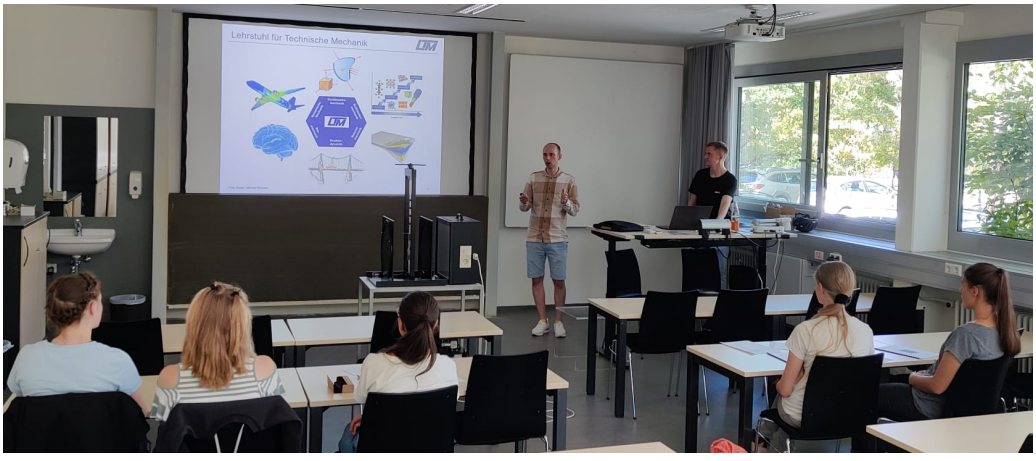
Girls' Day

(LSp) On the 'Girls' Day' in April, female high-school students were invited to visit the Technical Faculty of the FAU. This aimed at increasing their excitement towards technology and potentially inspire them to pursue a technical career in the future. The LTM participated in this project by offering the dynamics experiment 'Bad Vibes - when your cellphone vibration alarm becomes an earthquake' presented by Özge Akar and her student assistant Dominik Grützner. This year, many interested high-school students were eager to gain insights into the fascinating world of structural dynamics.

Mädchen und Technik Praktikum



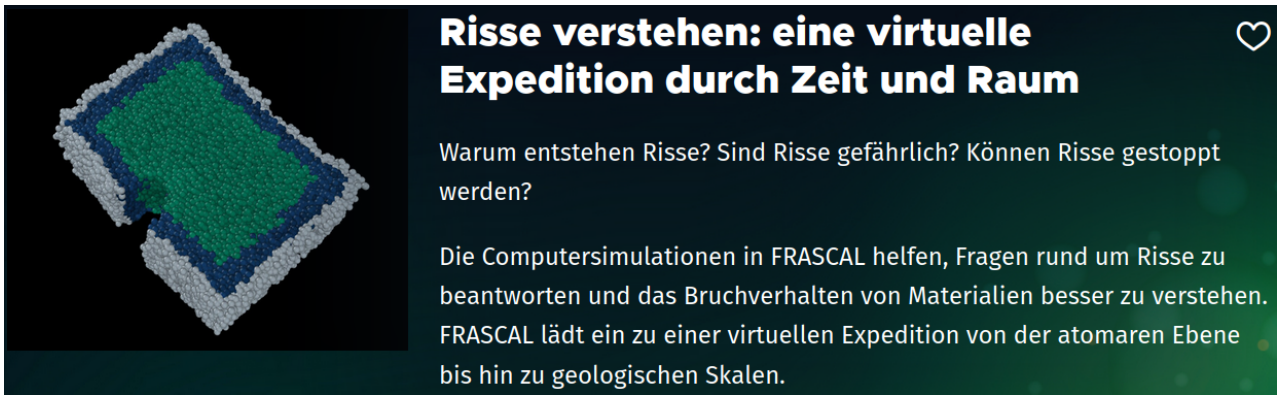
(LSp) In September, the LTM and LKM offered the experiment series 'Mechanics for future' within the scope of the 'Mädchen und Technik Praktikum' for the period of an entire week. We introduced several groups of high-school students to applied mechanics by performing four interactive experiments under the topic of stress analysis of a crane hook. The trials encompassed visual experiments, such as stress birefringence, measurements of material parameters, and recording strain maps via digital image correlation. Finally, the students learned how to set-up and perform basic Finite Element Method simulations of a crane hook subjected to loading. Using the parameters from the previous tests allows to roughly compare the simulation outcome with the performed experiments. This year, the experiments were supervised by five staff members (Alexander Greiner, Marie Laurien, Emely Schaller, Michael Schwarz, Felix Weber) to provide optimal support. Lucie Spannraft handled the coordination, the introductory presentation and scripts. Each student received a script comprising detailed information on the experiments and could complete the script by the obtained results, such as photos of the stress state and obtained material parameters. The participants showed high interest and excitement for our diverse experiments which allow a deeper understanding on some mechanical fundamentals and relations. In particular, the possibility to perform the experiments by themselves in small groups under our guidance was evaluated highly positively.



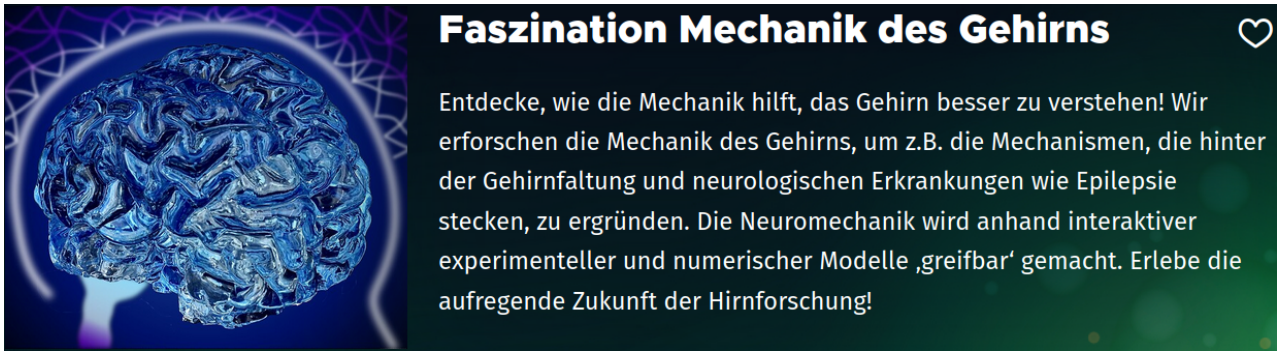
Die Lange Nacht der Wissenschaften

(LSp) Members of our institutes participated in the Long Night of Sciences (Die Lange Nacht der Wissenschaften) on Oktober 21, 2023 to communicate a selection of research topics to the interested public.

The RTG Fracture across Scales (https://www.frascal.research.fau.eu/) with 3 projects located at the LTM presented the topic 'Understanding cracks: A virtual expedition through time and space' discussing fracture behavior of different materials by means of a computer simulations from the atomar to the geological scale.



The CRC Exlporing Brain Mechanics (https://www.crc1540-ebm.research.fau.eu/) with several projects located at the LTM and LKM offered insights in the mechanics of brains by means of interactive experiments and numerical models under the theme 'Fascination Mechanics of Brains'.



Both participations were a success in terms of numerous excited visitors discussing the diverse topics of applied mechanics highly relevant to the public life.



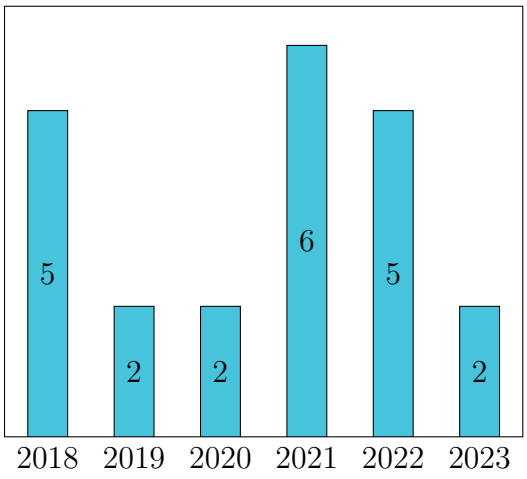


3 Scientific contributions

The following sections give a brief overview on the scientific output of LTM and LKM staff members during the year 2023. This does not only include multiple original contributions to international top-tier journals from the applied mechanics community, but also numerous presentations at international conferences, workshops, and symposia all around the globe. The high level of the scientific contributions is also emphasized by awards. Multiple research stays show the interconnectivity of the LTM and LKM with international research groups.

3.1 Awards and distinctions

Statistics of scientific/theses awards and distinctions 2018–2023



In 2023, **Prof. Dr.-Ing. Silvia Budday** has been awarded a Starting Grant from the European Research Council (ERC). She will use the funding of more than 2 million euros over a period of five years for the MAGERY project. This project aims to prevent damage to brain cells caused by mechanical stresses, e.g. during brain surgery.



Photo: FAU | Georg Pöhlein

Nina Reiter was elected as the speaker of the GAMM Juniors for the year 2023.

3.2 Research stays and summer schools

- Jessica Faber
  SFB/TRR 225 Summer school on Biofabrication. July 24 – 28, 2023. FAU Erlangen, Germany.

- Soheil Firooz
  Research stay upon invitation of Prof. Ali Javili. April 1st – May 31st, 2023. Bilkent University, Ankara, Turkie.

CISM Advanced Course on Virtual Elements for Problems in Mechanics. October 16 – 20, 2023. International Centre for Mechanical Sciences (CISM), Udine, Italy.
CISM Advanced Course on Peridynamic Models for Material Degradation: from Fracture/Fragmentation to Corrosion; from Models to Computer Codes. October 23 – 26, 2023. International Centre for Mechanical Sciences (CISM), Udine, Italy.
Research stay upon invitation of Prof. Daya Reddy. November 1st – 30th, 2023. University of Cape Town, Cape Town, South Africa.

- Paras Kumar
  CISM Advanced Course on Variational Methods for Complex Materials and Processes, coordinated by Prof. Klaus Hackl and Prof. Dorothee Knees. July 17 – 21, 2023. International Centre for Mechanical Sciences (CISM), Udine, Italy.
  8th GAMM Juniors Summer School on Scientific Machine Learning. July 31 – August 4, 2023. Gottfried Wilhelm Leibniz Universität Hannover, Hannover, Germany.

- Lukas Laubert
  BIO ART Kick-off Meeting upon invitation of PD Dr.-Ing. Sebastian Pfaller. July 19 – 22, 2023. Institut de Chimie et des Matériaux Paris-Est, Thiais, France.

- Marie Laurien
  CISM Advanced Course on Peridynamic Models for Material Degradation: from Fracture/Fragmentation to Corrosion; from Models to Computer Codes. October 23 – 26, 2023. International Centre for Mechanical Sciences (CISM), Udine, Italy.

- Michael Lengger
  Tribomechadynamics Research Camp upon invitation of Prof. Dr. Matthew Brake. June 19 – August 1, 2023. Rice University, Houston, Texas, USA.

- Oskar Neumann
  10th Summer School on Biomechanics of Soft Tissues: From the Heart to the Cardiovascular System to the Brain coordinated by Prof. Gerhard A. Holzapfel and Prof. Ray W. Ogden. September 11 – 15, 2023. Graz University of Technology, Graz, Austria.

- Dominic Soldner
  CISM Advanced Course on Batteries - Basic Principles, Experimental Investigations and Modeling Acress Scales. September 25 – 29, 2023. Udine, Italy (attended remotely).

- Yashasvi Verma
  10th Summer School on Biomechanics of Soft Tissues: From the Heart to the Cardiovascular System to the Brain coordinated by Prof. Gerhard A. Holzapfel and Prof. Ray W. Ogden. September 11 – 15, 2023. Graz University of Technology, Graz, Austria.
  Research Stay upon invitation of Prof. Luca Heltai. November 5 – 18, 2023. Scuola Internazionale Superiore di Studi Avanzati - via Bonomea, Trieste, Italy.

- Daniel van Huyssteen
  CISM Advanced Course C2317 on Virtual Elements for Problems in Mechanics. Ocotber 16 – 20, 2023. Udine, Italy (attended remotely).

- Jana Wedel
  Research stay upon invitation of Prof. Dr. Jure Ravnik and Prof. Dr. Matjaž Hriberšek. February 1 – July 31 and September 1 – December 31, 2023. University of Maribor, Maribor, Slovenia.

3.3 Conferences

Organization

- Silvia Budday and Paul Steinmann: Co-organizers jointly with Kristian Franze
  Special Session: Exploring brain mechanics at 18th Internation Symposium on Computer Methods in Biomechanics and Biomedical Engineering (CMBBE). May 3 – 5, 2023. Paris, France.

- Andrea Dakkouri-Baldauf, Maurice Rohracker and Paul Steinmann: Co-Organizers jointly with S. Shegufta
  FRASCAL Minisymposium: Connecting scales and disciplines to model fracture at 7th International Conference on Computational Modelling of Fracture and Failure of Materials and Structures (CFRAC). June 21 – 23, 2023. Prague, Czech Republic.

- Markus Mehnert and Miguel A. Moreno-Mateos: Co-Organizers jointly with M. Rambausek and E. Polukhov
  Minisymposium: Multiphysical Modeling of Complex Material Behavior at 10th GACM Colloquium on Computational Mechanics (GACM 2023). September 10 – 13, 2023. Vienna, Austria.

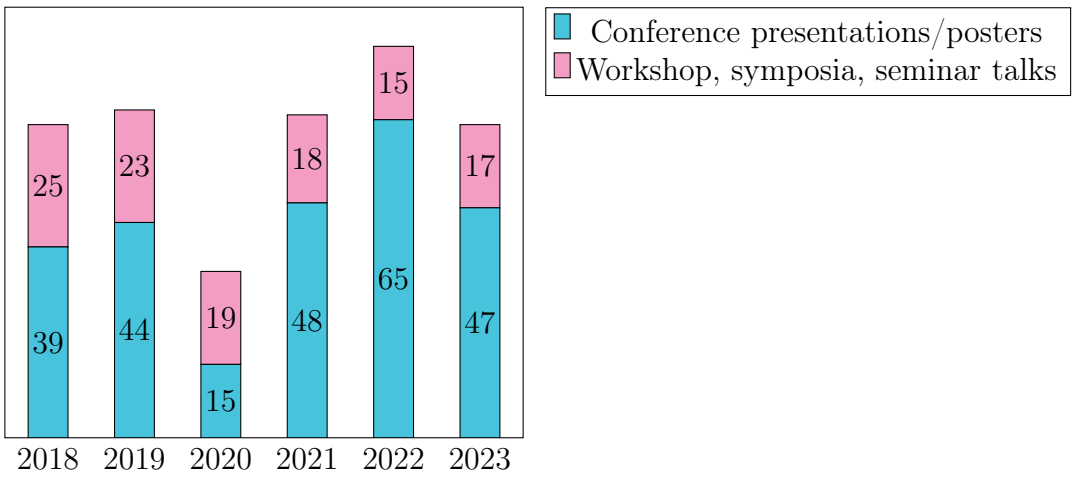
- Sebastian Pfaller and Wuyang Zhao: Co-Organizers jointly with F. Detrez and C. Wick
  Minisymposium: Fracture in Polymers and Polymer Composites at XVII International Conference on Computational Plasticity (COMPLAS 2023). September 5 – 7, 2023. Barcelona, Spain.

- Maximilian Ries and Felix Weber:
  Minisymposium: Computational treatment of polymer fracture across the scales at 7th Young Investigators Conference 2023 (YIC2023). June 19 – 21, 2023. Porto, Portugal.

- Dominic Soldner and Julia Mergheim:
  Minisymposium: Simulating Additive Manufacturing of Polymers - A Multi-Physics and Multi-Scale Challenge (IS11) at Simulation for Additive Manufacturing (SIM-AM 2023). July 25 – 28, 2023. Munich, Germany.

Conference presentations

Statistics of conference contributions and talks 2018–2023



After a significant drop in the number of conference contributions during the pandemic and a subsequent overcompensation of this restricted period, the number of conference contributions went back to a normal level during this year.

8th GAMM Workshop on Phase-field modeling
February 6 – 7, 2023. Zurich, Switzerland.

- Maurice Rohracker, Paras Kumar and Julia Mergheim:
  Comparison of Adaptive Spatial Refinement in Phase-Field Fracture Simulations of Brittle Materials.

Jahrestreffen 2023 GAMM Fachausschuss Computational Biomechanics
February 13 – 14, 2023. Saarbrücken, Germany.

- Emma Griffiths, Jan Hinrichsen, Nina Reiter and Silvia Budday:
  On the importance of using region-dependent material parameters for full- scale human brain simulations.

International Conference on Multiphase Flow (ICMF 2023)
April 2 – 7, 2023. Kobe, Japan.

- Jana Wedel, Paul Steinmann, Matjaž Hriberšek and Jure Ravnik:
  Towards modeling of soft deformable micro particles in dilute multiphase flow.

20th International Conference on Sheet Metal (SHEMET 2023)
April 3 – 5, 2023. Nürnberg, Germany.

- Johannes Friedlein, Julia Mergheim and Paul Steinmann:
  Influence of plastic orthotropy on clinching of sheet metal.

22nd Computational Fluids Conference (IACM–CFC 2023)
April 25 – 28, 2023. Cannes, France.

- Jana Wedel, Paul Steinmann, Matjaž Hriberšek and Jure Ravnik:
  A novel superellipsoid particle collision method.

18th Internation Symposium on Computer Methods in Biomechanics and Biomedical Engineering (CMBBE)
May 3 – 5, 2023. Paris, France.

- Emma Griffiths, Jan Hinrichsen, Nina Rieter and Silvia Budday:
  The Importance of Using Region-dependent Material Parameters for Full-scale Human Brain Simulations.

- Nina Reiter, Sarah Nistler, Katharina Mai, Friedrich Paulsen and Silvia Budday:
  Mechanical characterization of human and porcine brain tissue and human brain organoids.

- Emely Schaller, Ali Javili and Paul Steinmann:
  Poster: *Exploiting open system peridynamics for nonlocal bone remodelling.*

- Mohammad Saeed Zarzor, Ingmar Blümcke and Silvia Budday:
  A physical multifield computational model explains the role of different cell types in cortical folding.

ERCOFTAC Spring Festival 2023
May 11 – 12, 2023. Vienna, Austria.

- Jana Wedel, Paul Steinmann, Matjaž Hriberšek and Jure Ravnik:
  Development of dedicated computational models for modeling large numbers O(10^5) of micron- and submicron-sized (nonspherical) particles in fluiddominated two-phase flows.

93rd Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2023)
May 30 – June 2, 2023. Dresden, Germany.

- Johannes Friedlein, Julia Mergheim and Paul Steinmann:
  Gradient-plasticity vs Gradient-damage – What to choose for the Modelling and Calibration of Ductile Damage?

- Paras Kumar and Julia Mergheim:
  Phase-Field Modeling of Fracture in Polymer Nano-Composites via Graded Interphases.

- Dmytro Pivovarov, Paul Steinmann and Kai Willner:
  Incorporation of the IGA-FEM basis functions into the non-deterministic FEM-framework.

- Nina Reiter, Friedrich Paulsen and Silvia Budday:
  Modeling the finite viscoelasticity of brain tissue based on microstructural information.

- Felix Weber, Christof Bauer, Maximilian Ries, Wuyang Zhao and Sebastian Pfaller:
  Fracture Simulations of Polymers: Coupling Molecular and Continuum Models.

- Mohammad Saeed Zarzor, Ingmar Blümcke and Silvia Budday:
  Multifield computational model predicts the interplay between cellular processes and geometrical instabilities in the developing human brain.

- Mohammad Saeed Zarzor, Paul Steinmann and Silvia Budday:
  Multifield computational model for human brain development: Explicit numerical stabilization.

- Wuyang Zhao and Sebastian Pfaller:
  Multiscale modeling of fracture behavior of glassy polymers across molecular and continuum scales.

International Conference on Computational Methods for Coupled Problems in Science and Engineering (COUPLED PROBLEMS 2023)
June 5 – 7, 2023. Chania, Crete, Greece.

- Chaitanya Dev, Gabriel Stankiewicz and Paul Steinmann:
  Structural Topology and Shape Optimization of Electro-Active Polymers Immersed in Free Space.

- Gabriel Stankiewicz, Chaitanya Dev and Paul Steinmann:
  Advanced Study of the Design of Auxetic Piezoelectric Structures using Structural Optimization.

15th International Conference on Fracture (ICF-15)
June 11 – 16, 2023. Atlanta, Georgia, USA.

- Paras Kumar and Julia Mergheim:
  A Versatile Phase-Field Fracture Model for Polymer Composites: Capturing their Multi-Faceted Fracture Behavior via Graded Interphases.

5th International Conference on Uncertainty Quantification in Computational Sciences and Engineering (UNCECOMP2023)
June 12 – 14, 2023. Athens, Greece.

- Dmytro Pivovarov, Paul Steinmann and Kai Willner:
  Advantages of the (extended) isogeometrical basis for the general non-deterministic spectral FEM framework.

Computational treatment of polymer fracture across the scales at 7th Young Investigators Conference 2023 (YIC2023)
June 19 – 21, 2023. Porto, Portugal.

- Maximilian Ries, Vincent Dötschel, Felix Weber and Sebastian Pfaller:
  A coarse-grained molecular dynamics model to analyze fracture in polymer nanocomposites.

- Felix Weber, Christof Bauer, Maximilian Ries, Wuyang Zhao, and Sebastian Pfaller:
  Fracture in Polymers: Discrete-to-Continuum Coupling.

International Conference on Adaptive Modelling and Simulation (ADMOS)
June 19 – 21, 2023. Gothenburg, Sweden.

- Daniel van Huyssteen, Felipe Lopez Rivarola, Guillermo Etse and Paul Steinmann:
  Adaptive mesh refinement procedures for the virtual element method.

7th International Conference on Computational Modeling of Fracture and Failure of Materials and Structures (CFRAC 2023)
June 21 – 23, 2023. Prague, Czech Republic.

- Johannes Friedlein, Julia Mergheim and Paul Steinmann:
  Gradient-plasticity vs Gradient-damage for the Modelling and Calibration of Ductile Damage.

- Maurice Rohracker, Paras Kumar and Julia Mergheim:
  Comparison of Irreversibility Strategies in Phase-Field Fracture Simulations.

16th International Conference on Advanced Computational Engineering and Experimenting (ACEX)
July 3 – 7, 2023. Heraklion, Crete, Greece

- Gunnar Possart, Maximilian Ries, Eva Richter, Sebastian Pfaller and Paul Steinmann:
  An MD-based iterphase model for PS-silica nanocomposites: Implications and insights for engineering applications.

European Society of Biomechanics (ESBiomech 2023)
July 9 – 12, 2023. Maastricht, The Netherlands.

- Jessica Faber, Jan Hinrichsen, Anahita Ahmadi Soufivand, Hsuan-Heng Lu, Aldo Boccaccini and Silvia Budday:
  Tuning the mechanical properties of alginate dialdehyde-gelatin (ADA-GEL) bioinks for bioprinting approaches by varying the oxidation degree.

- Emma Griffiths, Jan Hinrichsen, Nina Reiter and Silvia Budday:
  Region-dependent material parameters for full-scale human brain simulations.

Simulation for Additive Manufacturing (SIM-AM 2023)
July 25 – 28, 2023. Munich, Germany

- Dominic Soldner, Paul Steinmann and Julia Mergheim:
  Thermo-Mechanical Modeling and Simulation of Powder-Bed based Additive Manufacturing of Polymers.

Tribomechadynamics Conference (TMD)
August 2 – 4, 2023. Houston, Texas, USA.

- Alexandre Spits, Michael Lengger, Matt Allen and Matthew Brake:
  On the use of adaptive chirp mode decomposition for modal coupling.

European Society of Biomaterials (ESB)
September 4 – 8, 2023. Davos, Switzerland.

- Sonja Kuth and Aldo R. Boccaccini:
  Designing a hydrogel for mimicking nervous tissue: development, optimization and application.

XVII International Conference on Computational Plasticity (COMPLAS)
September 5 – 7, 2023. Barcelona, Spain.

- Miguel Angel Moreno-Mateos, Mokarram Hossain, Paul Steinmann and Daniel Garcia-Gonzalez:
  Fracture-Resistant Ultra-Soft Magnetorheological Elastomers.

- Sebastian Pfaller, Maximilian Ries, Eva Richter and Gunnar Possart:
  Interphase Properties of Polymer Nanocomposites and their Role in Material Failure.

- Daniel van Huyssteen, Felipe Lopez Rivarola, Guillermo Etse and Paul Steinmann:
  Adaptive mesh refinement procedures for the virtual element method.

- Wuyang Zhao and Sebastian Pfaller:
  Fracture of glassy thermoplastics based on multiscale simulations across molecular and continuum scales.

10th GACM Colloquium on Computational Mechanics 2023 (GACM)
September 10 – 13, 2023. Vienna, Austria.

- Jan Hinrichsen, Lea Feiler, Nina Reiter, Friedrich Paulsen, Lars Bräuer, Martin Schicht and Silvia Budday:
  Exploring the mechanical landscape of the human brain.

- Jose Lara and Paul Steinmann:
  A gradient crystal plasticity formulation to model intergranular damage in polycrystals.

- Markus Mehnert and Paul Steinmann:
  Numerical modeling of photoelasticity.

- Miguel Angel Moreno-Mateos, Konstantinos Danas, Mokarram Hossain, Paul Steinmann and Daniel Garcia-Gonzalez:
  On the magnetostrictive and fracture behavior of soft magnetorheological elastomers: influence of magnetic boundary conditions.

- Simon Wiesheier, Julia Mergheim and Paul Steinmann:
  Discrete Data-Adaptive Approach to Hyperelasticity.

9th international conference on Discrete Element Methods (DEM9)
September 17 – 21, 2023. Erlangen, Germany.

- Dominic Soldner, Ludwig Herrnböck, Christian Burkhardt, Julia Mergheim and Paul Steinmann:
  Continuum Based Simulation for Additive Manufacturing.

- Jana Wedel, Paul Steinmann, Matjaž Hriberšek and Jure Ravnik:
  A novel superellipsoid particle collision model.

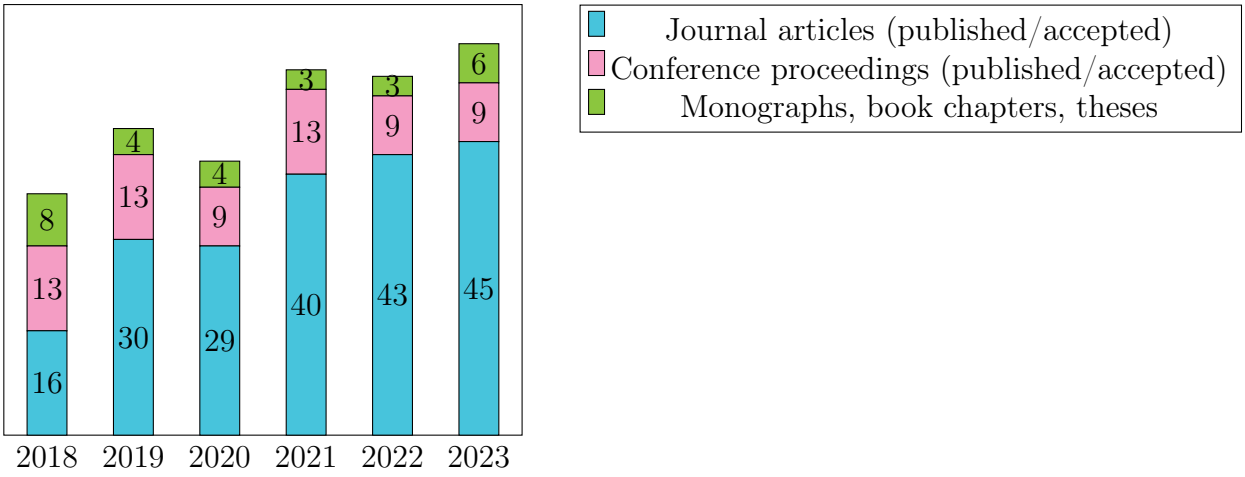
Computational Modeling of Complex Materials across the Scales (CMCS)
October 10 – 13, 2023. Eindhoven, The Netherlands.

- Maximilian Ries, Gunnar Possart, Paul Steinmann and Sebastian Pfaller:
  Poster: *Studying the mechanical performance of polymer nanocomposites with molecular dynamics-informed continuum models.*

- Lucie Spannraft, Julia Mergheim, Fredrik Larsson, Kenneth Runesson and Paul Steinmann:
  Poster: *Mechanics of Generalized Interfaces and Grain Boundaries.*

- Paul Steinmann, Andie de Villiers, Andrew McBride and Ali Javili:
  Towards configurational peridynamics: pas-de-deux of nonlocality and failure.

Statistics of publications 2018–2023



3.4 Journal articles

Published or accepted

[1] A. Ahmadi Soufivand, J. Faber, J. Hinrichsen, and S. Budday. "Multilayer 3D bioprinting and complex mechanical properties of alginate-gelatin mesostructures". *Scientific Reports* 13.1 (2023), p. 11253.

[2] S. Chayanun, A. Ahmadi Soufivand, J. Faber, S. Budday, B. Lohwongwatana, and A. R. Boccaccini. "Reinforcing Tissue-Engineered Cartilage: Nanofibrillated Cellulose Enhances Mechanical Properties of Alginate Dialdehyde–Gelatin Hydrogel". *Advanced Engineering Materials* (2023), p. 2300641.

[3] C. Dev, G. Stankiewicz, and P. Steinmann. "On the influence of free space in topology optimization of electro-active polymers". *Structural and Multidisciplinary Optimization* 66.187 (2023).

[4] V. Dötschel, S. Pfaller, and M. Ries. "Studying the mechanical behavior of a generic thermoplastic by means of a fast coarse-grained molecular dynamics model". *Polymers and Polymer Composites* 31 (2023).

[5] C. Fan, P. Steinmann, and J. Wang. "Modeling the dynamic magneto-mechanical response of magnetic shape memory alloys based on Hamilton's principle: The numerical algorithm". *Journal of the Mechanics and Physics of Solids* 180 (2023), p. 105408.

[6] S. Firooz, A. Javili, and P. Steinmann. "A versatile implicit computational framework for continuum-kinematics-inspired peridynamics". *Computational Mechanics* (2023).

[7] S. Firooz, D. Reddy, V. Zaburdaev, and P. Steinmann. "Mean zero artificial diffusion for stable finite element approximation of convection in cellular aggregate formation". *Computer Methods in Applied Mechanics and Engineering* (2023).

[8] M. Flaschel, H. Yu, N. Reiter, J. Hinrichsen, S. Budday, P. Steinmann, S. Kumar, and L. De Lorenzis. "Automated discovery of interpretable hyperelastic material models for human brain tissue with EUCLID". *Journal of the Mechanics and Physics of Solids* 180 (2023), p. 105404.

[9] J. Friedlein, J. Mergheim, and P. Steinmann. "Efficient gradient enhancements for plasticity with ductile damage in the logarithmic strain space". *European Journal of Mechanics - A/Solids* 99.104946 (2023).

[10] A. Hegendörfer, P. Steinmann, and J. Mergheim. "An implicitly coupled finite element-electronic circuit simulator method for efficient system simulations of piezoelectric energy harvesters". *Journal of Intelligent Material Systems and Structures* (2023), p. 1045389X231157359.

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[12] L. Herrnböck, A. Kumar, and P. Steinmann. "Two-scale off-and online approaches to geometrically exact elastoplastic rods". *Computational Mechanics* 71.1 (2023), pp. 1–24.

[13] J. Hinrichsen, L. Feiler, N. Reiter, L. Bräuer, M. Schicht, F. Paulsen, and S. Budday. "Identifying Composition-Mechanics Relations in Human Brain Tissue Based on Neural-Network-Enhanced Inverse Parameter Identification". *Mathematics and Mechanics of Solids* (2023).

[14] J. Hinrichsen, N. Reiter, L. Bräuer, F. Paulsen, S. Kaessmair, and S. Budday. "Inverse Identification of Region-Specific Hyperelastic Material Parameters for Human Brain Tissue". *Biomechanics and Modeling in Mechanobiology* 22.5 (2023), pp. 1729–1749.

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[16] D. van Huyssteen, F. L. Rivarola, G. Etse, and P. Steinmann. "On adaptive mesh coarsening procedures for the virtual element method for two-dimensional elastic problems". *Computer Methods in Applied Mechanics and Engineering* 418 (2023).

[17] M. P. Kainz, A. Greiner, J. Hinrichsen, G. Sommer, D. Kolb, E. Comellas, P. Steinmann, S. Budday, M. Terzano, and G. A. Holzapfel. "Poro-viscoelastic material parameter identification of brain tissue-mimicking hydrogels". *Frontiers in bioengineering and biotechnology* 11 (2023), p. 1143304.

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[19] M. Laurien, A. Javili, and P. Steinmann. "Peridynamic modeling of nonlocal degrading interfaces in composites". *Forces in Mechanics* (2023), p. 100124.

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[21] Z. Liu, A. McBride, A. Ghosh, L. Heltai, W. Huang, T. Yu, P. Steinmann, and P. Saxena. "Computational instability analysis of inflated hyperelastic thin shells using subdivision surfaces". *Computational Mechanics* (2023), pp. 1–20.

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[24] M. Moreno-Mateos. "A gradient micromechanical model to explore flexoelectric copolymers via stochastic chain growth". *European Journal of Mechanics-A/Solids* 102.1 (2023), p. 105106.

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[28] J. Pallares, A. Fabregat, A. Lavrinenko, H. B. Norshamsudin, G. J. G., D. Fletcher, K. Inthavong, M. Zasimova, V. Ris, N. Ivanov, R. Castilla, P. Gamez-Montero, G. Raush, H. Calmet, D. Mira, J. Wedel, M. Štrakl, J. Ravnik, D. Fontes, F. D. Souza, C. Marchioli, and S. Cito. "Numerical simulations of the flow and aerosol dispersion in a violent expiratory event: Outcomes of the 2022 International Computational Fluid Dynamics Challenge on violent expiratory event". *Physics of Fluids* 35.4 (2023), p. 045106.

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[30] N. Reiter, F. Paulsen, and S. Budday. "Mechanisms of mechanical load transfer through brain tissue". *Scientific Reports* 13 (2023).

[31] M. Ries, C. Bauer, F. Weber, P. Steinmann, and S. Pfaller. "Characterization of the material behavior and identification of effective elastic moduli based on molecular dynamics simulations of coarse-grained silica". *Mathematics and Mechanics of Solids* 28.5 (2023), pp. 1216–1231.

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[33] M. Rohracker, P. Kumar, and J. Mergheim. "A comparative assessment of different adaptive spatial refinement strategies in phase-field fracture models for brittle fracture". *Forces in Mechanics* 10 (2023), p. 100157.

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[37] P. Steinmann, A. M. de Villiers, A. T. McBride, and A. Javili. "Configurational peridynamics". *Mechanics of materials* 185 (2023), p. 104751.

[38] A. Titlbach, A. Papastavrou, A. McBride, and P. Steinmann. "A novel micromorphic approach captures non-locality in continuum bone remodelling". *Computer Methods in Biomechanics and Biomedical Engineering* (2023), pp. 1–14.

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[42] S. Wiesheier, J. Mergheim, and P. Steinmann. "Discrete data-adaptive approximation of hyperelastic energy functions". *Computer Methods in Applied Mechanics and Engineering* 416.1 (2023), pp. 116–366.

[43] M. Zarzor, I. Blümcke, and S. Budday. "Exploring the role of the outer subventricular zone during cortical folding through a physics-based model". *eLife* 12.e82925 (2023).

[44] L. Zhan, S. Wang, S. Qu, P. Steinmann, and R. Xiao. "A general continuum damage model for soft composites". *Journal of the Mechanics and Physics of Solids* 175 (2023), p. 105290.

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Under review

[1] Ö. Akar and K. Willner. "The Modal Behaviour of a Violin Corpus".

[2] E. Griffiths, J. Jayamohan, and S. Budday. "A comparison of brain retraction mechanisms using finite element analysis and the effects of regionally heterogeneous material properties".

[3] J. Hinrichsen, C. Ferlay, N. Reiter, and S. Budday. "Using Dropout Based Active Learning and Surrogate Models in the Inverse Viscoelastic Parameter Identification of Human Brain Tissue".

[4] D. van Huyssteen, F. L. Rivarola, G. Etse, and P. Steinmann. "On mesh refinement procedures for polygonal virtual elements".

[5] M. Laurien, A. Javili, and P. Steinmann. "Nonlocal interfaces accounting for progressive damage within continuum-kinematics-inspired peridynamics".

[6] M. Moreno-Mateos, M. Mehnert, and P. Steinmann. "Electro-mechanical actuation modulates fracture performance of soft dielectric elastomers".

[7] M. Moreno-Mateos and P. Steinmann. "Configurational force method enables fracture assessment in soft materials".

[8] T. Oberleiter and K. Willner. “Percentage comparison of fuzzy numbers using a newly presented method”.

[9] F. L. Rivarola, G. Chacón, D. van Huyssteen, P. Steinmann, and G. Etse. “Mesh refinement ergodicity in concrete fracture: a combined VEM-Interfaces Elements approach”.

[10] G. Stankiewicz, C. Dev, M. Weichelt, T. Fey, and P. Steinmann. “Towards advanced piezoelectric metamaterial design via combined topology and shape optimization”.

[11] R. Yamamoto, M. Schwarz, J. Mergheim, and K. Kakimoto. “Multisource energy harvesting using (Ba,Ca)(Zr,Ti)O_3 oscillating under temperature gradient”.

[12] W. Zhao, R. Xiao, P. Steinmann, and S. Pfaller. “Time-temperature correlations of amorphous thermoplastics at large strains based on molecular dynamics simulations”.

In preparation

[1] S. Kuth and A. Boccaccini. “Enzymatic in-situ crosslinking can improve hydrogel stability while maintaining matrix stiffness”.

[2] D. Pivovarov, K. Willner, and P. Steinmann. “The extended IsoGeometrical bases for non-deterministic spectral FEM”.

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

[4] D. Soldner, S. Cholewa, D. Drummer, P. Steinmann, and J. Mergheim. “Thermo-Mechanical characterization of polyamide 12 for selective laser sintering process simulation”.

[5] F. Weber, V. Dötschel, P. Steinmann, S. Pfaller, and M. Ries. “Evaluating the impact of filler size and filler content on the stiffness, strength, and toughness of polymer nanocomposites using coarse-grained molecular dynamics”.

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

[7] W. Zhao, P. Steinmann, and S. Pfaller. “A visco-hyperelastic-viscoplastic constitutive model for glassy polymers accounting for rate- and temperature-dependent strain hardening behavior”.

3.5 Conference proceedings articles

Published

[1] C. Bielak, M. Böhnke, J. Friedlein, M. Bobbert, J. Mergheim, P. Steinmann, and G. Meschut. “Numerical analysis of failure modeling in clinching process chain simulation”. In: *20th International Conference on Sheet Metal (SHEMET 2023)*. Vol. 25. Materials Research Forum LLC, 2023, pp. 263–270.

[2] M. Böhnke, C. Bielak, J. Friedlein, M. Bobbert, J. Mergheim, G. Meschut, and P. Steinmann. “A calibration method for failure modeling in clinching process simulations”. In: *20th International Conference on Sheet Metal (SHEMET 2023)*. Vol. 25. Materials Research Forum LLC, 2023, pp. 271–278.

[3] J. Friedlein, C. Bielak, M. Böhnke, M. Bobbert, G. Meschut, J. Mergheim, and P. Steinmann. "Influence of plastic orthotropy on clinching of sheet metal". In: *20th International Conference on Sheet Metal (SHEMET 2023)*. Materials Research Forum LLC, 2023.

[4] D. T. Huamani, W. Zhao, and S. Pfaller. "A particle-continuum coupling method for amorphous polymers with multiple particle-based domains". In: *Proceedings in Applied Mathematics and Mechanics*. Ed. by C. Böhm, K. Mang, B. Markert, S. Reese, M. Schmidtchen, J. Waimann, and M. Kaliske. Wiley, 2023.

[5] P. Kumar and J. Mergheim. "Computational modeling of fracture in polymer nanocomposites undergoing large deformations via the graded-interphase-enhanced phase-field fracture approach". In: *Proceedings in Applied Mathematics & Mechanics*. Wiley-VCH GmbH, 2023, e202300247.

[6] T. Oberleiter and K. Willner. "Approaches for optimizing surrogate models considering uncertain parameters". In: *Proceedings in Applied Mathematics and Mechanics*. Ed. by M. Kaliske. Wiley GmbH, 2023.

[7] T. Okada, M. Isobe, T. Kosaka, P. Steinmann, H. Matsumori, and N. Matsui. "Study on Electric Motor Vibration Suppression by Active Dynamic Vibration Absorber". In: *IEEE International Electric Machines and Drives Conference*. 2023.

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[9] M. Zarzor, P. Steinmann, and S. Budday. "Multifield computational model for human brain development: Explicit numerical stabilization". In: *Proceedings in Applied Mathematics and Mechanics*. Wiley Online Library, 2023, e202300288.

Under review

[1] D. Pivovarov, P. Steinmann, and K. Willner. "A hybrid fuzzy-stochastic finite element method for polymorphic microstructural uncertainties in heterogeneous materials". In: *LECTURE NOTES IN APPLIED AND COMPUTATIONAL MECHANICS*.

3.6 Workshops, symposia, and seminars

Workshops

[1] Ö. Akar and K. Willner. *Modal Analysis of a Violin*. Presentation, European Modal Analysis Users Group Meeting (EMAUG), Zuffenhausen, Germany. Sept. 2023.

[2] S. Budday. *Biomechanical modeling of the human brain*. Presentation, Workshop on Biophysics-based modeling and data assimilation in medical imaging, Berlin, Germany. Aug. 2023.

[3] M. Mehnert and P. Steinmann. *Experimental and Numerical Investigation of the Thermo-Electro-Mechanical Behavior of Dielectric Elastomers*. CISM Course on "Nonlinear Electro- and Magneto-Mechanics: Theory, Computations, and Experiments". June 2023.

[4] N. Reiter. *Human Brain Mechanics in Health and Disease*. Presentation, GAMM Juniors Fall Meeting, Zurich, Switzerland. Oct. 2023.

[5] M. Ries and S. Pfaller. *Generating scientific diagrams with pgfplots*. Frascal Special Seminar. May 2023.

Seminars

[1] J. Faber, F. Hofmann, T. Jüngst, and S. Budday. *Biofabricated gradients for functional tissue models*. Presentation, SFB/TRR 225 Retreat, Lichtenfels, Germany. Mar. 2023.

[2] D. van Huyssteen, F. L. Rivarola, G. Etse, and P. Steinmann. *Mesh refinement ergodicity in concrete fracture: a combined virtual and interface element approach*. Poster, FRASCAL: 3rd RTG Retreat, Kloster Banz, Bad Staffelstein, Germany. Nov. 2023.

[3] P. Kumar. *Microscale Modeling of Fracture Processes in Elastomeric Nano-Composites*. Poster, FRASCAL: 3rd RTG Retreat, Kloster Banz, Bad Staffelstein, Germany. Nov. 2023.

[4] M. Laurien, A. Javili, and P. Steinmann. *Peridynamic Fracture Mechanics*. Presentation, FRASCAL: 3rd RTG Retreat, Kloster Banz, Bad Staffelstein. Nov. 2023.

[5] M. Moreno-Mateos and P. Steinmann. *Soft Fracture: Electro-Magnetical Modulation & Configurational Mechanics*. Presentation, FRASCAL: 3rd RTG Retreat, Kloster Banz, Bad Staffelstein, Germany. Nov. 2023.

[6] M. Rohracker and J. Mergheim. *Comparative assessment of adaptive spatial refinement in 3D phase-field fracture simulations*. Presentation, FRASCAL: 8th RTG Seminar, Erlangen, Germany. Apr. 2023.

[7] D. Soldner, P. Steinmann, and J. Mergheim. *Simulation of Additive Manufacturing Processes of Polymers*. Guest Lecture at TU Munich upon invitation of Prof. Katrin Wudy for the Course: Additive Manufacturing with Plastics, Munich, Germany. Jan. 2023.

[8] L. Spannraft, J. Mergheim, F. Larsson, K. Runesson, and P. Steinmann. *Mechanics of Generalized Interfaces and Grain Boundaries*. Poster, FRASCAL: 3rd RTG Retreat, Kloster Banz, Bad Staffelstein, Germany. Nov. 2023.

[9] L. Spannraft, G. Possart, P. Steinmann, and J. Mergheim. *Generalized interfaces to model structural and soft adhesives and their failure*. Presentation, FRASCAL: 8th RTG Seminar, Erlangen, Germany. Apr. 2023.

[10] P. Steinmann, A. M. de Villiers, A. T. McBride, and A. Javili. *Configurational Peridynamics: The What, Why and How?* Presentation, GCEC Seminar, Glasgow, UK. Feb. 2023.

[11] F. Weber, M. Vassaux, and S. Pfaller. *Multiscale Fracture Simulations of Silica Glass*. Presentation, FRASCAL: 3rd RTG Retreat, Kloster Banz, Bad Staffelstein, Germany. Nov. 2023.

[12] F. Weber, C. R. Wick, A.-S. Smith, and S. Pfaller. *Coarse-Grained Molecular Dynamics Simulations of Polystyrene: Considering Bond Scission*. Presentation, FRASCAL: 8th RTG Seminar, Erlangen, Germany. Apr. 2023.

3.7 Monographs and book chapters

Abschlussbuch SFB814 - Additive Fertigung
Editors: D. Drummer et al.
Springer, tbp.

- C. Burkhardt, D. Soldner, J. Mergheim, P. Steinmann:
  Macroscopic Modelling, Simulation and Optimisation.

Abschlussbericht DFG-Forschungsgruppe FOR 2271, 2. Phase. Prozessorientiertes Toleranzmanagement mit virtuellen Absicherungsmethoden
Editors: S. Wartzack
FAU University Press, 2023.

- T.Oberleiter, K.Willner:
  Teilprojekt 2: Fuzzy-arithmetische Modellierung von Prozessen mit unsicheren Parametern

3.8 Doctoral and habilitation theses

- A. Hegendörfer:
  System Simulations of Piezoelectric Energy Harvesters with the Finite Element Method. Submitted Dissertation. Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 2023.

- L. Herrnböck:
  Numerische Methoden zur Modellierung elastoplatischer Balken und ihre Anwendung auf periodische Gitterstrukturen. Dissertation. Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 2023.

- T. Hiller:
  Schwingungsverhalten von Abgasanlagen mit Entkoppelelementen. Dissertation. Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 2023.

- P. Kumar:
  Enhanced Computational Homogenization and Phase-Field Fracture Approaches for Polymer Nano-Composites. Submitted Dissertation. Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 2023.

- M. Ries:
  Characterization and modeling of polymer nanocomposites across the scales - A comprehensive approach covering the mechanical behavior of matrix, filler, and interphase. Dissertation. Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 2023.

- W. Zhao:
  Multiscale modeling of fracture behavior of glassy polymers across the atomistica nd continuum scale. Dissertation. Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 2023.

4 Ongoing research projects

The following pages allow a short overview on the various ongoing research projects pursued at the Institute of Applied Mechanics and the Institute of Continuum Mechanics and Biomechanics during 2023. These are mainly financed by third-party funding of various (public and industrial) funding sources and are in addition supported by the core support of the university. We have a nice mix of continuations of previous projects with projects that started afresh in 2023.
Also the complementing expertise – as displayed in the five working groups for continuum mechanics, structural mechanics, computational mechanics, multi-scale simulation 'Capriccio' and the Emmy-Noether Group 'BRAIn mechaNIcs ACross Scales' established at the Institute of Applied Mechanics and the Institute of Continuum Mechanics and Biomechanics – is reflected by the variety of research that is performed. This spans from atomistic approaches to material modeling, from experimental investigations to computational challenges and from frictional contact to structural problems. Certainly, the research on these topics constantly produces new insights, thus the following reports can only shed a spot-light on the current state of affairs.

– Biomechanics –

Mechanical characterization, modeling, and simulation to advance 3D bioprinting

Anahita Ahmadi Soufivand, Silvia Budday

3D bioprinting as an additive manufacturing technology has been widely used in tissue engineering and enables fabricating geometrically complicated tissue and organ replacements. Besides the great potential of this technology for regenerative medicine, there are many challenges to overcome. For example, the replacement must bear the mechanical loadings of the tissue and organ under physiological conditions. For tuning the mechanical properties of the printed construct, computational simulations can help through prediction before any fabrication.

Initially, we quantified the mechanical properties of alginate/gelatin hydrogels as a matrix material through an inverse FEM and experimental data of cyclic compression-tension. Then, we predicted the mechanical properties of different hydrogel mesostructures fabricated through various print patterns. Finally, we validated our results through corresponding experiments. Figure 1(A) illustrates that the fabrication process significantly affects the material properties and parameters of the one-term Ogden model. Figure 1(B) shows that we can predict the mechanical properties of different mesostructures using porous sample material parameters, especially under compression loading. The presented methodology can be extended for cell bioprinting applications and can help save time, material, and cost for biofabrication applications.

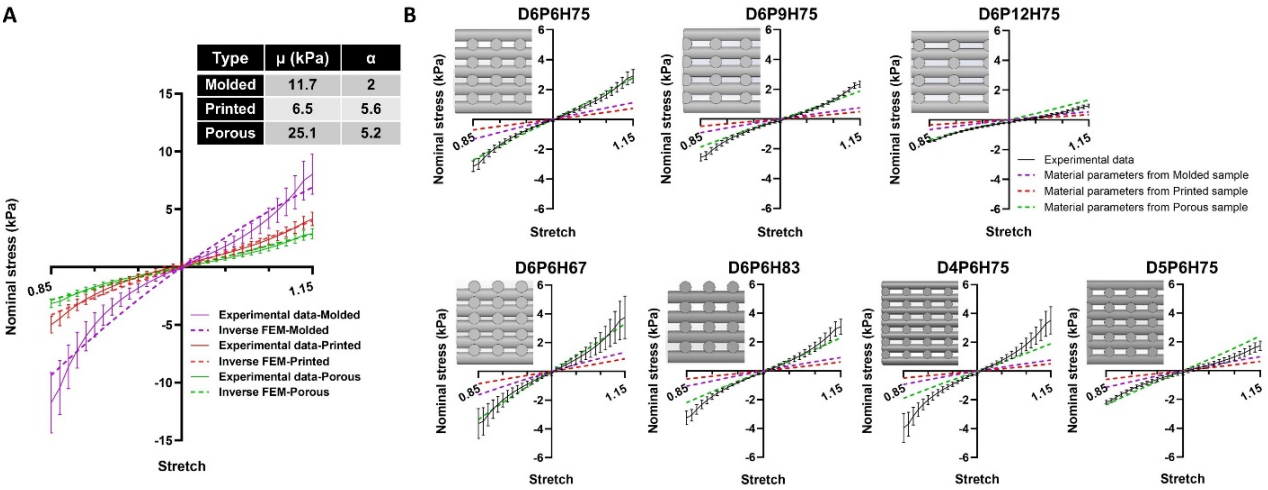

Figure 1: Predicting the hyperelastic properties of alginate-gelatin hydrogels and 3D bioprinted mesostructures. A) Comparison of experimental data and one-term Ogden finite element model predictions for molded, printed, and porous samples. B) Comparison of nominal stresses during compression-tension loadings from experiments with predictions from finite element (FE) simulations using material parameters determined from molded, printed, and porous samples.

Inverse identification of oxidation-specific material parameters for ADA-GEL hydrogels

Jessica Faber, Jan Hinrichsen, Anahita Ahmadi Soufivand, Silvia Budday

Alginate dialdehyde-gelatin (ADA-GEL) hydrogels with tailored biological and mechanical properties depending on the oxidation degree (OD) of ADA are promising bioinks for extrusion-based 3D bioprinting approaches and tissue engineering applications. While the biological properties of ADA-GEL have been intensively investigated, knowledge about the multi-modal mechanical properties remains limited. Therefore, we establish an inverse parameter identification scheme [1] using hyperelastic Ogden models and experimental data from multi-modal large-strain mechanical testing of ADA-GEL hydrogels. Considering the conditioned response in compression and tension simultaneously, we calibrate the modified modified one-term and two-term Ogden models and inversely identify corresponding hyperelastic material parameters of ADA-GEL hydrogels with varying OD. Figure 1 shows the performance of the hyperelastic modified one-term Ogden (left) and two-term Ogden model (right) to represent the conditioned ADA-GEL response of molded and 3D printed samples with 6 % and 25 % OD during compression and tension, simultaneously. It is clearly visible that the modified one-term Ogden with one nonlinearity parameter α is sufficient to capture ultrasoft ADA-GEL hydrogels (25 % OD) including their compression-tension asymmetry well. Nevertheless, only the two-term Ogden model with two nonlinearity parameters α_1 and α_2 can resemble the compression-tension asymmetry, as well as the distinct nonlinear, S-shaped response in compression and tension of molded and 3D printed ADA-GEL hydrogels with 6 % OD. These findings highlight the importance of precise computational models for a predictive understanding of hydrogels to further optimize them and 3D printing parameters in the future.

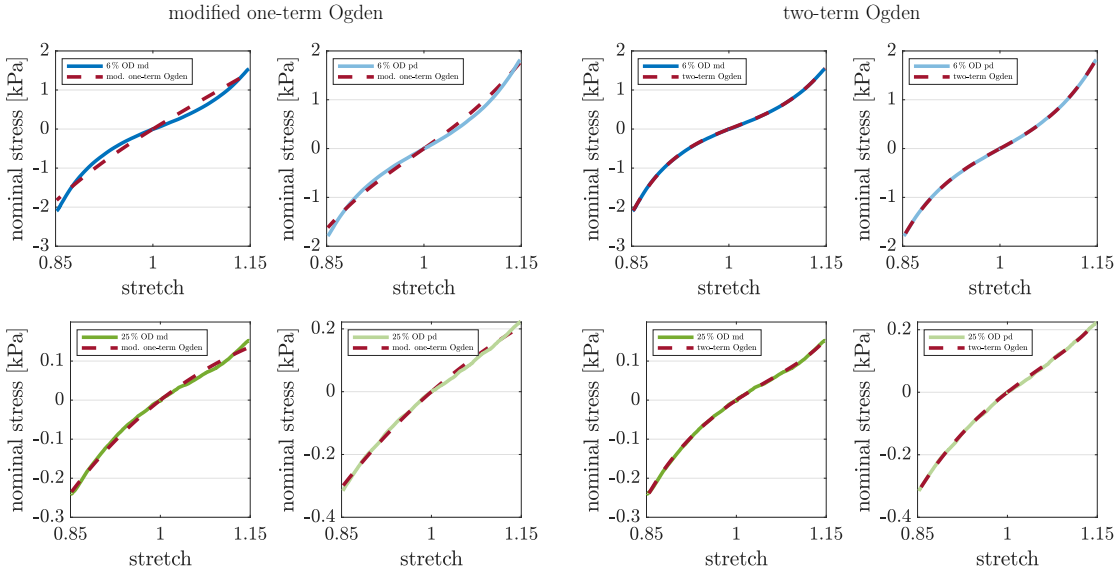

Figure 1: Performance of the modified one-term and two-term Ogden model to capture the mechanical response in compression and tension of molded (md) and 3D printed (pd) ADA-GEL hydrogels with 6 % and 25 % OD, simultaneously.

References

[1] J.Hinrichsen, N. Reiter, L. Bräuer, F. Paulsen, S. Käßmair, and S. Budday. "Inverse identification of region-specific hyperelastic material parameters for human brain tissue". *Biomechanics and Modeling in Mechanobiology* 22 (2023), pp. 1729–1749.

Mean zero artificial diffusion for stable finite element approximation of convection dominated problems

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[2] Department of Biology, FAU

Convection-diffusion problems mainly describe the distribution or transfer of a physical quantity inside a physical system. Examples of such physical quantities include temperature, enthalpy, chemical or biological species and turbulence parameters. In this project (EBM C01), the quantity of interest is the cellular species whose aggregate formation is investigated. Such an analysis can be further extended to represent tumor growth in human brain. In convection-diffusion problems, it is well-known that instabilities in finite element discretization may occur in the form of physically unrealistic and oscillatory solutions In this project, we developed a novel mean zero artificial diffusion method which not only circumvents the instabilities, but also does not require any higher-order elements [1]. Via introducing a new variable to represent the cell number density gradient, the mass conservation equation is enhanced by a diffusion term which is enforced to be zero on average. Figures 1 and 2 render the evolution of the cell number density and the velocity (x, y, z components) in a convection dominated biological problem. As mentioned before, classical coupled-field FE with equal order approximations lead to unstable oscillatory solutions whereas our developed mean-zero artificial diffusion scheme yield stable smooth solutions. Our proposed framework proves to be computationally more robust when compared to a mixed-order finite element method.

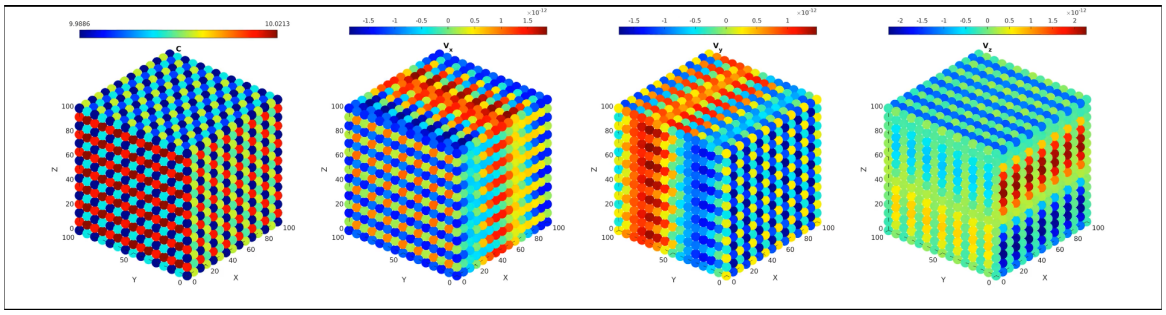

Figure 1: Unstable solution obtained by classical coupled-field FEM..

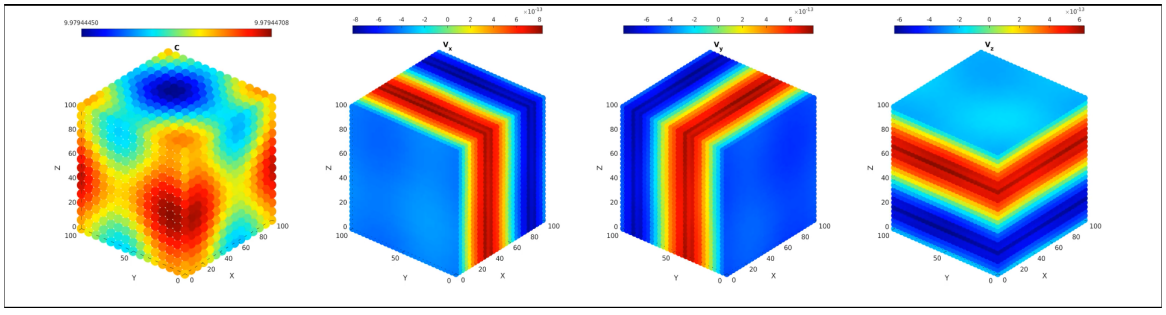

Figure 2: Stable solution using mean-zero artificial diffusion method..

References

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Modeling the porous properties of brain tissue

Alexander Greiner[1], Ester Comellas[3], Paul Steinmann[2], Silvia Budday[1]

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The porous properties of brain tissue remain poorly understood and their investigation requires profound experimental setups and modeling approaches. We identified a strong coupling between the volumetric response of the solid and the porous effects in our nonlinear poro-viscoelastic model [1], thus, making material parameter identification even more challenging. The solid volumetric Kirchhoff stress $\boldsymbol{\tau}_{\mathrm{E}}^{\mathrm{vol}} = \lambda^*[1-n_{0\mathrm{S}}^{\mathrm{S}}]^2[J_{\mathrm{S}}/[1-n_{0\mathrm{S}}^{\mathrm{S}}] - J_{\mathrm{S}}/[J_{\mathrm{S}}-n_{0\mathrm{S}}^{\mathrm{S}}]]\mathbf{1}$ depends on the initial solid volume fraction $n_{0\mathrm{S}}^{\mathrm{S}}$, the Jacobian J_{S} of the biphasic material and the first Lamé parameter λ^*. As indicated in Figure 1, left, low values of λ^* lead to a gradual increase of the volumetric stress response towards the compaction point, i.e., when all fluid has left the tissue. In contrast, high values of λ^* lead to an immediate, strong volumetric response – even for small volumetric changes, i.e., $J_{\mathrm{S}} \approx 1$. Therefore, the overall biphasic tissue response is highly sensitive to the choice of λ^*. In fact, high values of λ^* obliterate the porous effects such that our biphasic model acts like an incompressible solid model.
Figure 1 shows compression relaxation and cyclic loading simulations using a poroelastic one-term Ogden model for different choices of λ^* and the intrinsic permeability K_0. For $\lambda^* = 10^2$, the permeability clearly affects the overall material response and we observe porous relaxation as well as hysteresis. For $\lambda^* = 10^5$, we observe a hyperelastic response independent of the permeability. Our results highlight that both λ^* and the permeability need to be chosen very carefully when modeling brain tissue behavior, and new experimental insights are needed.

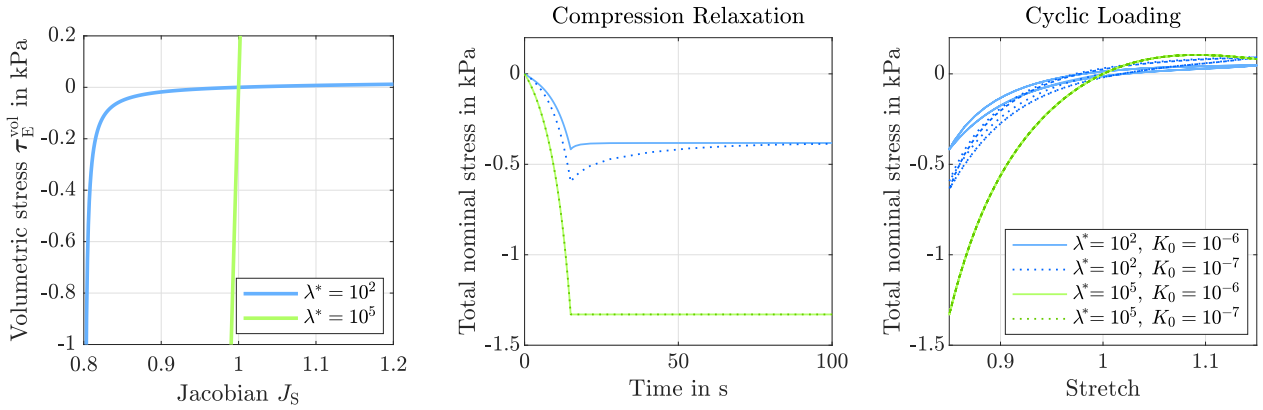

Figure 1: Evolution of the solid volumetric stress $\boldsymbol{\tau}_{\mathrm{E}}^{\mathrm{vol}}$ over the Jacobian J_{S} of the biphasic material for an initial solid volume fraction $n_{0\mathrm{S}}^{\mathrm{S}} = 0.8$ (left). Poroelastic compression relaxation (middle) and cyclic loading (right) using a one-term Ogden model with $\alpha = -12.76$ and $\mu = -43.84$ for the human brain cortex [2]. Results for $\lambda^* = 10^2$ (blue) and $\lambda^* = 10^5$ (green) and two intrinsic permeabilities $K_0 = 10^{-6}$ (solid) and $K_0 = 10^{-7}$ (dotted).

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[1] E. Comellas, S. Budday, J.-P. Pelteret, G. A. Holzapfel, and P. Steinmann. "Modeling the porous and viscous responses of human brain tissue behavior". *Computer Methods in Applied Mechanics and Engineering* 369 (2020), p. 113128.

[2] J. Hinrichsen, N. Reiter, L. Bräuer, F. Paulsen, S. Kaessmair, and S. Budday. "Inverse identification of region-specific hyperelastic material parameters for human brain tissue". *BioRxiv* (2022), pp. 2022–12.

Full-scale brain modeling and simulation

Emma Griffiths, Silvia Budday

Brain retraction is often necessary during neurosurgery in order to access hard to reach deep areas of the brain. Secondary damage, which refers to surrounding tissue damage that was not initially accounted for, is often an unfortunate result. Traditionally spatulas are used for brain retraction but recently tubular retractors (with circular or elliptical cross sections) were introduced as a safer alternative.

This year we used our three dimensional full scale brain model accounting for region-dependent properties to investigate the effects of different surgical instruments used in the retraction of healthy tissue [2].
Due to high variability in testing conditions, clinical comparisons between these devices is difficult. On the other hand, finite element (FE) simulations provide a means to negate these variabilities and even probed them whilst ensuring that there is no risk to harm the patient. We, thus, compared three different retraction mechanisms and compared their simulated effects on the surrounding cortical and subcortical structures. Based on our simulations, we found that traditional spatulas cause higher predicted stresses in the brain in several different locations. We believe that further work into into this direction will be greatly beneficial in understanding and improving the surgical procedures.

Additionally we studied the importance of a heterogeneous brain model by investigating regionally specific viscoelastic parameters. Using the parameters of Budday et al. [1], we found that both region-dependent hyperelastic and viscoelastic parameters should be used especially when modelling the inner structures of the brain such as the corpus callosum.

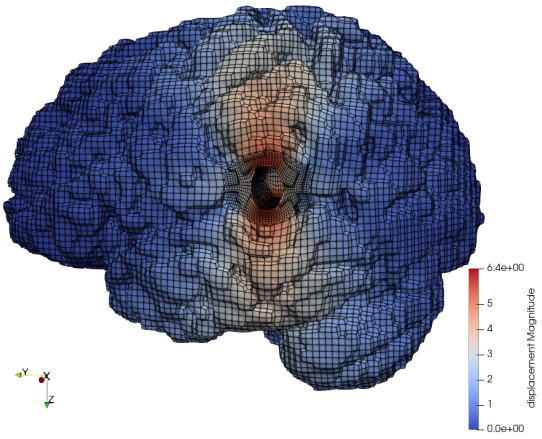

Figure 1: Simulated brain retraction.

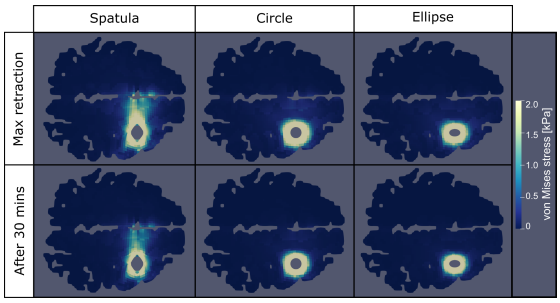

Figure 2: Simulated von Mises stress for a slice of the brain 2cm below the surface of retraction for each retraction mechanism. Showing elevated stresses using a traditional spatula.

References

[1] S. Budday, G. Sommer, J. Haybaeck, P. Steinmann, G. Holzapfel, and E. Kuhl. "Rheological characterization of human brain tissue". *Acta Biomaterialia* 60 (2017), pp. 315–329. ISSN: 1742-7061.

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Inverse mechanical characterization of human brain tissue

Jan Hinrichsen[1], Carl Ferlay [3], Lea Feiler [1], Nina Reiter[1], Lars Bräuer[2], Friedrich Paulsen[2], Silvia Budday[1]

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[2] Institute of Functional and Clinical Anatomy, FAU,
[3]Ecole polytechnique, 91128 Palaiseau, France

The human brain is arguably the most complex organ in the human body with its mechanical behavior still not being fully understood. We have combined inverse parameter identification with the results of enzyme-linked immunosorbent assays (ELISA) that quantify specific tissue components. We have found strong correlations between hyperelastic parameters and levels of Iba1, collagen IV, collage VI, and GFAP (see Figure 2) [1]. Furthermore, we have investigated how we can accelerate the computationally demanding inverse parameter identification [2]. To this end, we have incorporated recurrent neural networks as surrogate models for viscoelastic finite element simulations. However, it is still necessary to run simulations in order to produce pairs of in- and output data that are curcial for the training of these data-driven models. Therefore, we have implemented a Monte-Carlo dropout-based active learning approach that seeks to select the next best point in the parameter space during training. Our hybrid approach incorporates the surrogate model for parameter identification and effortlessly transitions into a higher precision finite element model. This results in dependable accuracy and computational economy. Figure 1 shows the final viscoelastic model output for experimental data from the human frontal cortex.

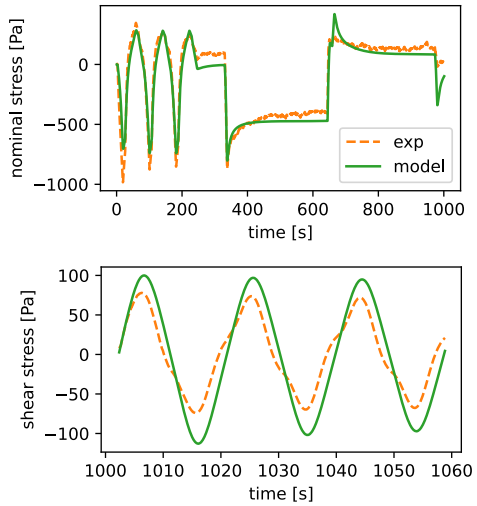

Figure 1: Final model output for the viscoelastic characterization for experimental data from the human frontal cortex.

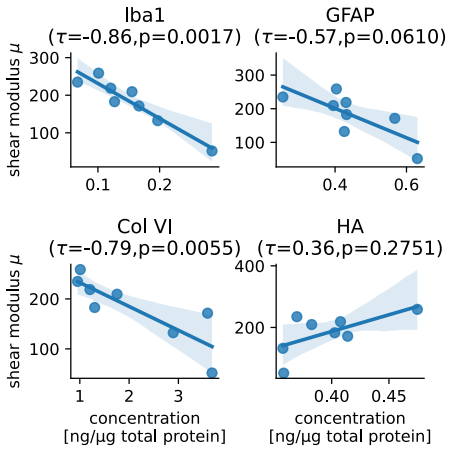

Figure 2: Correlation of the shear modulus μ from fitting the one-term Ogden model and component concentrations.

References

[1] J. Hinrichsen, L. Feiler, N. Reiter, L. Bräuer, M. Schicht, F. Paulsen, and S. Budday. "Identifying Composition-Mechanics Relations in Human Brain Tissue Based on Neural-Network-Enhanced Inverse Parameter Identification". *Mathematics and Mechanics of Solids* (2023).

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Modeling the Viscoelasticity of Human Spinal Cord Tissues During Indentation Loading

Stephen Melly[1], Oskar Neumann[2], Silvia Budday[2], Paul Steinmann[1]

[1] Institute of Applied Mechanics, FAU

[2] Institute of Continuum Mechanics and Biomechanics, FAU

A pivotal component of research within the field of biomechanics aims at formulating accurate mathematical models to describe the complex mechanical characteristics of biological tissues. To model the viscoelastic properties of the human spinal cord, we conducted nanoindentation tests on specimens extracted from the cervical region with average dimensions, $D = 12\,mm$ and $H = 5\,mm$ with loading speeds spanning from $1.25\,\mu m/s$ to $5.0\,\mu m/s$, using a spherical indenter with $r = 250\,\mu m$.

The specifics of the computational model are obtained from the reference [1], in which isotropic material response is assumed for both elastic and viscoelastic behavior. The equilibrium and non-equilibrium components of the model are represented by the modified one-term Ogden model in terms of total and isochoric principal stretches, respectively. Material parameters were obtained through an inverse scheme developed by [2], in which a Python optimization routine is coupled with finite element simulation in deal.ii. As illustrated in Fig. 1 (a), we observed a strong alignment between our simulation and experimental results. Examination of relative errors, depicted in Fig. 1 (c) revealed the need for improvements in the low indentation depth region. Nevertheless, the average relative errors displayed in Fig. 1 (d) hover around approximately 10%, a generally acceptable level. With the optimized parameters, the model should be able to predict the behavior under different loading scenarios including at high loading speeds, as depicted in Fig. 1 (b).

In summary, the model performs satisfactorily, especially in light of the experimental uncertainties and substantial computational costs. Our next step involves developing an axisymmetric formulation, which promises a significant reduction in computational costs.

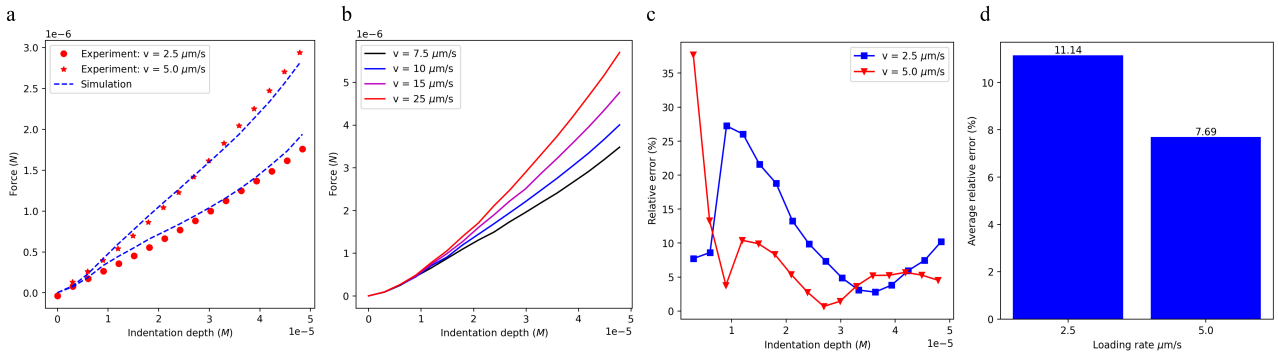

Figure 1: (*a*) Comparison between simulation and experimental load-depth data, (*b*) prediction for high loading speed behavior, (*c*) graphical depiction of relative errors at every indentation depth point for the two loading speeds, and (*d*) average relative errors for each loading speed.

References

[1] S. Budday, G. Sommer, J. Haybaeck, P. Steinmann, G. Holzapfel, and E. Kuhl. "Rheological characterization of human brain tissue". *Acta Biomaterialia* 60 (2017), pp. 315–329.

[2] J. Hinrichsen, N. Reiter, L. Bräuer, F. Paulsen, S. Kaessmair, and S. Budday. "Inverse identification of region-specific hyperelastic material parameters for human brain tissue". *Biomechanics and Modeling in Mechanobiology* 22 (2023), pp. 1729–1749.

Mechanical testing of human spinal cord tissue

Oskar Neumann, Paul Steinmann, Silvia Budday

The mechanical properties of the human spinal cord and possible correlations with microstructural characteristics remain insufficiently understood. To fill this knowledge gap and open up potential application areas at the interface between engineering and medical technology, we have performed spherical indentation testing on 31 specimens taken from the cervical, thoracic, and sagittal segments of the human spinal cord, obtained from three different donors. In addition, a rheometer was used to test the mechanical response of spinal cord tissue under compression-tension and torsional shear. These tests were performed on a subset of ten samples that had previously been tested by indentation. A comprehensive experimental setup was developed for conducting nanoindentation on spinal cord tissue. This setup includes the general procedure of preparing and conducting the experiments as well as the digital documentation. A strategic framework was conceptualized for the development of a protocol specifically tailored for human spinal cord tissue indentation experiments. Initial efforts were made to explore the potential influence of the sequence of applied loading rates. In addition, a suitable post-processing software was developed to fulfil two key functions: localization of indentation points in grey and white matter and filtering, smoothing, and segmenting the recorded force indentation paths. The preliminary evaluations show that the Chiaro Nanoindenter, our chosen instrument, appears to be well-suited for gaining valuable insights into the mechanical properties of spinal cord tissue. Based on currently available experimental data from indentation tests, it is suggested that spinal cord grey matter exhibits greater stiffness compared to white matter.

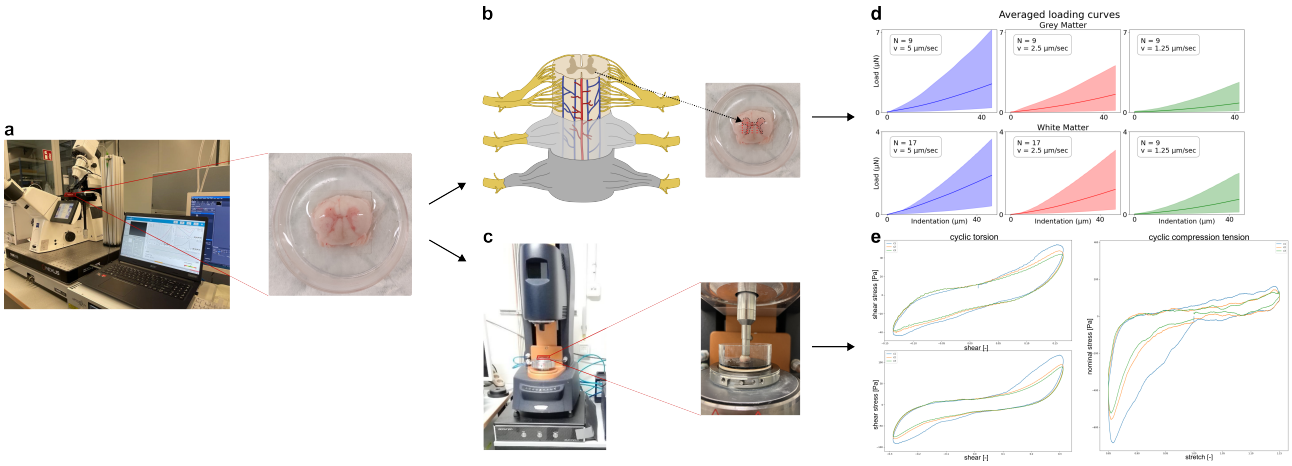

Figure 1: Experimental protocol for the characterisation of the mechanical properties of human spinal cord. (**a**) Nanoindentation setup (Optics11Life, Chiaro Nanoindenter) and spinal cord slice. (**b**) Identification of grey and white matter with indications of indentation locations. (**c**) Post-processed loading paths of indentation experiments. (**d**) Rheometry setup (TA instruments, Discovery HR-3 Rheometer). (**e**) Raw data of rheometer torsion and compression-tension testing..

In the future, further experiments will be conducted with porcine spinal cord to explore possible influences of our experimental design on the measurement of the tissues mechanical response. These considerations encompass factors such as tip diameter, cantilever stiffness, experiment duration, post-mortem time, and tissue staining. A well-defined staining protocol will be established for the spinal cord to enhance our ability to distinguish between grey and white matter.

Modeling the finite viscoelasticity of human brain tissue based on microstructural information

Nina Reiter[1], Anne-Mareike Schäfer[1], Sophia Auer[2], Friedrich Paulsen[2], Silvia Budday[1]

[1] Institute of Continuum Mechanics and Biomechanics, FAU

[2] Institute of Clinical and Functional Anatomy, FAU

In contrast to existing phenomenological material models, which only provide adequate estimates for brain regions with a similar microstructure as those used for calibration, microstructurally motivated constitutive models can account for regional and temporal changes through microstructural parameters. In a previous study, we have proposed a microstructure-informed finite viscoelastic constitutive model for porcine brain tissue based on experimental insights into the link between macroscopic deformations and cell displacements during compression tests with strains up to 7.5% [1]. Here, we show that the model can simulate the material response of human brain tissue from the cerebellum during compression and tension tests with strains up to 15% [2]. As illustrated in Figure 1, we calibrate the model using a combination of cyclic loadings and stress relaxation experiments and include cell densities and the percentage area covered by cell nuclei into the model. Our results show that the microstructure-based time constant that we had determined for porcine brain tissue is also valid for human tissue. Furthermore, the microstructure-informed material model is capable of capturing the pronounced compression-tension asymmetry of brain tissue. The model performance was improved by introducing the nonlinearity parameter α as a function of the area percentage covered by cell nuclei A_c instead of the cell density ρ_c, highlighting that A_c is a promising candidate for a microstructural parameter in future microstructure-informed constitutive models for brain tissue.

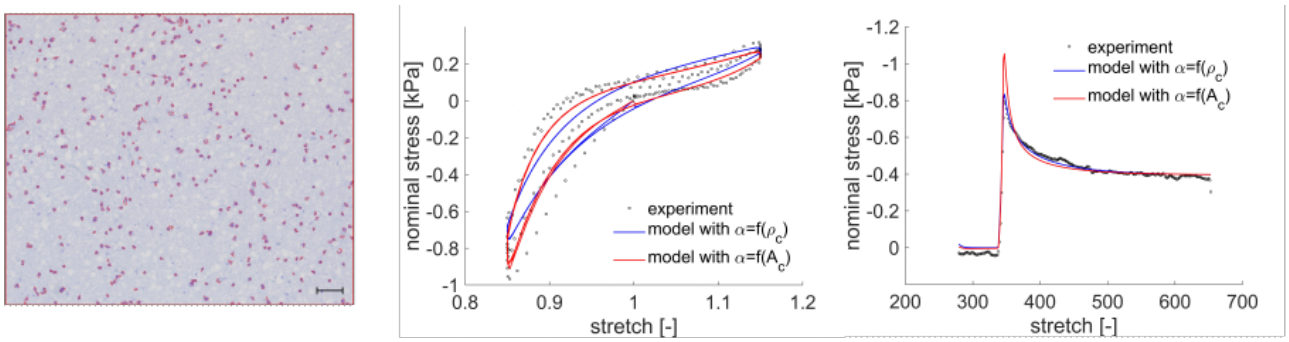

Figure 1: Model calibration. Representative histologically stained image with detected cells (left) and mechanical response of a sample from the human cerebellar white matter during cyclic loading (middle) and stress relaxation tests (right). Scale bars = 50 µm..

References

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Mechanical characterization of soft tissue in time and high frequency domain

Laura Ruhland, Kai Willner

Contradictory mechanical responses are a persistent problem concerning experimental studies of ultrasoft materials such as brain tissue when using different testing techniques. Reasons for these inconsistent responses are mainly attributed to the varying testing conditions of the different techniques. Particularly challenging is the use of multiple time and length scales across the experiments. The aim of this project is to reconcile the results of different testing methods using a wide strain and frequency range.

As a first step quasi-static experimental data in the time domain was conducted by performing experiments at the rheometer. A phantom material based on alginat (ALG) and gelatin (GEL), mimicking the viscoelastic behavior of the brain, was used for the measurements. The material parameters of the hydrogel were established with a parameter identification procedure based on an Abaqus model of the experiments. Fig.1 shows the hysteresis and stress relaxation data for compression, tension and shear loading of ALG-GEL and the calculated Abaqus results of the mechanical behavior.

Further a table-top magnetic resonance elastography system was established to obtain material responses in a high frequency range. The measurements were performed on a 0.5T magnet, which determines the vibration in the material induced by a piezoelectric actuator. With this measurement technique vibration data up to several kHz can be obtained. The material parameters of those experiments were identified by fitting the 1D-wave field of every frequency to the viscoelastic Maxwell or Kelvin-Voigt equations. Fig.2 shows the storage and the loss module for ALG-GEL in a frequency range from 300Hz to 4100Hz.

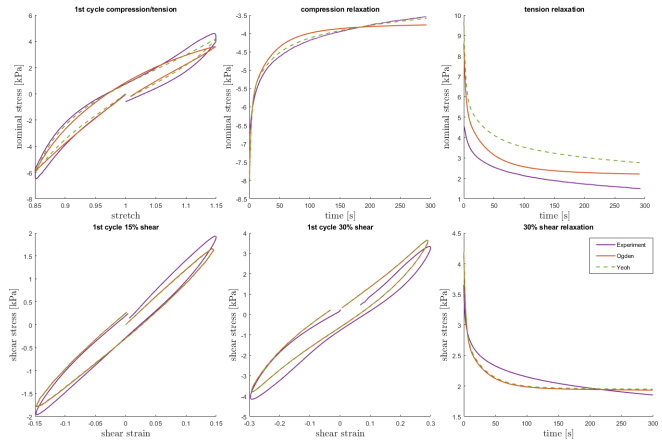

Figure 1: Mechanical behavior of ALG-GEL under cyclic loading and stress relaxation in compression-tension (first row) and shear (second row) and the calculated material responses by using a hyperelastic Ogden and Yeoh model both combined with a viscoelatic Prony series.

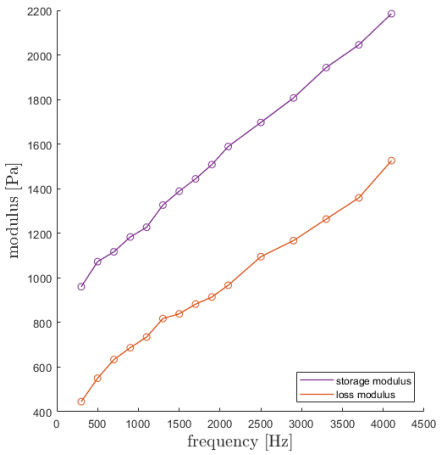

Figure 2: Storage and loss modulus of ALG-GEL calculated with the viscoelastic Maxwell model.

Computation-driven reconciliation of ex vivo and in vivo experimental data of brain tissue

Yashasvi Verma, Paul Steinmann

The experimental testing of brain tissue *in vivo* and *ex vivo* has reportedly given contradictory results which have been attributed to the different testing modalities and hence the different testing conditions. The aim of this project is to develop a computational model that can suitably predict the results of the various testing modes and methods.
In this effect, we employ a non-linear poroviscoelastic model of the brain [1]. This model is founded on the hypothesis that the brain is intrinsically biphasic in nature, and the porous and viscoelastic parameters interact with each other. It has previously shown promising results by predicting the contradicting nature of the stiffer white matter in indentation experiments, while the stiffer gray matter in large strain compression testing [2]. The model is implemented by using the deal.ii library and is being enhanced by including a full dynamic range over various time and length scales. This approach also involves a comprehensive consideration of specific loading, initial, and boundary conditions tailored to diverse testing setups.
In this context, another important aspect is the inclusion of the vascular structure present in the brain into the model. The overlay of this discretized network and the integration of the blood pressure will serve as an enhancement of the model especially when *in vivo* measurements will be considered. The basis for adding the vascular tree into our model will be a code that generates a dendritic tree and a tool that exports it into the deal.ii model [3]. This step will also incorporate the mathematical coupling of our biphasic nonlinear poroviscoelastic brain model with an additional vascular network.

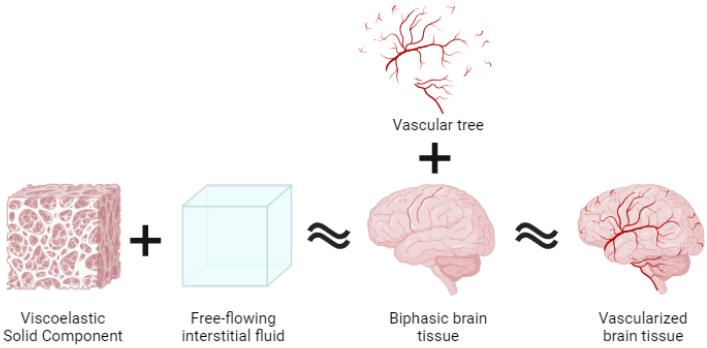

Figure 1: Approximation of the brain tissue in the computational model.

References

[1] E. Comellas, S. Budday, J.-P. Pelteret, G. A. Holzapfel, and P. Steinmann. "Modeling the porous and viscous responses of human brain tissue behavior". *Computer Methods in Applied Mechanics and Engineering* 369 (2020), p. 113128.

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A physical multifield computational model explains the role of different cell types in cortical folding

Mohammad Saeed Zarzor, Silvia Budday

The human brain is one of the most intriguing organs in our body. It undergoes a wide range of changes on both micro- and macroscopic scales during development. During embryonic life, different types of cells are generated, and each of these types plays an essential role in forming the brain. On the one hand, neuroscientists have carefully assessed the pedigree relationship between different cell types. They have successfully investigated the behavior and role of each type on the microscopic scale [1]. On the other hand, the link between the changes on the microscopic scale and the formation of cortical folds on the macroscopic scale remains less well understood. From a mechanical point of view, mechanical forces generated as a result of cellular processes and brain growth play an important role in forming cortical morphology. In our work, we mathematically link the changes on the microscopic scale with the forming cortical folds on the macroscopic scale. To do so, we establish a multifield computational model that couples a system of advection-diffusion equations (ADEs) with the theory of finite growth. Each ADE is formulated in such a way to mimic the biological behavior of a certain cell type, including cell proliferation, cell migration, and connectivity, Eq.1 [2]. We consider four cell types, i.e., radial glial cells, intermediate progenitor cells, outer radial glial cells, and neurons. Here, the differential growth of the cortex is controlled by the density of the neurons in the cortical layers. Figure 1 shows the final folding pattern observed around gestational week 36 with the obtained cell density distribution of the earlier-mentioned cell types.

$$\frac{\dot{J}}{J}\, c + \dot{c} = -\boldsymbol{\nabla}_{\boldsymbol{x}} \cdot [\hat{\mathbf{v}}(c, \boldsymbol{x})\, c - \boldsymbol{d}^{cc}(\boldsymbol{x}) \cdot \boldsymbol{\nabla}_{\boldsymbol{x}}\, c] + r^{c}(\boldsymbol{x}, s), \tag{1}$$

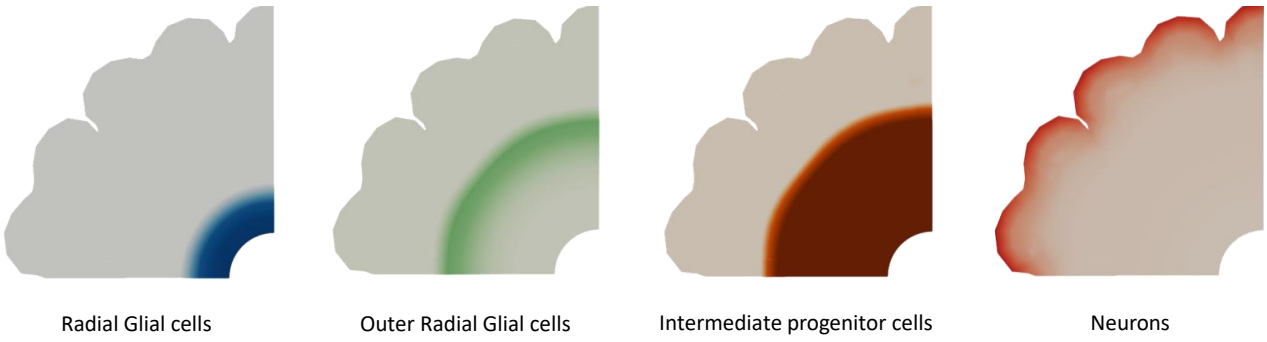

Figure 1: Final folding pattern at gestational week 36 with the final state of the cell density distribution of the radial glial cells, outer radial glial cells, intermediate progenitor cells, and neurons from left to right, respectively.

References

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– Material mechanics –

Damage modelling for the simulation of mechanical joining processes

Johannes Friedlein, Julia Mergheim, Paul Steinmann

Clinching is a mechanical joining method for assembling sheet metal, which relies on the controlled local deformation of the sheet material. Thereby, accurate and robust material models are needed to reliably predict the joint formation and strength. Moreover, large deformation, mesh distortion, and frictional contact, being inherent to mechanical joining processes, result in complex simulation models with high computational cost.

To enable the use of comprehensive material models in this context, particular attention needs to be paid to the computational efficiency. Therefore, the Mathematica-based AceGen-package was utilised to ease the code implementation, apply automatic code optimisation, and automatically generate the code for multiple programming languages. This framework, for instance, enabled the efficient implementation of own element formulations with reduced integration, hourglass control, and coupled plasticity-damage material models with gradient-enhancement. This code is at once available, for instance, in the commercial FEM software LS-DYNA in FORTRAN and the open-source C++ FE library DEAL.II.

With these efficient models in hand, also simultaneous inverse material parameter identification based on multiple large-scale experiments becomes possible. The so-called modified punch test in Fig. 1 is one example standing out due to its closeness to the clinching process yet with an improved visual insight exploited in [1] for the failure calibration. During the calibration of ductile damage even more challenges arise. For example, the non-locality of damage, introduced by an internal length ℓ, can render an excessive specimen size dependency, revealed in Fig. 2.

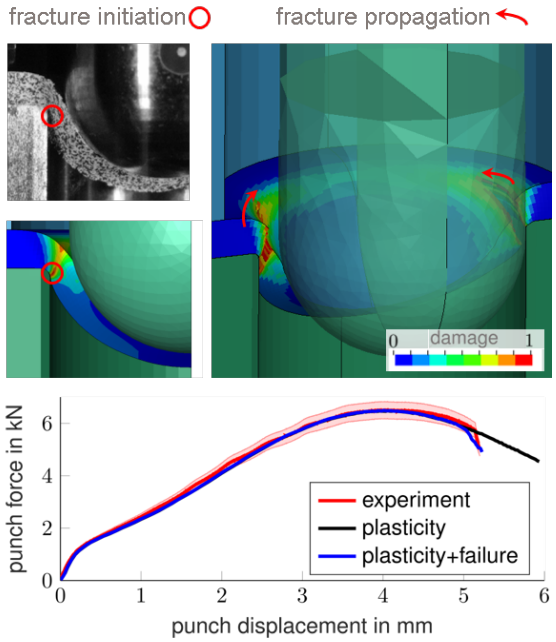

Figure 1: Modified punch test variant probing 1.5 mm thick dual-phase steel HCT590X. Deformation and process force.

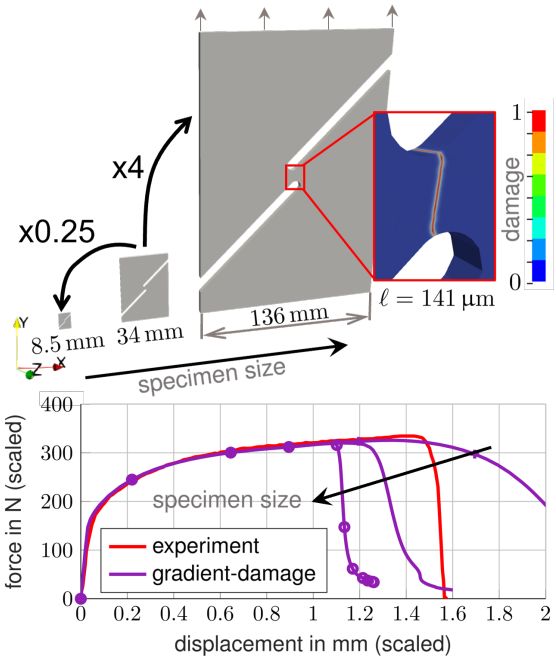

Figure 2: Specimen size dependency of gradient-damage. Scaled shear specimens.

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Phase Fracture Modeling of Polymer Nano-Composites Undergoing Large Deformations

Paras Kumar, Julia Mergheim

The graded-interphase-enhanced phase-field fracture (PFF-GI) approach [2], facilitates the modeling of a wide range of microscale fracture responses observed experimentally in case of particulate polymer composites, polymer nano-composites in particular. Herein, we consider a continuous grading or variation in the elastic and fracture properties, by means of a power law type interpolation ansatz, within an interphase region of finite thickness around the filler particles. Appropriate tuning of the graded interphase parameters, thus, enables us to capture a wide spectrum of microscale fracture phenomena including cohesive failure between the inclusion and the matrix; see Figure 2 for example.

The adopted finite-deformation setting enables the modeling of fracture response in materials such as elastomeric nano-composites which undergo large strains prior to fracture. As discussed in detail in [1], we consider a double-edge-notched tension (DENT) specimen comprising of a stiff and tough circular inclusion embedded in a rubber matrix and subjected to a displacement controlled loading on its top face; cf. Figure 1. As depicted by the force-displacement curve, the standard or no graded interphase (GI) case results in complete failure occurring at an applied strain of around 30 %. A weak GI, on the other hand leads to complete failure at a lower applied strain of around 15 % but with a different cracking pattern wherein crack nucleation and void growth occurs within the GI region followed by the propagation of the side cracks which ultimately coalesce with the void to culminate in complete failure of the specimen; cf. Figure 2.

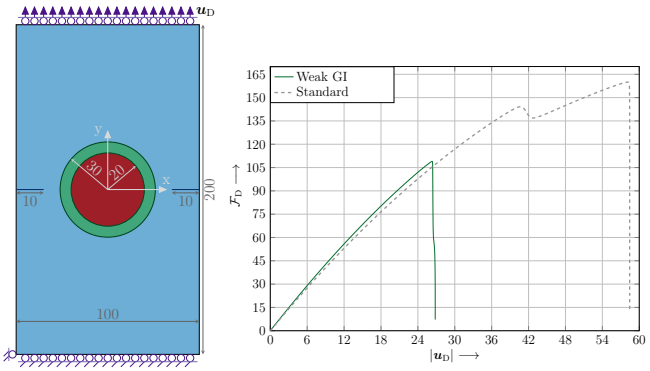

Figure 1: Problem setup (left) and the force-dispalcement curves for the single-particle DENT test.

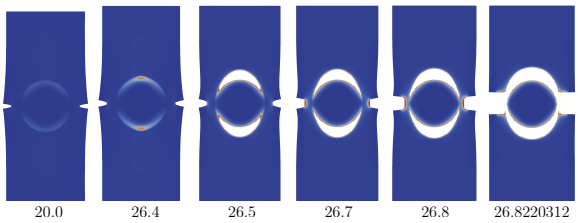

Figure 2: Evolution of the diffuse crack for the case of weak GI. The number below each contour plot denote the applied displacement.

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Development and optimization of hydrogels based on oxidized hyaluronic acid for the mimicry of brain-tissue

Sonja Kuth[1,2], Silvia Budday[1], Aldo R. Boccaccini[2]

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[2] Institute of Biomaterials, FAU

Many applications require materials that closely mimic the intricate mechanical and biochemical properties of brain tissue. Hydrogels are most commonly used in the engineering of soft tissue as they can closely resemble the microstructure of native extracellular matrix. In a previous study, we developed and assessed a hydrogel material for its mechanical properties similar to human brain tissue [2]. We confirmed that, through material selection, we can achieve brain-mimicking compr./tens. asymmetry and an eff. stiffness similar to that of brain tissue. Besides material selection, crosslinking characteristics play a crucial role in the successful development of a hydrogel matrix for biomedical applications. By reducing crosslinking time or concentration, one can lower the network density and, consequently, the stiffness of the matrix. However, this often leads to a significant reduction in the stability, resulting in rapid degradation of the hydrogel structure.

In this study [1], we evaluate and compare two crosslinking approaches, post-crosslinking (postCL) and *in-situ* crosslinking (in-situCL), while maintaining the material chemistry. The hydrogel system consisted of oxidized hyaluronic acid (OHA), and gelatin (GEL). The matrix was crosslinked using microbial transglutaminase (mTG), an enzyme native to the human body. Our findings indicate that, by employing in-situCL instead of postCL, we can significantly enhance the stability of the hydrogel constructs while maintaining matrix stiffness (see 1). These findings allow us to independently modify hydrogel parameters that are typically interdependent, thus providing the opportunity to conduct a broader range of experiments.

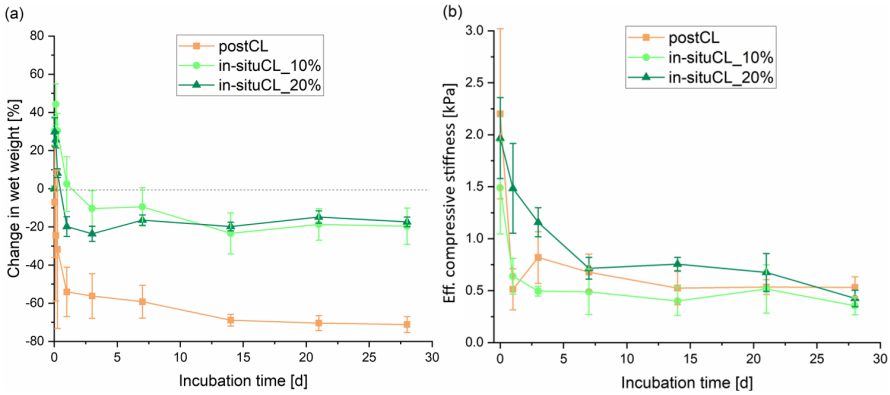

Figure 1: Degradation behavior of postCL and in-situCL OHA/GEL samples over 28 days under cell culture conditions. (a) Change of wet weight. (b) Eff. compressive modulus..

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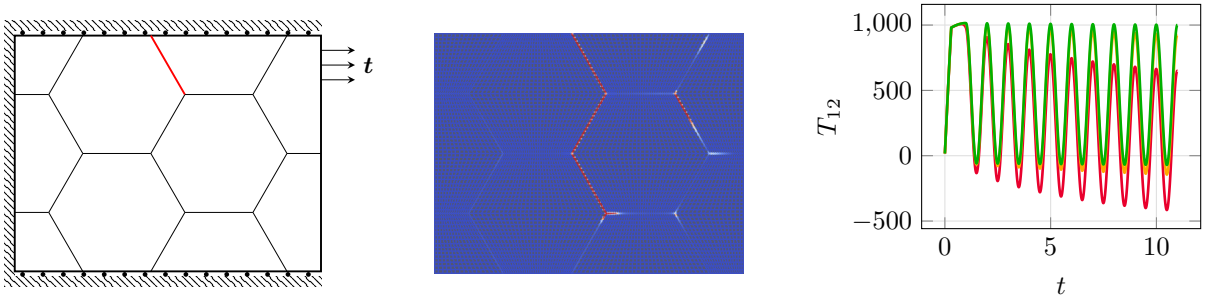
Intergranular damage modelling in polycrystalline materials

Jose Lara, Paul Steinmann

Structural components subjected to cyclic loading can eventually lead to an failure in what is known as fatigue. This is caused by the propagation of microcracks that initiate at imperfections inside the material. Considering the grain boundaries as the predominate defect leading to microfractures, a damage-enhanced strain-gradient crystal plasticity formulation has been proposed in which the grain boundaries are modeled as a cohesive zone. On the one hand, the non-locality allows not only to capture size-dependent effects but also quantifies the interaction of the plastic slips of adjacent crystals as proposed by Gurtin [1], on which the formulation is based upon. On the other hand, the cohesive zone model establishes a framework in which a damage variable can be naturally introduced, as advocated by Spannraft et al. [3]. To showcase the material behavior described by the proposed formulation, the boundary value problem shown in Fig. 1a is solved. As can be seen in the damage field after 10 load cycles depicted in Fig. 1b, the damage evolution has been adapted such that fatigue can be reproduced both in its initiation and propagation stage.
The rate-independent formulation is approximated in its numerical implementation by a visco-plastic regularization. As a result of a numerical study regarding the regularization scheme [2], it was determined that the fidelity of the approximation plays a deciding role in the material response during cyclic loading. As the number of cycles to simulate increases the regularization parameter has to decrease, otherwise a fatigue-like material response is caused by the introduced rate-dependence as seen in Fig. 1c.



(a) **(b)** **(c)**

Figure 1: (a) The boundary value problem subjected to a cyclic traction load $\boldsymbol{t}$ and with a pre-inserted crack marked in red. (b) Damage field after 10 load cycles with random crystal orientations. (c) Evolution of the shear stress on the upper boundary of an infinite strip composed of a single crystal subjected to cyclic simple shear for different values of the regularization parameter (— $\lambda = 1 \times 10^{-3}$, — $\lambda = 1 \times 10^{-4}$ and — $\lambda = 1 \times 10^{-5}$).

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

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Peridynamics (PD) is an emerging nonlocal continuum theory that is increasingly applied to model physical phenomena that are not accurately captured in classical local models. Nonlocality is introduced to the governing equations of PD through an integral term which computes the interactions of a continuum point and its neighboring points within a finite distance. In this work, continuum-kinematics-inspired peridynamics (CPD) is employed, which considers the interactions between pairs, triplets and quadruplets of points to capture the kinematic changes in terms of length, area and volume. A major advantage of PD is the straightforward modeling of damage through bond breakage. In [1], we developed a CPD model accounting for progressive damage within a finite-thickness interface, as opposed to the more common practice of abrupt bond breakage across a zero-thickness interface. A thorough derivation of the theoretical framework employing a rate-variational principle demonstrates the compliance of the damage formulation with thermodynamics and balance laws. The model allows to investigate the effects of nonlocality that accompany a PD model and are of particular interest for small-scale applications. The two aspects of nonlocality and progressive interfacial damage are linked for the first time to study the wrinkling and delamination behavior of a stiff film bonded to a substrate, see Fig. 1.

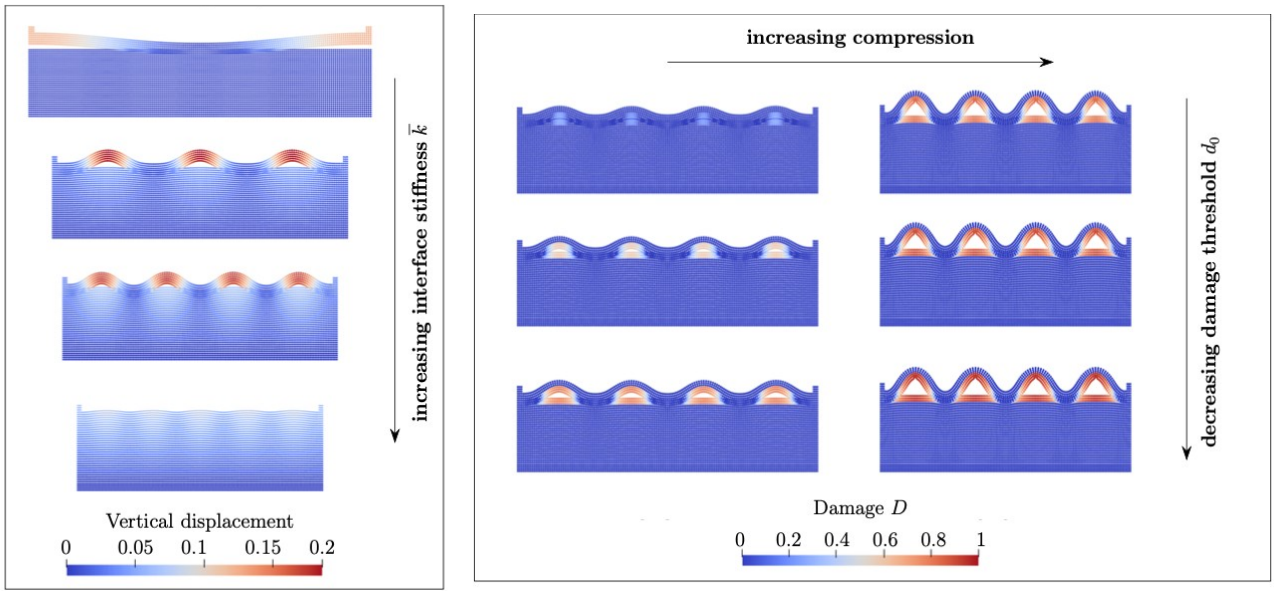

Figure 1: Wrinkling and delamination of a compressed bilayer: A decrease in wrinkling wavelength is observed with increasing interface stiffness (left). Damage is mitigated when larger interface damage thresholds are modeled (right).

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Experimental Investigation of Light-Matter Interactions in Polymers

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[2] University Gießen

Photostrictive materials form a subclass of smart materials in which light-matter interactions result in a mechanical response that does not correspond to thermo-mechanical effects. This unique feature enables the design of adaptive structures powered and controlled simply through activation by light sources. It effectively eliminates the need for hard-wired connections for the transmission of sensor signals or control voltages and additional power sources. A promising examples for photo-sensitive materials can be fabricated by embedding molecular switches, such as Azobenzene, into a polymer matrix. The application of light of a specific wave length triggers a transformation of the molecular switches from the straight trans to the kinked cis state which then induces volumetric changes or a bending motion of the material.
Using Azobenzene molecules supplied by Prof. Wegner from Gießen and the silicone Elastosil P7670^{TM} we produced soft material samples that are able to undergo large deformations and that are not temperature sensitive. This ensures that any effect visible in photo-mechanical experiments is not due to the heating of the material but the influence of the switching molecules. The result of a multistep relaxation experiment is presented in Figure 1. Here the material is deformed in eight steps to a maximum of 200 %. Following each deformation step is a relaxation period of 5 minutes. As it is known that the polymer chains orient in the direction of the deformation we investigate if the randomly distributed switching molecules align with the polymer chains. The experiments were performed with different Azobenzene concentrations. The results show that the strength of the photomechanical coupling increases with increasing deformation. This indicates that the Azobenzene molecules orient with the polymer chains resulting in a more pronounced effect.

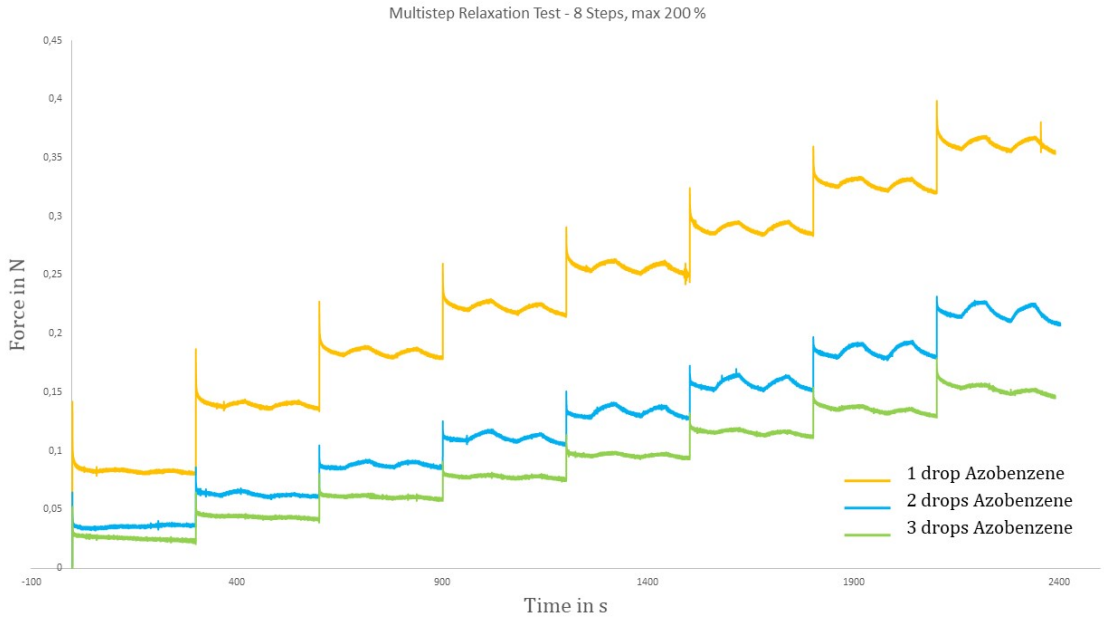

Figure 1: Material response of a multistep relaxation test with azobenzene doped Elastosil.

Soft Fracture: Electro-Magnetical Modulation & Configurational Mechanics

Miguel Angel Moreno-Mateos, Paul Steinmann

Soft magneto-rheological elastomers (MREs) and dielectric electro-active elastomers (DEAP) respond to magnetic and electric stimuli, respectively, by undergoing large deformations and changes in their material properties. We explore the fascinating response of an ultra-soft elastomer to the multiphysical coupling and its effects on the fracture performance [1, 2]. In conjunction with the experiments, we employ bespoke fracture phase-field models that integrate the physics. The comprehensive study reveals that the magneto-mechanical and electro-mechanical effects induce beneficial stress de-concentration and delay in crack propagation. Furthermore, we are highly interested in the application of configurational mechanics to soft materials. Configurational mechanics offers a framework for quantifying the tendency of defects to alter the material configuration. When applied to fracture mechanics, configurational forces can be used to quantify the propensity of cracks to propagate. By integrating advanced computational and experimental techniques, we aim at paving the way for future applications where configurational forces are calculated from advanced constitutive modeling frameworks. In this context, the configurational force method can be used in a standalone manner [3].

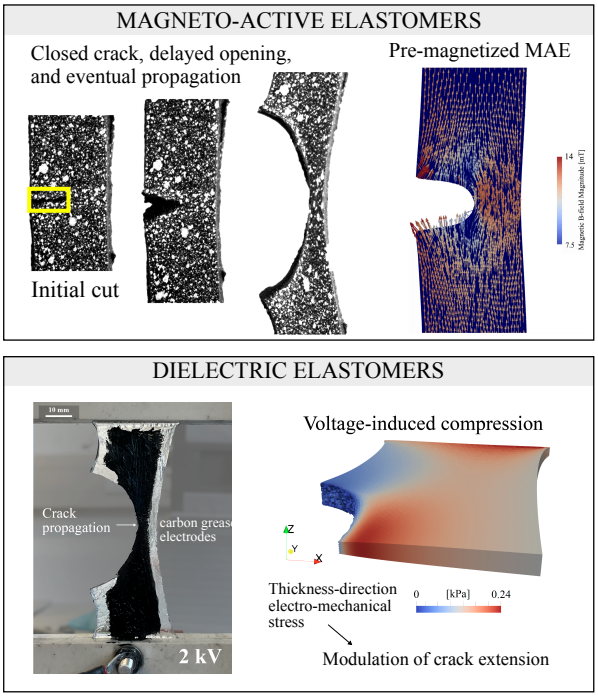

Figure 1: MREs/DEAPs: Soft Fracture.

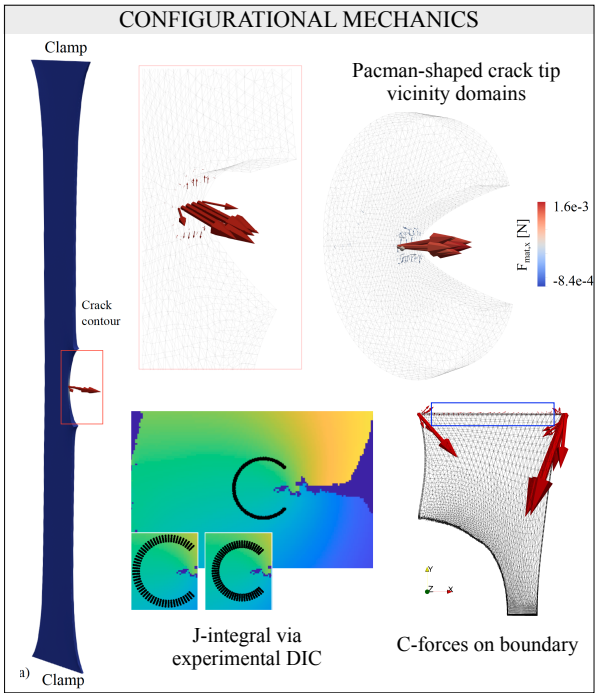

Figure 2: C-Forces and Soft Fracture.

References

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Influence of the irreversibility strategies in phase-field fracture simulations

Maurice Rohracker, Julia Mergheim

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

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

For an accurate resolution of the phase-field function, suitable finite element meshes are required which could lead to very computationally expensive simulations due to the high number of elements. In our recent publication (Rohracker et al. [2]), we introduced three different error indicators for adaptive spatial refinement (ASR) of the finite element mesh and compared them to each other. Particular emphasis has been placed on the accuracy (error measure of the load-displacement curve) and efficiency (speedup) of the simulations. We extended this comparative assessment to 3-dimensional numerical examples for crack growth in the single edge notched shear (SENS) test (cf. Figure 2). For suitable parameters, they show a very good accuracy and efficiency compared to the simulation on on a pre-refined mesh. Further interest was also

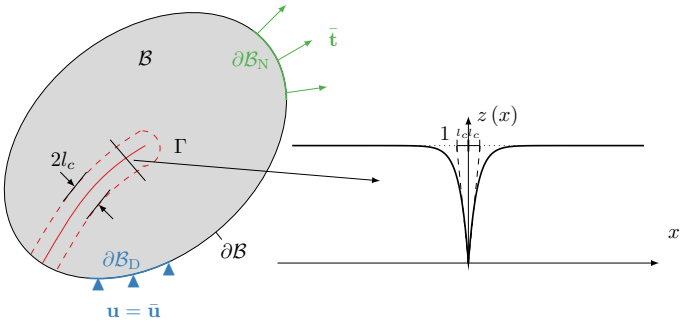

Figure 1: Smeared model of the phase-field fracture model.

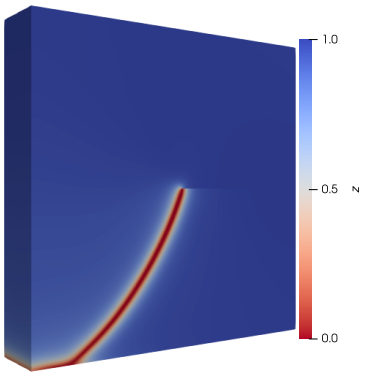

Figure 2: Phase-field contour of the 3D SENS test.

devoted to the crack irreversibility or in other words to methods to prevent crack healing. Working with a crack driving force based on the phase-field values of only the previous load step decouples both field equations but requires small time-step sizes to accurately capture the crack propagation. Hence, other strategies, i.e. the History current, the Dirichlet-type, and the damage formulation irreversibility techniques have been discovered. The strategies result in a strong coupling of the two field equations requiring multiple outer iterations until convergence in the critical loading regime. Our goal here is to provide a new convergence criteria for the iterative solution scheme for accurate and efficient phase-field fracture simulations.

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Novel cubatures in peridynamics

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[2] Department of Mechanical Engineering, Bilkent University, Turkey

Peridynamics (PD) [1] is a nonlocal continuum mechanics formulation, where every continuum point interacts with continuum points in its finite-sized neighbourhood, the so-called horizon $\mathcal{H}_0$. The pointwise governing equations depend consequently on the integration over $\mathcal{H}_0$.
In PD models, the continuum is typically discretized by a finite number of collocation points, at which the governing equations are evaluated. The collocation points can additionally serve as integration points for the cubature of $\mathcal{H}_0$, as indicated in Fig. 1 (left and middle). This

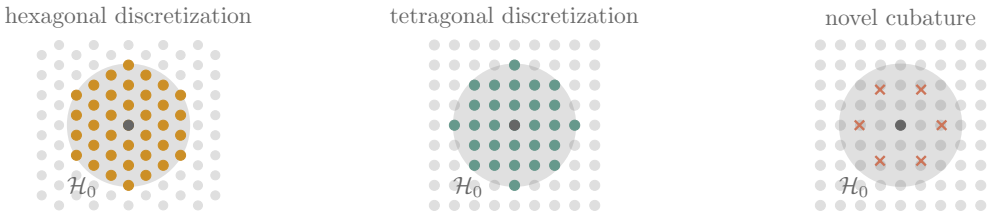

Figure 1: Integration points for cubatures dependent (left and middle) and independent (right) on the discretization.

method is commonly used for PD models despite its dependence of the integration accuracy and computational cost on the discretization. To address this problem, we established novel cubatures for PD, where integration and collocation points no longer necessarily coincide. We align the integration points in a hexagonal pattern, as depicted in Fig. 1 (right), and use linear or quadratic interpolation schemes to evaluate the governing quantities at the integration points. The bending example in Fig. 2 depicts one of our validation tests and shows that the resulting vertical displacement of the cubature with quadratic interpolation (bottom right) is in good agreement with the cubatures dependent on the discretization (top). In contrast, the cubature with linear interpolation (bottom left) can not capture the bending exactly as it is based on lower order interpolation functions. However, for other load cases, e.g. extension and shear test, we obtain reasonable results for both novel cubatures that are independent on the discretization.

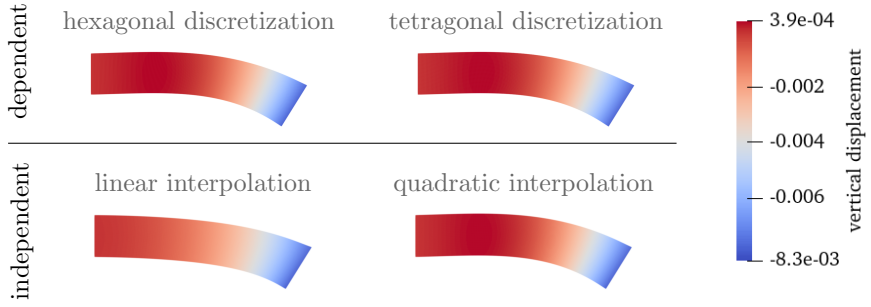

Figure 2: Bending test with cubatures of $\mathcal{H}_0$ dependent and independent on the discretization.

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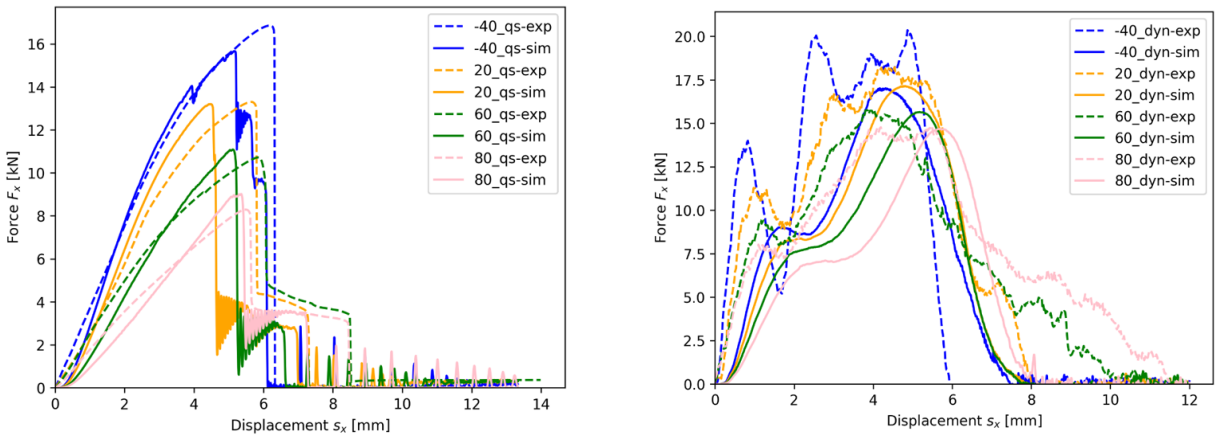
Temperature and strain rate dependent modeling of adhesive joints - validation on sample components

Lars Schmelzle, Gunnar Possart, Julia Mergheim

The mechanical properties of polymers depend significantly on temperature and strain rate. For a safe design of adhesive joints, it is therefore critical to identify and describe those dependencies. In a first step we already successfully extended the TAPO (Toughened Adhesive Polymer) material model to temperature dependency [1]. This quasi-static model could be validated using a diagonal pull specimen. So in a consecutive step we could confidently extend the model to temperature dependent rate dependency in the same fashion.
The resulting model was then used to simulate a T-test specimen under transverse loading for a final validation. Four temperatures $T \in \{-40, 20, 60, 80\}$ [°C] and two impact velocities $v \in \{0.0001\bar{6}, 2.0\}$ $[\frac{m}{s}]$ were considered. The simulation of the T-test proofed to be sensitive to the actual thickness of the adhesive layer, the filling of the gaps between the adherents as well as the modeling of the shock absorbing impact plate. The thickness of the adhesive and the gap filling were therefor measured experimentally and the temperature and rate dependent elastic parameters of the HDPE (high density polyethylene) impact plate were identified by DMA (dynamic mechanical analysis). Taking all this information into account lead to the successful



(a) quasi-static. **(b)** dynamic.

Figure 1: Validation using the T-test specimen under transverse loading.

validation results shown in Figure 1. For the quasi-static loading, pictured in Figure 1a, a very good agreement of the simulation results and experiments can be observed. Not only the initial stiffness and maximum force match very well, but also the displacement at damage initiation and final material failure coincide. At a temperature of -40 °C the specimen fails abruptly in both experiment and simulation, whereas higher temperatures show a two step failing pattern, whereby the force first drops and then plateaus until failure. The results for the dynamic load case shown in Figure 1b further proof, that the model very well captures both temperature as well as rate effects.

References

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Mechanics of Generalized Interfaces and Grain Boundaries

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Interfaces play an important role in numerous engineering applications, such as grain boundaries and adhesive layers. On the one hand, interfaces can increase the material's toughness, e.g by acting as dislocation obstacles in polycrystalline metals. On the other hand, interfaces can be considered as a weak link, predestined for decohesion and in-plane damage.
Our publications [1–3] present thermodynamically consistent interface laws for grain boundaries and generalized interfaces; and analyze their effects in FEM simulations. The grain boundary model (embedded in a gradient-extended crystal inelasticity framework) accounts for crystallographic mismatch and decohesion. The microtractions along the grain boundary reduce for increasing decohesion, cf. [1]. Generalized interfaces allow for anisotropic decohesion (introducing additional shear-like stresses for nonlinear kinematics) and interface inelasticitiy (introducing membrane stresses in the interface). Our models account for interactions between the damage modes in-plane (m) and normal/tangential cohesive (cm/ct), cf. [2, 3].

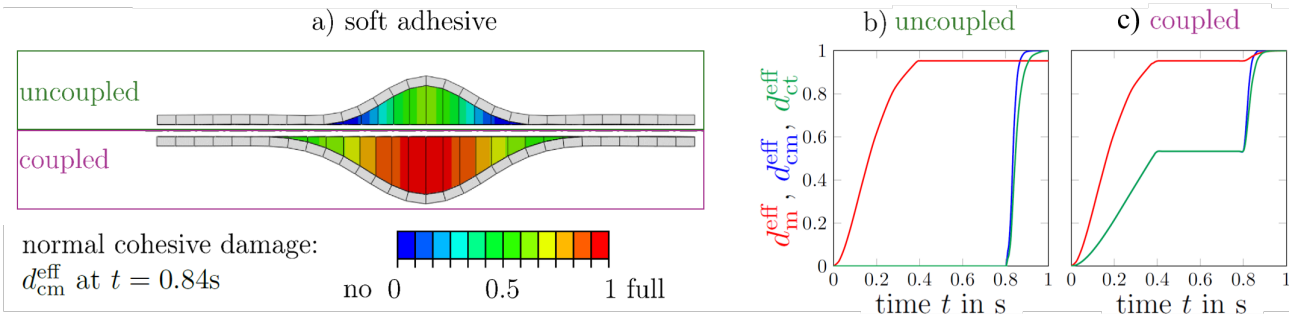

Figure 1: a) The cohesive damage in a soft adhesive connecting two substrates during buckling. The damage variables d_i^{eff} for the b) uncoupled and c) coupled damage modes over time t, cf. [3].

Such generalized interfaces allow modeling sealing applications and convenience products suffering in-plane deformations critical to their integrity, e.g. during manufacture or assembly. Figure 1 depicts the results of stretching such a structure up to 300% strain ($t = 0.4$s), unloading to its original state ($t = 0.8$s) and causing a buckling by means of compression. Accounting for a damage mode interaction (coupled), the structure fails earlier, cf. Figure 1 a), since the in-plane damage caused by stretching impairs the cohesion. Compare Figure 1 b) and c) which juxtapose the damage variables for the cases of b) uncoupled and c) coupled damage modes.

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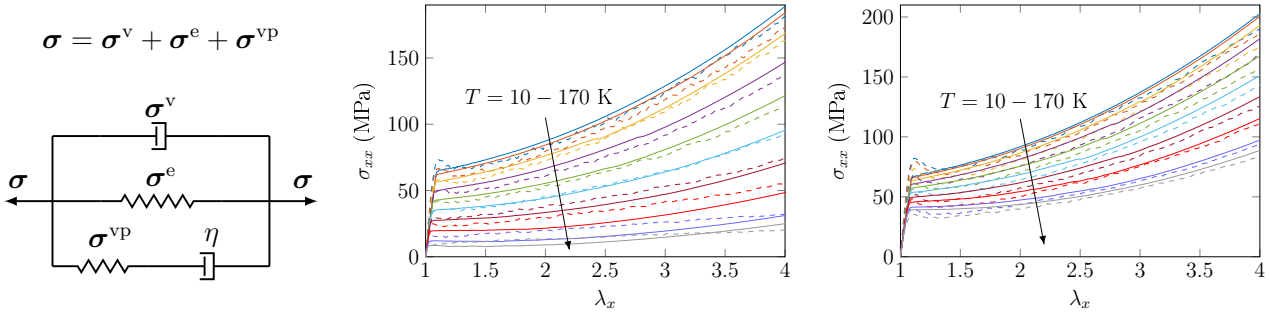
A visco-hyperelastic-viscoplastic constitutive model for rate- and temperature-dependent strain hardening behavior of glassy polymers

Wuyang Zhao, Paul Steinmann, Sebastian Pfaller

The strain hardening of glassy polymers at large deformation plays an important role in increasing their toughness by inhibiting the localized failure induced by strain softening. To predict the rate- and temperature-dependence of hardening, various constitutive models have been developed, e.g. by incorporating a deformation-dependent viscosity [2], considering dissipative orientation-induced back stress [3], or assuming a rate-dependent effective shear modulus [5], etc. In contrast to these models, which attribute strain hardening to internal variables, we use the rate of the total strain to account for the rate-dependent hardening. Using the viscous potential $\Psi^{\mathrm{v}} = \Psi^{\mathrm{v}}(\boldsymbol{C}, \dot{\boldsymbol{C}})$ with the right Cauchy Green tensor $\boldsymbol{C}$ and its rate $\dot{\boldsymbol{C}}$ proposed in [1], and adding it to an elasto-viscoplastic model, we propose a thermo-dynamically consistent visco-hyperelastic-viscoplastic model [4] as schematically illustrated in Fig 1(a). This model has been validated by comparing the stress responses with molecular dynamics (MD) simulations of coarse-grained polystyrene in uniaxial tension simulations as shown in Fig 1(b) and 1(c), where a strain rate of $\dot{\varepsilon} = 1\%/\mathrm{ns} - 100\%/\mathrm{ns}$ at the temperatures across a wide range of $T = 10\,\mathrm{K} - 170\,\mathrm{K}$ below the glass transition temperature $T_{\mathrm{g}} = 171.5\,\mathrm{K}$ has been considered.



(a) Rhelogical model. (b) $\dot{\varepsilon} = 1\%/\mathrm{ns}$. (c) $\dot{\varepsilon} = 100\%/\mathrm{ns}$.

Figure 1: Comparison between the constitutive model (solid curves) and the MD simulations (dashed curves) in uniaxial tension deformations at different temperatures and strain rates.

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– Fluid mechanics –

In the treadmill: the weirdness of flow-immersed soft particles

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Flows of particles suspended in fluids remain a challenge in various branches of science and engineering. This is especially true for particles in the micron-size range, since there the complexity and cost of experimental techniques and corresponding computational models of particle-fluid interactions is highly demanding. When dealing with the case of microparticles in the form of vesicles or bacteria, these particles not only display non-spherical shapes but also posess the ability to deform according to loads originating from the fluid flow conditions, most typically due to fluid shear stress. As the change of microparticle shape gives rise to the change in particle's translational as well as angular momentum dynamics, the resulting particle trajectories could significantly be altered.

Thus our work focuses on developing a novel model for simulating motion of soft deformable microparticles in dilute flows using hyperelastic particles of initially spherical shape by assuming creeping flow conditions around the particle as well as affine transformation. For the case of deformed ellipsoidal particle shapes the Jeffery model, [2] with Roscoe modification, [3], is implemented.

The Euler Equation of pseudo-ridgid body motion with spatially constant body forces renders

$$\ddot{\boldsymbol{F}} \cdot \boldsymbol{\Theta} + \boldsymbol{P}\mathrm{vol}(\mathcal{B}_0) = \int_{\partial\mathcal{B}_0} \boldsymbol{t}_0 \otimes \boldsymbol{\Xi} dA\,. \tag{1}$$

As we assume a hyperelastic material and Neo-Hooke constitutive law ($\boldsymbol{P} = \partial W/\partial \boldsymbol{F}$), we can express $\boldsymbol{P}$ as

$$\boldsymbol{P} = \mu\left[\boldsymbol{F} - \boldsymbol{F}^{-t}\right] + \lambda \ln\left[\det \boldsymbol{F}\right]\left[\boldsymbol{F}^{-t}\right]\,, \tag{2}$$

where λ and μ denote the first and the second Lamé parameter, respectively. As displayed in Fig. 2, we achieve good agreement to Gao & Hue [1], who studied particle deformation in simple shear flow conditions, by employing the Roscoe correction, [3].

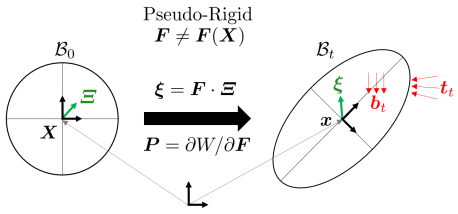

Figure 1: Pseudo-rigid body.

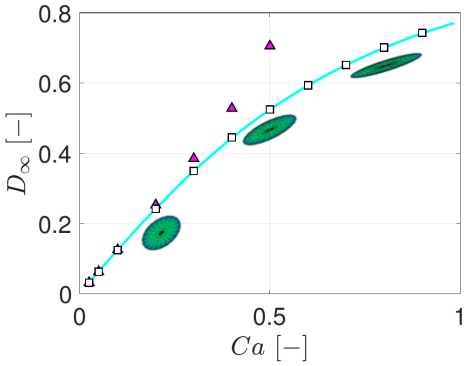

Figure 2: Particle deformation $D_\infty = [a-b]\,/\,[a+b]$ as a function of the capillary number Ca: ▬ [1], △ present model (Jeffery's Eqs. [2]), □ present model (Roscoe's Eqs. [3]).

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– Multi-scale modeling and simulation –

Characterization and modeling of polymer nanocomposites across the scales covering matrix, filler, and interphase

Maximilian Ries

Polymers represent a highly versatile material class and can be further enhanced to meet the requirements of highly demanding applications by adding filler particles. Particularly with nano-sized fillers, remarkable improvements in polymer nanocomposites' (PNCs') mechanical performance could be achieved experimentally. The outstanding mechanical properties of PNCs are mainly attributed to the matrix-filler interphase, which has a major impact, especially for nano-sized fillers. Therefore, a detailed understanding of the interphase and its impact on the overall behavior is necessary to exploit the full potential of PNCs. For this purpose, precise numerical models are required, to complement the challenging experimental investigation at the nano-scale. Particle-based methods such as molecular dynamics (MD) provide a detailed resolution of the microstructure, but are too expensive to solve problems at the engineering scale. To this end, computationally more efficient continuum approaches like the finite element (FE) method are commonly employed. However, these methods require accurate constitutive laws that capture the impact of the interphase and are usually not available. To this end, we introduce a methodology to derive continuum mechanical models for PNCs based on molecular dynamics and thus combines the advantages of particle-based and continuum approaches [1]. This interdisciplinary work contributes significantly to understanding polymer nanocomposites, especially the crucial matrix-filler interphase, and thus complements experimental insights. Moreover, the transfer of molecular-scale insights into continuum mechanical models forms an essential link between the chemistry and engineering communities for the numerical modeling of polymer nanocomposites. [1]

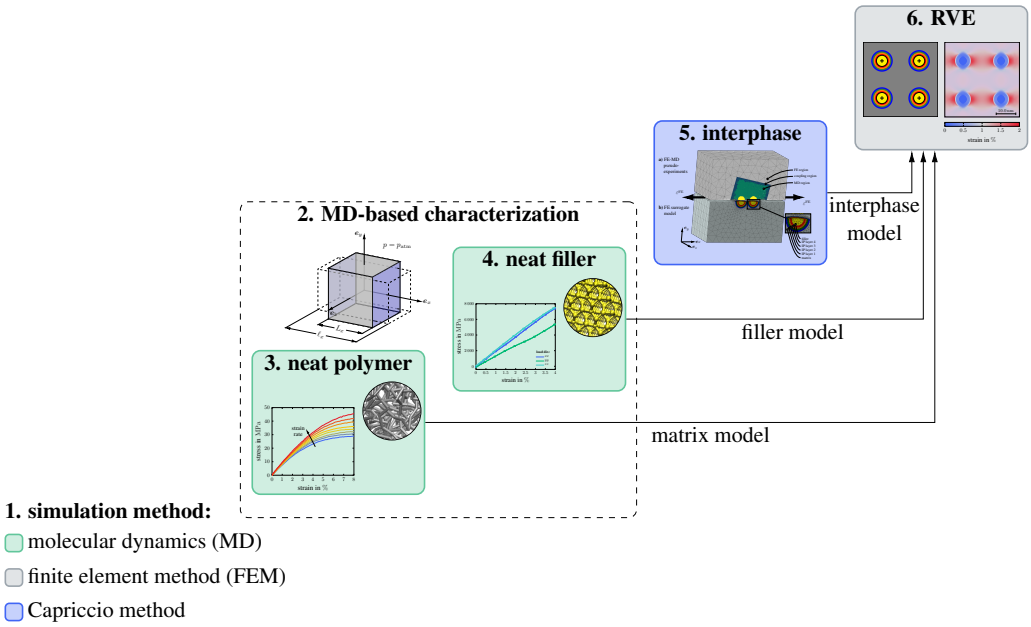

Figure 1: Schematic representation of the employed methodology in [1].

References

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Studying failure of polymer nanocomposites with a generic MD model

Felix Weber, Vincent Dötschel, Paul Steinmann, Sebastian Pfaller, Maximilian Ries

Their great versatility makes polymer nanocomposites (PNCs) an important class of engineering materials. To gain detailed insights into the nanoscale mechanisms underlying their macroscopic mechanical properties, molecular dynamics (MD) simulations have become a valuable tool to complement experimental studies. In [2], we modify the analytical potential functions of an efficient bead-spring model representing a generic polymer nanocomposite [1] to allow for breakage of covalent bonds. We then perform uniaxial tensile simulations of double-notched samples, see Figure 1. Here, we replace the classical periodic boundary conditions with nonperiodic ones on the precracked surfaces and apply Dirichlet boundary conditions in the x direction to regions of width L_d (plane strain condition in the z direction).
Validation of the model against experimental trends in stiffness, strength and toughness measurements is performed in two stages: First, we investigate the effects of specimen size, pre-crack geometry, strain rate, temperature, and degree of polymerization for the pure polymer. In a further step, we analyze the influence of filler size and filler content on the behavior of the PNCs. With this study, we show that when developing new materials or optimizing established ones, it is possible to use a simple MD setup to gain initial valuable insights into the effects of key parameters, which can then be extended by increasing the complexity of both the material description and the boundary conditions.

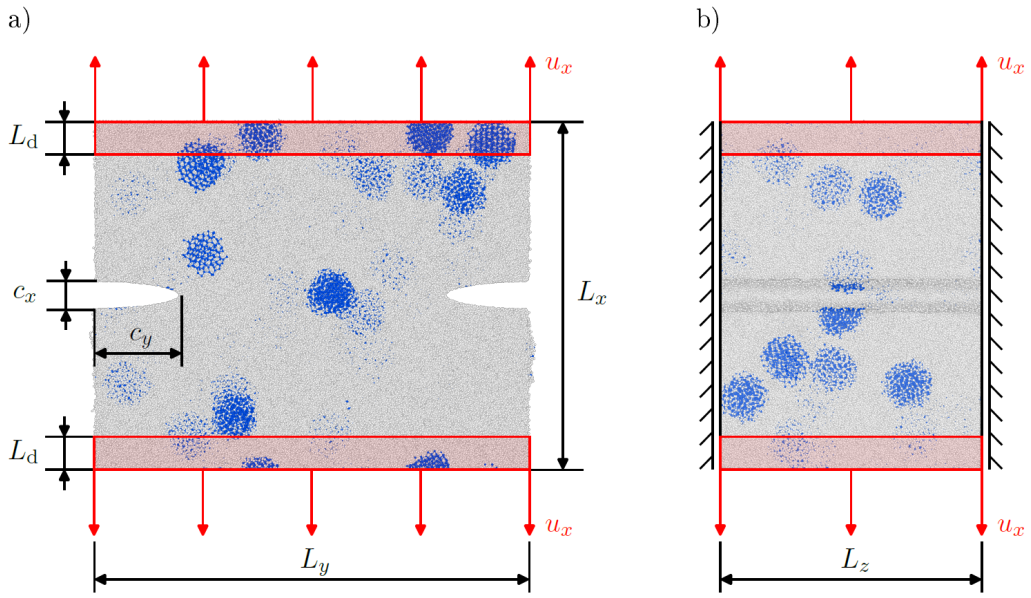

Figure 1: Setup of the double-notched samples of polymer nanocomposites subjected to uniaxial tension: Exemplary specimen in a) x-y-plane and b) x-z-plane [2].

References

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– Multi-physics simulation –

Finite element simulation of pyropiezoelectric energy harvesting

Michael Schwarz, Julia Mergheim

Piezoelectricity is the basis for a variety of energy harvesting devices that generate electrical energy from ambient energy such as mechanical vibrations. It describes the property of certain crystalline materials (PZT-5A, $BaTiO_3$, etc.) that show a distinct interaction between mechanical and electrical phenomena. Figure 1 shows this interaction for a cube with uniaxial displacement in **z**-direction. Typically, the energy harvesting structure is connected to an electric circuit to extract the energy. An example energy harvester structure with a resistor as electric circuit is shown in figure 2. In addition to the connection between mechanical and electrical properties, some piezoelectric materials also exhibit a distinct interaction between electrical and thermal properties. The effect of a changing electric polarization due to temperature changes is called pyroelectricity. Since pyro- and piezoelectricity are closely related and both occur simultaneously in some types of materials, pyropiezoelectricity describes in general the interaction between mechanical, electrical and thermal properties, thus combining both effects. From a modeling perspective, these effects can be taken into account by linear thermopiezoelectricity [2]. In addition to a balance equation and the kinematics for each field, the three fields are coupled via three constitutive equations.

The simulation of a thermopiezoelectric structure together with its electrical circuit is the overall goal of the current efforts. This requires a discretization of the continuous structure in time and space. While the finite element method is used for the spatial discretization, the time domain is discretized differently for each field. The balance of linear momentum is integrated in time using the Bossak-Newmark method, while the generalized midpoint rule is used for the transient heat equation. Since Gauss's law does not depend on time, no time integration is required for the electric field. The discretization in space and time results in an algebraic linear system of equations that can be solved for the unknown displacement, electric potential and temperature field. In the next steps, the influence of temperature on the energy harvesting is investigated.

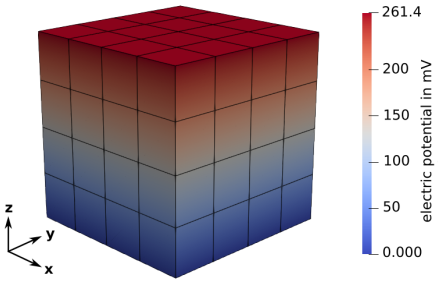

Figure 1: Electric potential distribution for a piezoelectric cube (PZT-5A, edge length 1mm) with a uniaxial displacement of 1% on the top surface in negative **z**-direction.

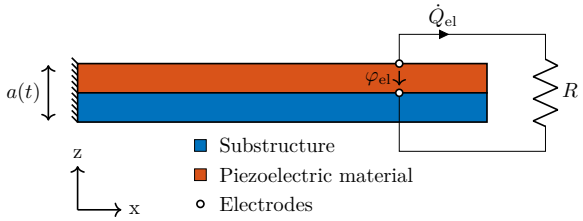

Figure 2: Schematic energy harvester beam based on [1].

References

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– Optimization and inverse problems –

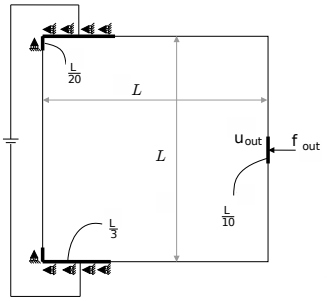
Free Space Matters in Optimizing Electro-Active Polymers

Chaitanya Dev, Gabriel Stankiewicz, Paul Steinmann

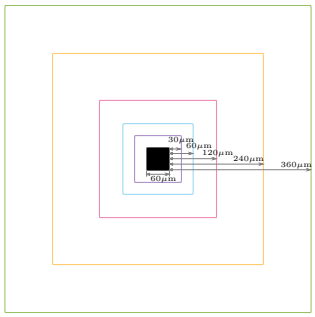
We examine the impact of free space on the optimization of electro-active polymers (EAPs). EAPs undergo deformation under electric fields and find use in engineering applications such as actuators and valves, as well as in biomedical applications such as artificial muscles. To effectively utilize density-based topology optimization in the design process, it is essential to comprehend the role of free space.

In a benchmark study involving a linear guiding actuator, we increased the truncation size of free space. Figure 1 displays optimized structure illustrations for different truncations of free space. The optimized structures converge when the free space reaches six times the bulk dimension. Moreover, the difference in objective value between considering no free space and considering a free space size of six times the bulk material is approximately 9.98%. For a more comprehensive analysis of our results, we refer readers to our paper [1].

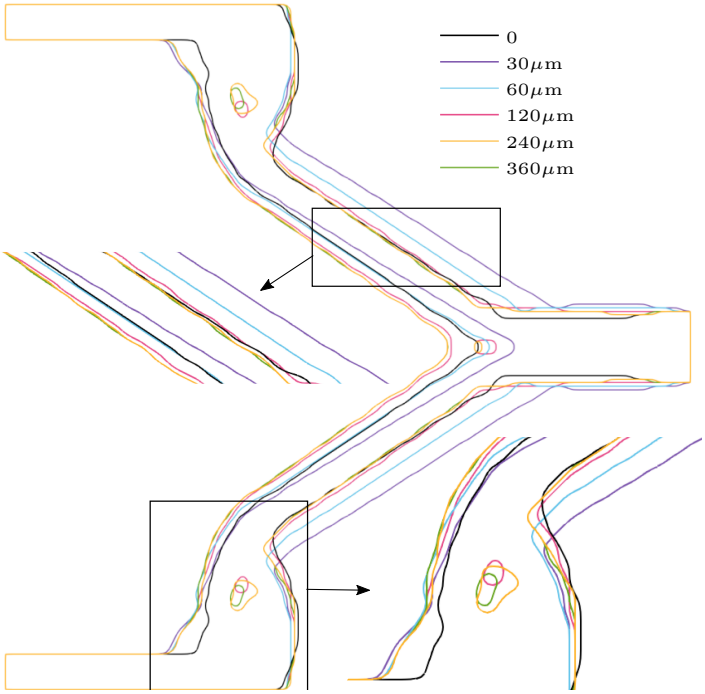
In conclusion, this study emphasizes the impact of free space on the optimization of EAPs. Although these visual disparities may be inconspicuous, performance deviations are non-negligible. Consequently, we suggest a minimum magnitude of free space equaling six times that of the bulk material in order to provide genuine samples.



(a) Linear guiding actuator problem setup.



(b) Visualization of free space truncation.



(c) Shape comparison.

Figure 1: Optimization results for the linear guiding actuator problem with a domain size of $L = 60\mu$m and varying free space truncations. Subfigure **(a)** shows the problem setup, **(b)** visualizes different free space truncations, and **(c)** compares optimized structure outlines for various free space truncations..

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Structural optimization of energy harvesting structures using a Ground-Structure approach

Andre Sommer, Paul Steinmann

Many technical applications and natural phenomenons show up energy-frequency spectra that can be exploited in the sense of energy harvesting; it is differentiated between technical and natural stochastic excitations. To harvest from these supplied mechanical energies, suitable structures are necessary. In order to design such structures, an optimization procedure is needed, determining the best suitable one out of an initial structure that comprises many different potential ones. In order to achieve this, we optimize discrete structures, building on a so called ground-structure approach. Different types of ground-structures exist, from variants with all nodes being connected to other types that for instance only connect neighboring nodes. The structure is modeled with geometrically linear frame elements, where the Euler-Bernoulli theory is used for the bending-part. Through the current optimization procedure not only the frame elements are optimized in their dimensions but also the nodes in their spatial positions. An example of the 2D simulation is shown in figure 1, while the optimized result is shown in figure 2. Regarding the node movement, Hetrick and Kota [1] have shown that optimizing compliant mechanisms as truss-networks using a modular ground-structure with moving nodes instead of a full ground-structure with fixed nodes can lead to results with higher energy efficiency. In our optimization sequential linear programming (SLP [2]) is used in order to solve the optimization problem, which currently consists of minimizing the structural volume with respect to stress constraints. An extract of future extensions of the model comprises investigations on the dynamical behavior of the structure and the incorporation of piezoelectric materials.

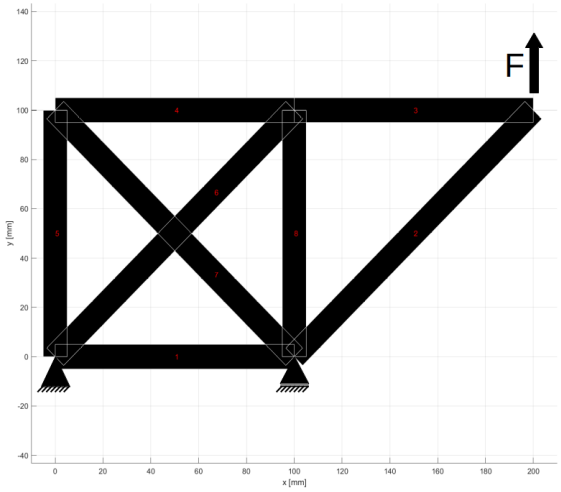

Figure 1: Initial Ground-Structure (8 Elements, 5 Nodes).

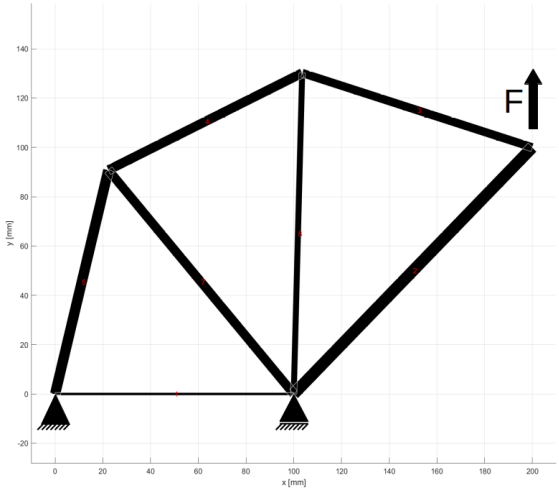

Figure 2: Optimized Ground-Structure: Load F is 1000N.

References

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Piezoelectric metamaterial design using combined topology and shape optimization

Gabriel Stankiewicz, Chaitanya Dev, Paul Steinmann

Metamaterials offer artificially engineered properties that cannot be achieved with conventional bulk materials. They allow for the creation of lightweight materials with high hydrostatic piezoelectric coupling coefficients and negative Poisson's ratio, making them ideal for use in electromechanical energy conversion systems.
In this project we explore the design possibilities of piezoelectric metamaterials through the use of structural optimization. More specifically, we use a sequential framework of topology and shape optimization to create piezoelectric metamaterials with negative Poisson's ratio for electromechanical energy conversion under uniform pressure. Initially, topology optimization generates the layout, while shape optimization refines the design and increases the durability and manufacturability of the structures with a curvature constraint. An embedding domain discretization (EDD) method using adaptive domain and shape refinement is employed for efficient and accurate computation of the state problem during the shape optimization stage.
Several case studies were conducted to assess the significance of desired stiffness characteristics, symmetry conditions, and objective formulations on piezoelectric metamaterials design. Objective formulations and symmetry conditions were also found to have a non-negligible impact. Findings indicate a strong correlation between desired stiffness characteristics and the resulting designs. Furthermore, the inclusion of the EDD-based shape optimization phase brings about noteworthy alterations to the schemes, ratifying the practicality of the sequential methodology.
In Fig. 1 a graphical summary of the project is shown.

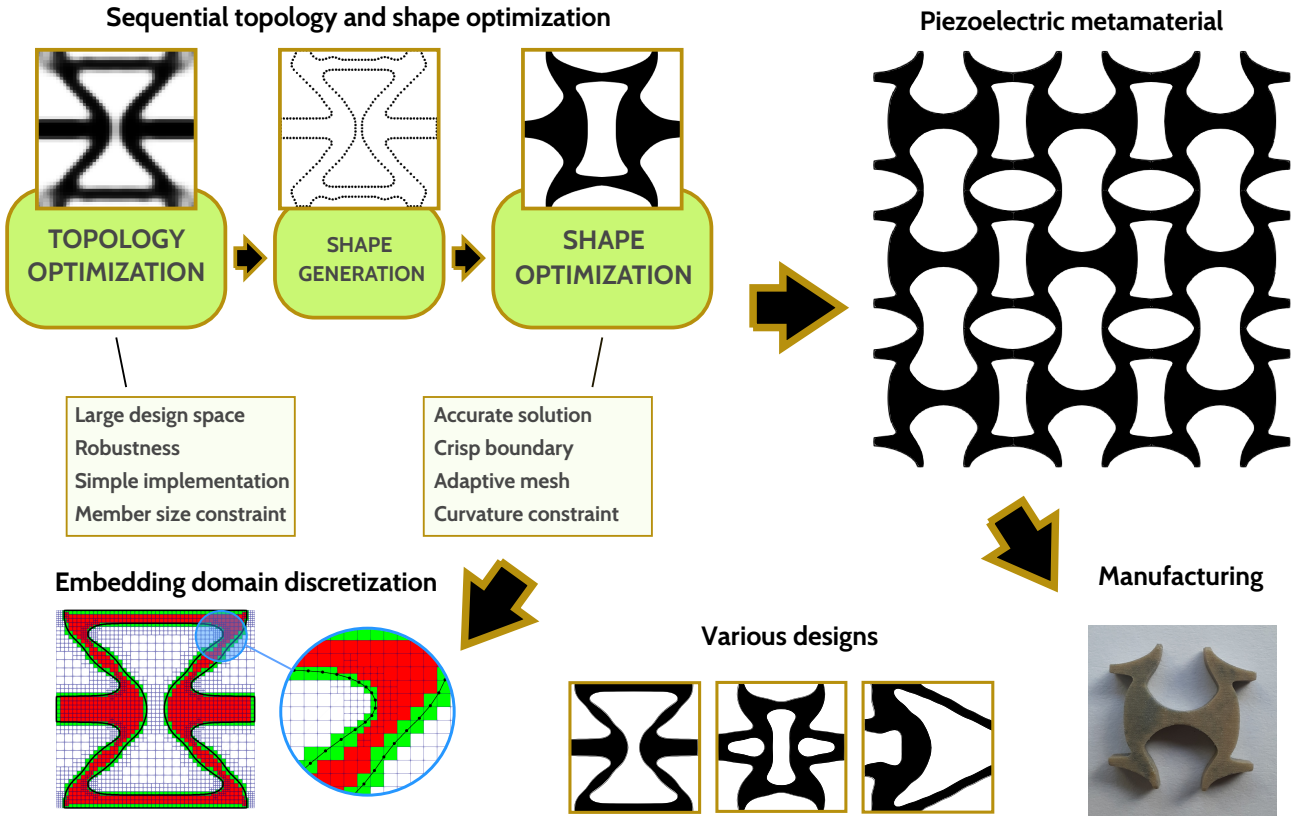

Figure 1: Graphical summary of combined topology and shape optimization for the design of piezoelectric metamaterials..

Adaptive mesh coarsening procedures for the virtual element method

Daniel van Huyssteen[1], Paul Steinmann[1], Felipe Lopez Rivarola[2], Guillermo Etse[2]

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[2] Facultad de Ingeniería, Universidad de Buenos Aires

This work is part of a larger ongoing research project that is jointly funded by the DFG (Germany) and CONICET (Argentina). Current work is focused on complimenting previously proposed adaptive mesh refinement procedures for the virtual element method (see for example [2]) with suitable adaptive mesh coarsening procedures [1]. The combination of adaptive refinement and coarsening procedures promises to yield significant improvements in computational efficiency, particularly in the case of dynamic/transient problems such as fracture.
The performance of one of the proposed adaptive coarsening procedures is demonstrated using the example problem of an L-shaped body that is stretched both horizontally and vertically (see Figure 1). A sample coarsened mesh, generated from an initially uniform and dense mesh, is depicted in Figure 2. The finest mesh is retained in the region surrounding a stress singularity, while the rest of the mesh is much coarser. Thus, demonstrating the efficacy of the procedure. Additionally, the $\mathcal{H}^1$ error is plotted against the number of nodes in the discretization in Figure 3. The proposed procedure significantly improves the efficiency of the solution, for any level of initially uniform mesh density, by eliminating a large portion of the number of nodes while introducing only a small amount of error [1].

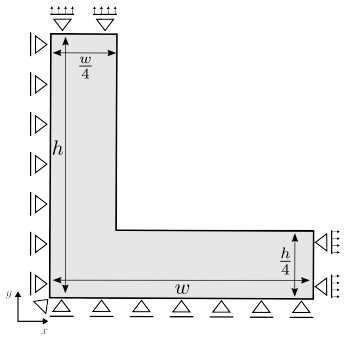

Figure 1: L-shaped body.

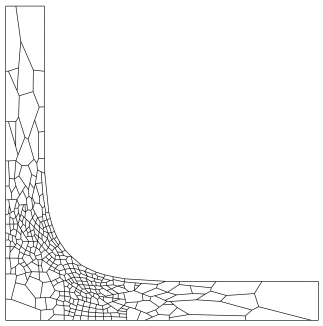

Figure 2: Coarsened mesh.

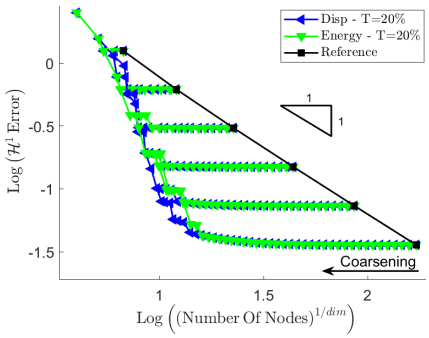

Figure 3: Error vs cost.

In addition to the work on adaptive remeshing, concurrent work is focused on developing a stochastic approach to brittle fracture analysis using a combined virtual element and interface element technique. The technique involves determining the average behaviour of a large number of randomly generated coarse mesh simulations to predict complex fracture behaviour. Numerical results indicate that this technique can produce more accurate and more reliable results than those generated from a single fine mesh simulation [3].

References

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Data-adaptive approximation of hyperelastic energy functions

Simon Wiesheier, Julia Mergheim, Paul Steinmann

Data-driven approaches are a promising alternative to constitutive modeling. The first work in this direction is by Kirchdoerfer and Ortiz from 2016. Our proposed data-adaptive approach combines the advantages of phenomenological hyperelasticity with the data-driven paradigm of directly including experimental data in calculations. Import constraints, such as thermodynamic consistency, material objectivity and frame indifference and material symmetry are satisfied a priori. In essence, we suggest formulating a finite-element-like approximation of the strain energy function E as a sum of basis functions multiplied by parameters:

$$E \approx E^h = \sum_{a=1}^{n} N_a(\mathfrak{i}^h) E_a \qquad \text{with} \qquad \mathfrak{i} \approx \mathfrak{i}^h = \sum_{a=1}^{n} N_a(\mathfrak{i})\mathfrak{i}_a \tag{1}$$

The basis functions N_a are expanded over the space of invariants $\mathfrak{i}$ which is, in the most generic form, formed by the principal invariants of the right Cauchy-Green tensor. Support points $\mathfrak{i}_a$ are distributed in the space of invariants, which are the points at which the parameters E_a are defined. In other words, the parameters are the values of the discrete strain energy function at the support points, see Fig. 1 for illustration, and are determined based on measured full-field displacements, e.g. obtained from Digital-Image-Correlation, and reaction forces by solving a non-linear optimization problem.

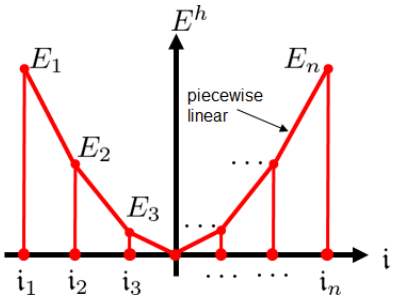


Figure 1: Exemplary piecewise linear approximation of the strain energy function to visualize the quantities introduced in eq. (1).

Fig. 2 indicates that a moderate number of parameters is sufficient to approximate smooth energy functions quite accurate. Here, the parameters match a compressible Yeoh model at the support points resulting in an interpolation error between the support points.

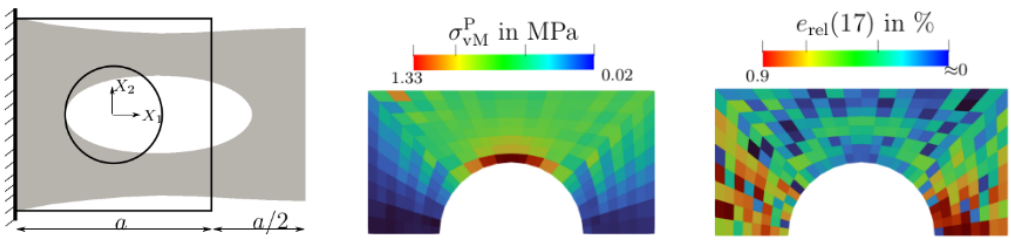


Figure 2: Contour plot of the Von-Mises stress $\sigma^{\mathrm{P}}_{\mathrm{vM}}$ (middle) corresponding to the plate benchmark (left) using a phenomenological compressible Yeoh strain energy function model to solve the boundary-value-problem. If this model is approximated with 17 parameters using eq. (1), the relative difference in the Von-Mises stress (right) is nearly zero.

– Process simulation and materials characterization –

Franco-German Research Project BIO ART

Lukas Laubert, Sebastian Pfaller

BIO ART (Optimization of the mechanical properties of BIO-sourced epoxy resins through ARTificial intelligence) is a DFG and ANR funded joint research project of four institutes, namely the Institut de Chimie et des Matériaux Paris-Est (ICMPE) at the Université Paris-Est Créteil Val de Marne (UPEC), the Laboratoire Modélisation et Simulation Multi-Échelle (MSME) at the Université Gustave Eiffel (UGE), the Department of Polymer Engineering (PE) at the University of Bayreuth (UBT), and the Capriccio group at the Institute of Applied Mechanics (LTM), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU). BIO ART's main goal is to develop a fully bio-based epoxy-fibre composite at a competitive price with thermal and mechanical properties comparable or even superior to classical petro-sourced epoxy composites. The work package designated to the LTM is mainly concerned with multiscale modeling of the epoxies and related composites developed by the ICMPE and PE. This task covers two domains, namely the "rheological properties of the continuum", which develops and calibrates a continuum mechanical constitutive law that establishes a link between the network structure of the epoxy formulations and their mechanical properties at larger scales as well as "Multiscale simulations of fracture", which develops a multiscale simulation tool that couples a fine-scale network model capable of polymer fracture at the network level with the coarse-scale continuum model providing realistic boundary conditions.
In order to enable the MSME to train an epoxy network model based on the mechanical properties of biobased epoxy synthesized by the ICMPE in a next step, a continuum mechanical model has been selected and calibrated during Lukas Laubert's master thesis, aiming to reproduce experimetal data from creep recovery experiments (exp) via FE simulations (sim/eval). The plane

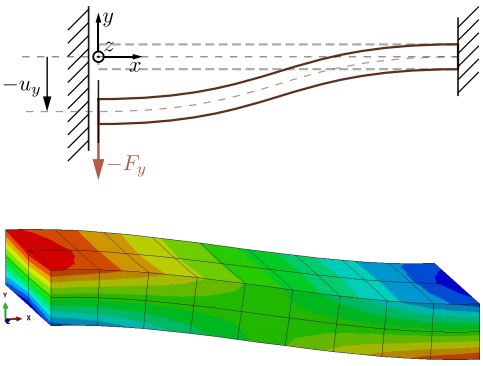


Figure 1: Schematical setup representation and deformed FE visualization.

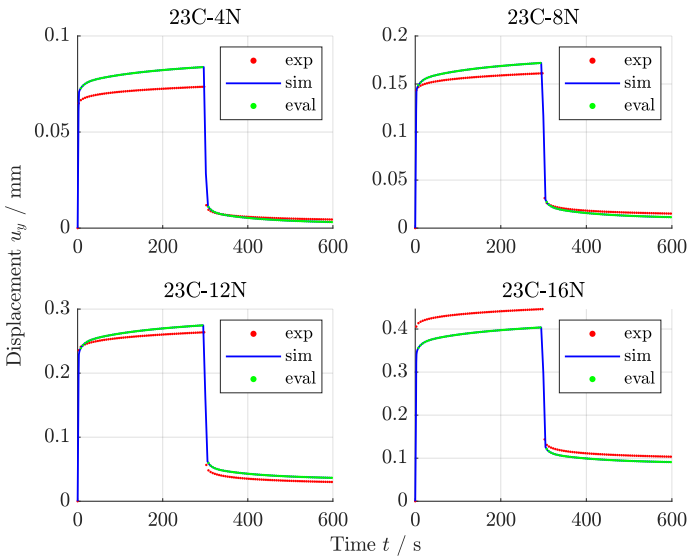


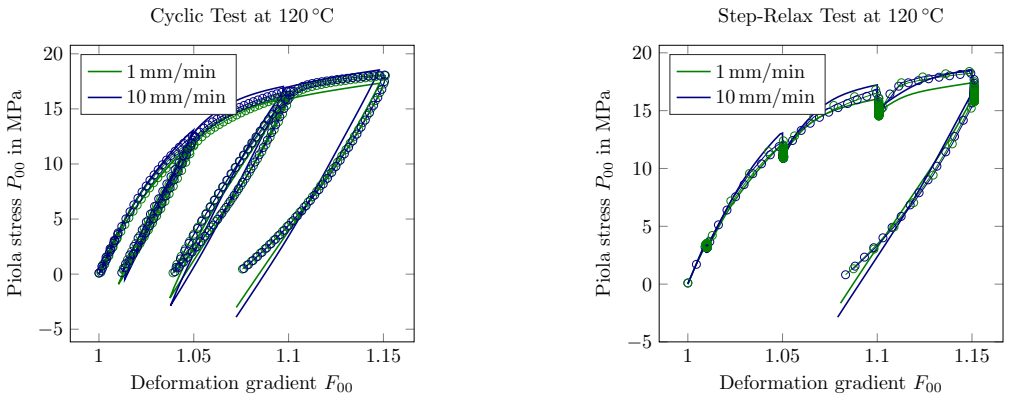
Figure 2: Comparison between experimental (exp) and simulation (sim/eval) results.

stress setup is depitcted in Figure 1, showing a schematical representation including the boundary conditions on the top and a deformed FE representation on the bottom. The results of four comparisons at 23 °C and different force levels during the creep phase are displayed in Figure 2. As the simulation results revealed certain shortcomings with regard to the hyperelastic law of the VEVP model employed, this area will be addressed in the follow-up work.

Thermo-Chemo-Mechanical Process Simulation for Powder Bed-Based Additive Manufacturing of Polymers

Dominic Soldner, Paul Steinmann, Julia Mergheim

Selective Laser Sintering (SLS) of polymers belongs to the powder bed-based additive manufacturing (AM) techniques and is widely used in industry and academia. During the manufacturing process, the material undergoes phase change from powder to molten and subsequently to solid/crystallized material. The latter transition is accompanied by volumetric shrinkage. Hence, a thermo-chemo-mechanical approach at finite strains is chosen to model the process. The modeling ansatz combines the ones proposed in [2, 3] and represents a visco-elastic-visco-plastic formulation with a crystallization dependent yield function and relaxation time. The identification of the material parameters is carried out using multi-/many objective optimization with genetic algorithms, building on the open-source library *PYMOO*[1]. The characterization of the solid material relies on step-relaxation and cyclic uniaxial test at various temperatures (performed by the Insitute of Polymer Technology (LKT) from the FAU Erlangen-Nürnberg). The comparison of experimental and numerical data (one-element tests with prescribed displacement boundary conditions) at 120 °C are presented in figure 1 and show an acceptable accuracy of the model. One challenge in the parameter identification process was given by the observation, that the higher strain rate lead to slightly lower stress values at larger strains. This can not be accounted by the current model and would require further investigation.



(a) Uniaxial cyclic test, circles refer to experimental data.

(b) Uniaxial step-relaxation test, circles refer to experimental data.

Figure 1: Comparison of experimentally measured (circles) and numerically obtained data (lines) for cyclic and step-relaxation tests at different strain rates. The rates refer to the velocity used in the machine and translate to approximately $\dot{F}_{00} \approx 1/6\,\%\,\mathrm{s}^{-1}$ and $\dot{F}_{00} \approx 1/60\,\%\,\mathrm{s}^{-1}$ respectively.

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– Structural dynamics –

Modal Analysis of a Violin

Özge Akar, Kai Willner

From a structural dynamics perspective, studying a bowed string instrument holds significant interest due to its intricate design marked by anisotropic material behavior and numerous interfaces. The present work seeks to gain a thorough understanding of the structural dynamics of a particular violin using a novel step-by-step approach. Firstly, we gather the raw material parameters of wood for each component of the violin through numerical and experimental modal analysis. In the second phase, we perform experimental modal analyses on the violin's subcomponents, which are crafted by a luthier, to ascertain the modal parameters. Simultaneously, we conduct a numerical investigation employing finite element models of the sub-components, integrating the material parameters determined earlier. After conducting a thorough comparison between the numerical and the experimental results, the violin maker proceeds to assemble the parts of the violin until its final stage of completion. Throughout this process, we investigate each production step utilizing numerical and experimental modal analysis. The high degree of correspondence between the modal parameters derived from the experiment and the numerical results obtained at different production stages illustrates the practicality of utilizing traditional modal analysis methods for intricate mechanical systems such as the violin. Additionally, the use of experimental modal analysis in examining the finalized violin enables us to make conclusive statements regarding the impact of the violin soundpost and the strings. Figure 1 illustrates the crafting process, with modal analysis conducted for each step depicted. [1]

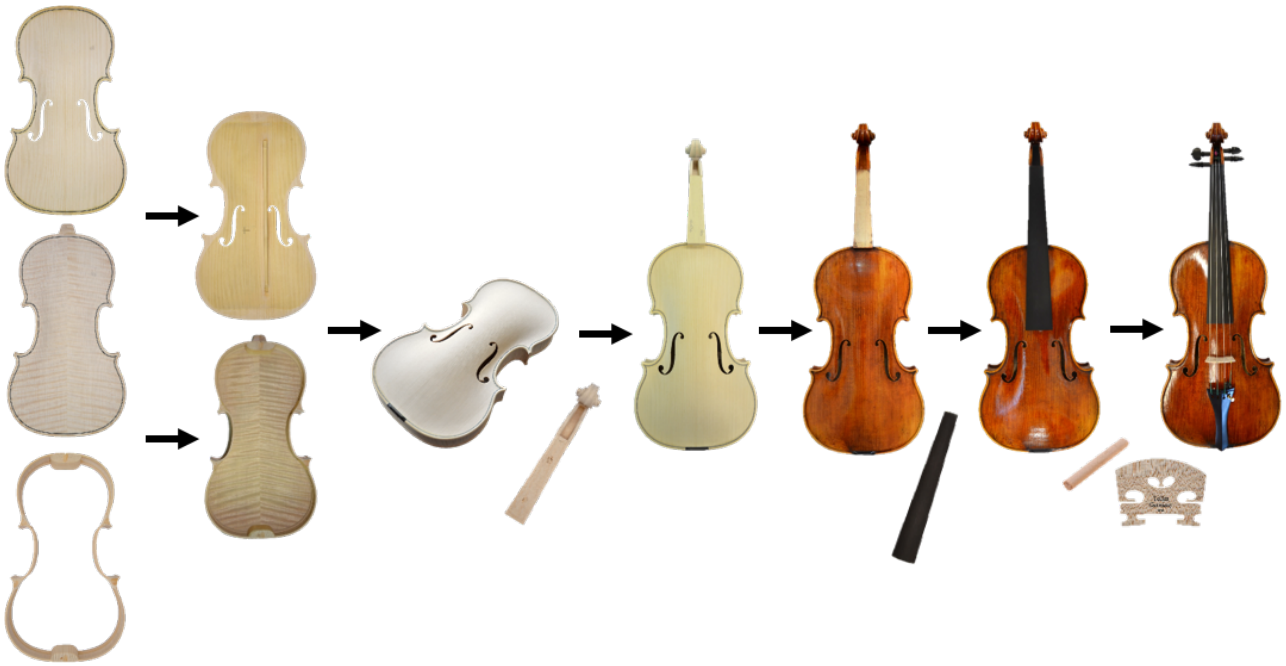

Figure 1: Crafting steps and phases of modal investigation.

References

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Quasi-periodic oscillations in dynamical systems

Michael Lengger, Kai Willner

In view of an economical and reliable design of a dynamical system, numerical predictions of its oscillatory behavior are vital to identify possible harmful vibrations. A strong focus is commonly on the steady-state response of a system under operational conditions prescribed by the number of excitation mechanisms, corresponding load amplitudes, and frequencies.

Here, small changes in the operating conditions have a significant impact on the resulting steady-state behavior, as demonstrated by the time-marching results of a single degree-of-freedom oscillator ($m = 1$ kg, $d = 0.02$ N/(ms) and $k = 4$ N/m) equipped with a Jenkin-element ($k_{\mathrm{nl}} = 5$ N/m and $f_{\max} = 3$ N). While the steady-state motion of the nonlinear system subject to a single harmonic excitation is periodic and vibrates with integer multiples of the excitation frequency, cf. Fig. 1 (top row), the response gets more involved in the case of a bi-harmonic loading with incommensurable excitation frequencies, cf. Fig. 1 (bottom row). As a result of the incommensurability, the resulting motion never repeats itself in physical time and exhibits frequencies at linear combinations of the two excitation frequencies [1]. This type of oscillation is called *quasi-periodic*.

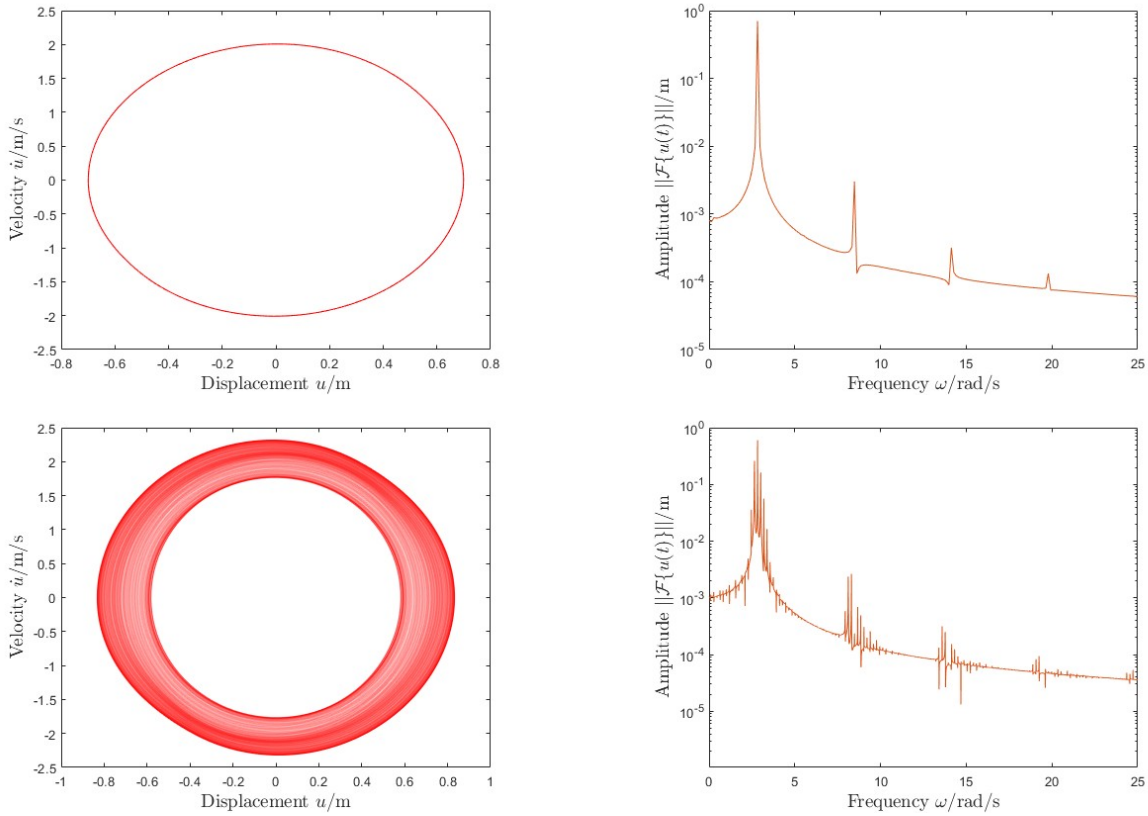

Figure 1: Phase-space representation (*left*) and frequency spectrum (*right*) of steady-state motion of Jenkin oscillator due to harmonic ($g(t) = 0.7\sin(\sqrt{8}t)$ N) (*top* row) and bi-harmonic external excitation ($g(t) = 0.6\left[\sin(\sqrt{7}t) + \sin(\sqrt{8}t)\right]$ N) (*bottom* row).

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[1] S. Bäuerle, R. Fiedler, and H. Hetzler. "An Engineering Perspective on the Numerics of Quasi-Periodic Oscillations". *Nonlinear Dyn* 108.4 (2022). Accepted, pp. 3927–3950.

– Uncertainty quantification –

Uncertainties in the context of surrogate models

Thomas Oberleiter, Kai Willner

The consideration of uncertainty in existing mechanical systems is nowadays a common method to optimize virtual computations. However, in addition to the advantage of improved reality replication, the disadvantages of the more complex calculation systems need to be considered. In the environment of interdisciplinary tolerance management, this project relies on the fuzzy uncertainty method for uncertainty analysis. Thereby, parameters are defined as fuzzy numbers. Fuzzy uncertainty requires a high number of system evaluations and is thus often only indirectly applicable. It requires substitute models for complex systems, which are applied in this work in the form of surrogate models [2]. In interdisciplinary tolerance management, complex process simulations, which appear as a kind of black box, and time-consuming real experimental setups have to be transferred into a virtual approach. A suitable approach is offered by the Kriging method or the radial basis functions. Especially the interaction of fuzzy uncertainty and these surrogate models is interesting for interdisciplinary tolerance management and offers sufficient potential for investigation.
The focus of this project is therefore on the optimization of surrogate models considered in an interconnection of several surrogate models regarding fuzzy uncertainty. Thus, fuzzy uncertainty can be better integrated in the step of creating using a new-valued sampling plan (FOSS) [1]. An evaluation and result interpretation via fuzzy numbers using the O-index or a fuzzy-based sensitivity analysis for the surrogate models has been developed and offers a feasible approach in dealing with the accuracy of the surrogate models. A detailed summary of the results is presented in [3].

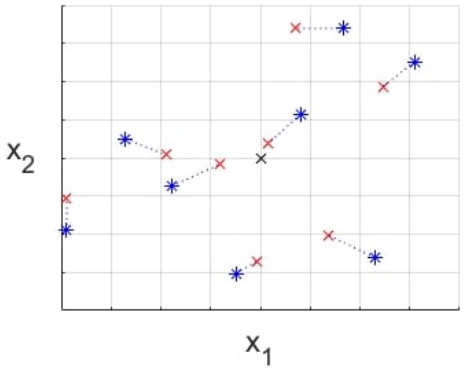


Figure 1: Scheme of the FOSS sampling plan [2].

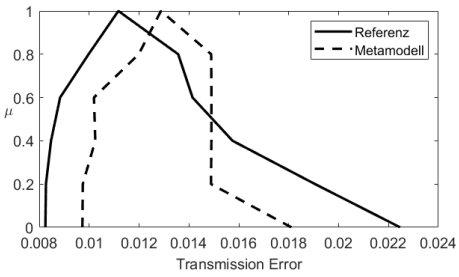


Figure 2: Example of two result fuzzy numbers (reference and surrogate model) of a characteristic variable in the gear transmission (transmission error), which are to be compared (see [3]).

References

[1] A. Forrester, A. Sóbester, and A. Keane. *Engineering Design via Surrogate Modelling.* Wiley, 2008. ISBN: 978-0-470-06068-1.

[2] T. Oberleiter and K. Willner. "Sampling strategy for fuzzy numbers in the context of surrogate models". *SN Applied Sciences* 3.831 (2021).

[3] T. Oberleiter and K. Willner. "Teilprojekt 2: Fuzzy-arithmetische Modellierung von Prozessen mit unsicheren Parametern". In: *Abschlussbericht DFG-Forschungsgruppe FOR 2271, 2. Phase. Prozessorientiertes Toleranzmanagement mit virtuellen Absicherungsmethoden.* Ed. by S. Wartzack. Erlangen: FAU University Press, 2023, pp. 39–64.

Reduced order modeling with an adaptive sampling

Dmytro Pivovarov, Paul Steinmann and Kai Willner

Reduced order modeling is a powerful technique which allows to reduce the computational costs of FEM simulations by using the data from previous calculations. One of the most efficient and widely used methods is the proper orthogonal decomposition (POD). This methods uses snapshots of the previously calculated system states to evaluate new basis vectors for further FEM simulations. The generalization of the POD to the many-parameter system is known as the low-rank tensor decomposition. However the low-rank tensor decomposition works only is the data has a tensor structure, i.e. is evaluated on a rectangular grid of samples. This sampling approach is however known for its high computational costs and is not optimal. On the other hand the strong reduction of the computational costs is achieved by using the adaptive sampling. In this project we modify the low-rank tensor decomposition to be used with the adaptive sampling approach, i.e. on a data from the unstructured grid of samples. This approach allows for a further reduction of computational costs and also for an (quasi-) optimal selection of new samples "on fly".

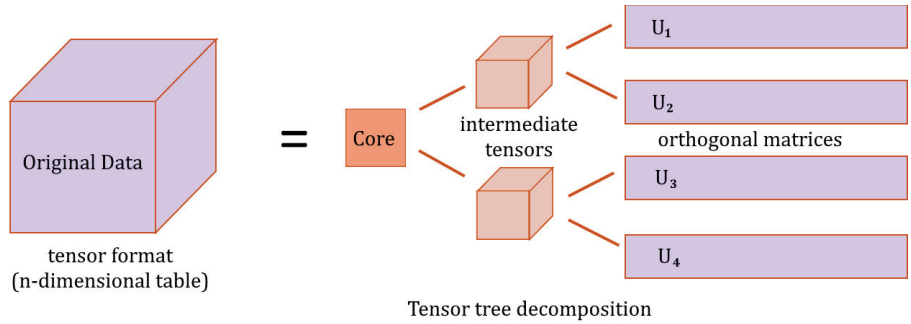


Figure 1: The tensor tree is an advanced variant of the low-rank tensor decomposition.

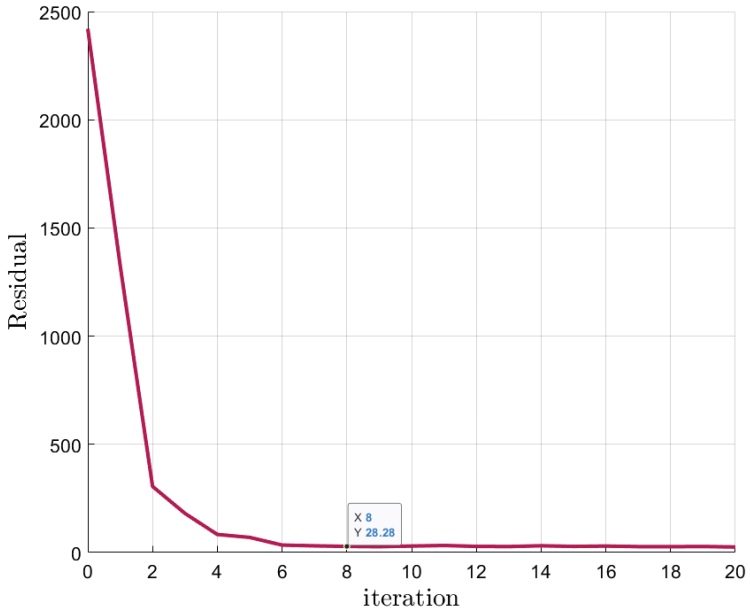


Figure 2: Rapid residual (error) decrease achieved using the adaptive sampling algorithm.

5 Highlights and social activities

5.1 LTM Band

(LSp) After a two-year break due to Covid, some old band members reunited for LTM's Xmas Party in 2022 winning a few new colleagues over:

- Julia wowing everyone with her singing and rocking her performance
- Domi playing the most modern electric 'Cajon' existing ;-)
- Özge – after doing extensive research in the field of structural dynamics on the violin – mastering its play
- Felix & Lucie at the pianos sounding like 5 pianos with Felix's talent
- Soheil at the guitar in all songs since the other 2 players were finishing their doctoral theses.

Seeing the crowd going wild during the band's performance of 7 songs and 2 encores, the rehearsals were not only fun for the band members but totally worth the effort. Thank also goes to Alexander Greiner who supported us with his amazing sound system during all the rehearsals and the performance.

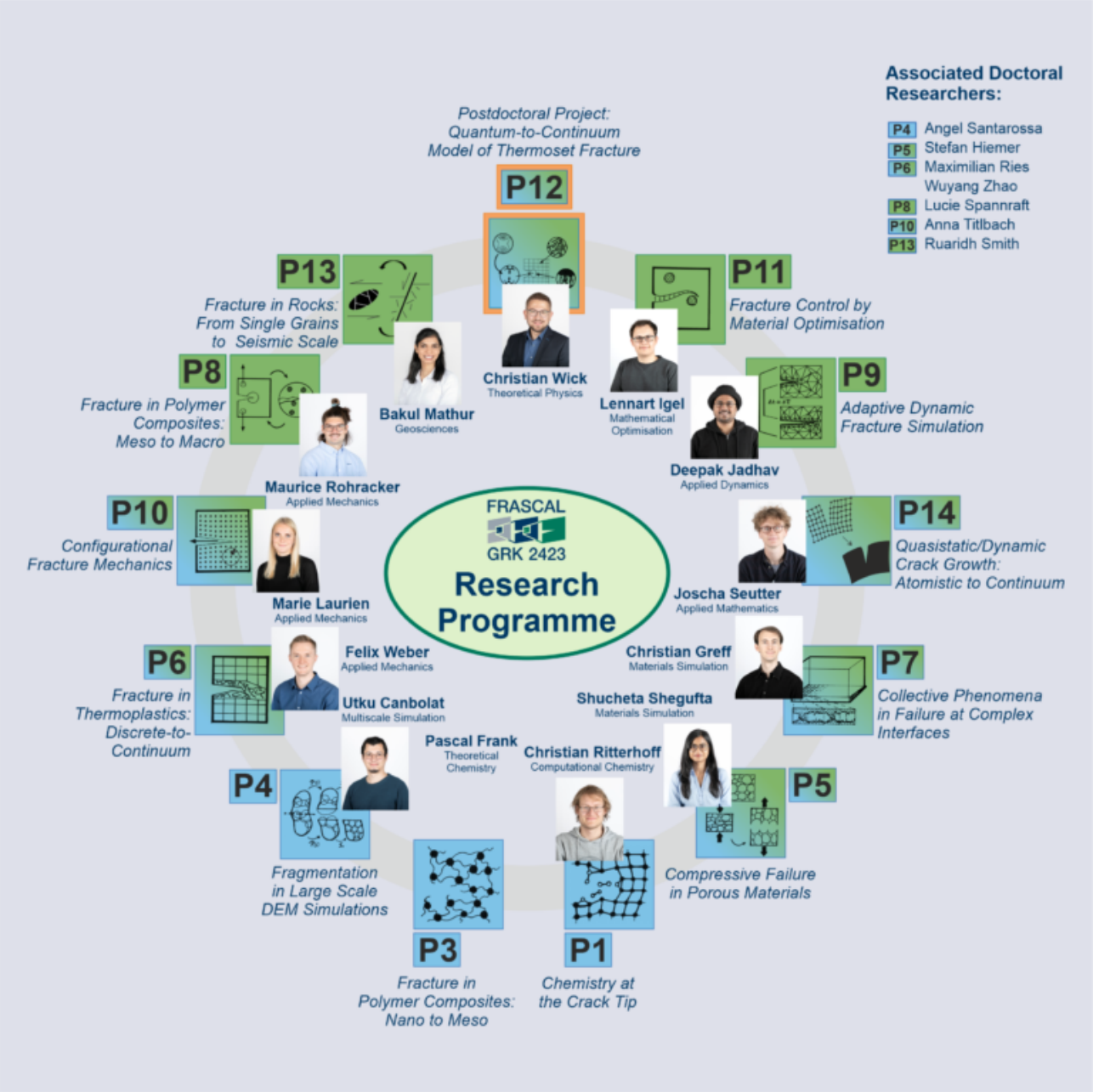


Top: The band performing at LTM's Xmas Party 2022. Bottom left: Having fun at one of the rehearsals in the LTM Seminar room after working hours. Bottom right: LTM members enjoying the musical performance.

After an expensive and fun trip to Thomann early 2023, the band was equipped with a new e-violin and Alex's new sound system.

5.2 FRASCAL activities

(LSp) The research training group GRK2423–FRASCAL (Fracture across scales) consists of 13 projects from different departments of the Faculty of sciences (Physics, Chemistry, Mathematics) and the Faculty of Engineering (Chemical and Biological Engineering, Materials Science, Mechanical Engineering). FRASCAL aims to improve the understanding of fracture in brittle heterogeneous materials by developing simulation methods at (and across) different length and time scales able to capture the multiscale nature of failure.



FRASCAL projects of the second cohort, cf. https://www.frascal.research.fau.eu/

On January 30 and 31, FRASCAL's on-site review took place in Erlangen. Based on the recommendation formulated by the group of reviewers, the DFG announced on May 5 the approval of FRASCAL's second funding phase of another 4.5 years with a funding of around 5.6 million euros.

FRASCAL Symposium

(text: Ann-Sophie Herzner; images: A. Dakkouri-Baldauf, N. Güthlein, LSp; captions: LSp)
On 15 March 2023, the 2nd FRASCAL Symposium was held at the venerable Orangerie of Erlangen. The symposium aimed to provide a platform for the FRASCAL principal advisors and prospective future Mercator fellows to share their insights on the fracture problem from a higher-level perspective. As expected, the event was well-attended by colleagues and young researchers from various institutions who had an interest in the fracture problem.

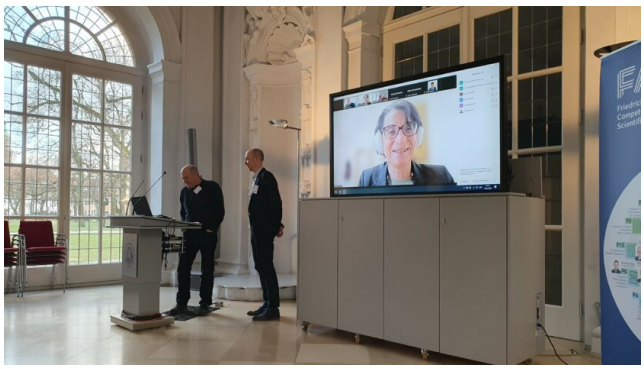



FRASCAL's spokesperson Prof. Steinmann opening the event (left). Group photo of all attendees (right).

Throughout the day, seven guest speakers delivered talks that provided valuable insights into the fracture problem. Laura De Lorenzis from ETH Zurich opened the stage with her talk on "The role of multi-physics and multi-scale approaches in fracture mechanics". Manuel Friedrich from FAU followed with a talk on "Modeling of the fracture process using cohesive zone models". Paolo Moretti from FAU reported thereupon on "Fracture of thin films and interfaces". Christian Wick, also from FAU, shared his insights on "Microstructure and fracture of advanced materials", while Erik Bitzek from MPIE Düsseldorf presented "Atomistic simulations of fracture: From continuum to discrete models". Daniel Koehn from FAU dived into "Machine learning approaches for fracture prediction", and Anna Pandolfi from Politecnico di Milano wrapped up the symposium with a talk on "Fracture of biological and soft materials".

Each talk was followed by a stimulating discussion among the attendees, which helped to deepen their understanding of the fracture problem. The symposium concluded at 4:15 p.m., with closing remarks from the organizers.





Principal advisor Prof. Moretti (left) and Mercator Prof. Pandolfi (right) presenting.

In summary, the 2nd FRASCAL Symposium provided a valuable opportunity for principal advisors, doctoral researchers and prospective Mercator fellows to share their insights on the fracture problem. Overall, it was a successful event that contributed to the advancement of knowledge in the field of fracture mechanics.





Pictures of the coffee and lunch break area prior to intense discussions.

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

We are also pleased to announce that Heidi Zinser will be taking her place in the role of FRASCAL Coordinator. We extend a warm welcome to our newest team member!





Andrea Dakkouri-Baldauf receiving flowers and vouchers for dinner and cultural events. Finally, Andrea Dakkouri-Baldauf was awarded by the FRASCAL (associate) doctoral researchers with a 3D-printed FRASCAL hyper-performer award – in the spirit of last year's high-performer awards which were given to all (associate) doctoral researchers of the first and second cohort.

FRASCAL RTG Seminar

(LSp) On April 28, the 8th FRASCAL Seminar took place, allowing scientific exchange among all FRASCALi, i.e. (associate, post-)doctoral researchers and (co-)principal advisors.
Six doctoral researchers, two associate doctoral researchers and one start-up fellow gave 20 minute presentations on their projects with subsequent ten minute Q&A sessions. Afterwards, a 'peripatetic closing discussion' was held. Of course all FRASCALi came fully prepared to the seminar – meaning having looked up the word 'peripatetic' under the initial assumption of a new 'Steinmann'sche Wortbildung' (word formation). Due to the bad weather, it was less peripatetic in the sense of 'Aristoteles & friends' walking outside during their discussions, but rather typical FRASCALesque standing around a rich buffet sipping coffee and intensifying the previous discussions.

PROGRAMME

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

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

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

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

10:40 – 11:00 COFFEE BREAK

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

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

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

PROGRAMME

12:30 – 13:40 LUNCH BREAK

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

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

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

15:10 – 15:40 PERIPATETIC CLOSING DISCUSSION



FRASCAL members at the 2nd FRASCAL Symposium (March 2023)

www.frascal.fau.eu

FRASCAL Soft Skills

(LSp) The qualification program of FRASCAL includes soft skills seminars. **'Unconscious bias in academia: How our brain tricks us'** was one of this year's seminars.

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

It is an integral part of the FRASCAL curriculum to create awareness of decision-making processes regarding gender, equality and diversity. In this context, PhD students annually invite an expert on this topic to gain further knowledge in this area.

On April 14th, the PhD students welcomed Dr. Iris Wangermann, who visited the Graduate College to hold a workshop on our unconscious biases. Dr. Iris Wangermann is an expert in inclusive leadership, intercultural team building, and consciousness.

> „We underestimate or overestimate the competence of people or allow ourselves to be influenced by the group. Talents are overlooked, people who are not necessarily best suited for the position are promoted and needs are not met, which has massive effects on your overall team performance." (Dr. Iris Wangermann)

During the workshop "Unconscious bias: how our brain tricks us" participants studied the neuroscientific and psychological basics of unconscious biases. Through personal examples and experiences, participants discovered their blind spots.

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

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

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





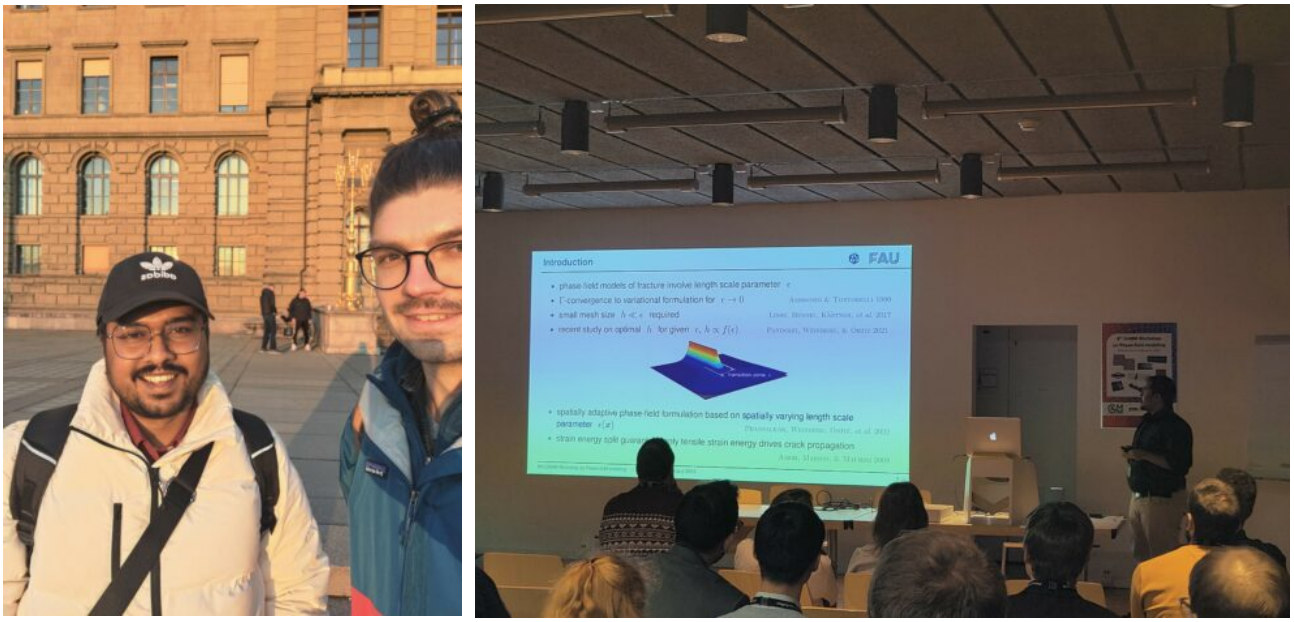
FRASCAL goes Conferences

(LSp) FRASCALi attend numerous conferences during the year. One highlight was certainly CFRAC2023 with a minisyposium organized by FRASCAL. Besides, FRASCALi enjoyed specific workshops at conferences.

(text & images: Maurice Rohracker, Deepak Jadhav) At the eighth edition of the **GAMM workshop on phase-field modeling** at the ETH Zürich Deepak Jadhav and Maurice Rohracker participated and gave a talk about their research within FRASCAL.

In this two-day workshop, different researchers from several disciplines met together in the Alumni Pavilion at ETH to talk about their recent insights of their research with a focus on theoretical and application-related aspects of the phase-field approach to study physical phenomena such as fracture. Further, also other physical phenomena, such as diffusion, thermal conduction, ferro- and piezo-electric effects, phase transformation and separation processes, biomechanics, fluid mechanics, as well as coupled problems involving multiple processes, have been presented. On top of everything, also, the development of novel, efficient numerical algorithms has been discussed along with innovative approaches based on data-driven and/or machine-learning methods.

Deepak Jadhav showed his investigations of different forms of fracture using a spatially adaptive phase-field model, and Maurice Rohracker presented a comparison of different adaptive spatial refinement strategies in phase-field fracture simulations of brittle materials. One highlight of the event was the dinner in the Dozentenfoyer on top of the main building of ETH Zürich with a very nice view over the city. A special thanks to the organizers of this event and FRASCAL for the assumption of all travel costs.



Deepak Jadhav and Maurice Rohracker exploring Zurich (left). Deepak Javdhav during his talk (right).

(Maurice Rohracker)

The **7th International Conference on Computational Modelling of Fracture and Failure of Materials and Structures (CFRAC)** took place from June 21 to 23, 2023 in the beautiful city of Prague.

FRASCAL organized a **mini-symposium "Connecting scales and disciplines to model fracture"** at CFRAC comprising three sessions with four presentations each. We were very pleased to welcome Prof. Marc Geers from the Eindhoven University of Technology as the keynote speaker at our symposium. Christian Greff and Maurice Rohracker also presented their current work in one of the sessions. Furthermore, Stefan Hiemer gave a talk on his research covered in his recently achieved doctoral degree.

A special thanks go to Maurice Rohracker and Shucheta Shegufta for co-organizing the mini-symposium.

Besides the very interesting scientific discussions at the conference, the organizers also convinced with a very fitting social program. In addition to the conference dinner at Letenský zámeček, in the heart of Letná Park next to the popular beer garden, there was also an invitation to the classical concert by the soloists Marie Fajtová and Roman Patočka accompanied by the Bohemia Chamber Orchestra in the Bethlehem Chapel – presenting a further highlight at CFRAC 2023.

Many thanks to the organizers of CFRAC 2023.





Kick-off event of CFRAC (left), FRASCAL doctoral researcher in Prague (middle), classical music concert in Bethlehem Chapel (right).

FRASCAL RTG Retreat

On November 17–18, the 3rd FRASCAL Retreat took place at Kloster Banz in Bad Staffelstein, located in the so-called 'Franconian Switzerland'. This idyllic community is known far and wide for its breathtaking scenery and health resort. What a fitting place for a scientific exchange in a quiet and thought-provoking environment! Kloster Banz serves as an educational centre that will generously open its doors to the FRASCAL Research Training Group. FRASCAL retreats are usually held as two-day seminars away from the FAU campus, accompanied by social activities to allow for informal get-togethers.

PROGRAMME

Friday, November 17

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

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

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

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

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

10:30 - 11:00 COFFEE BREAK

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

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

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

12:00 - 13:00 LUNCH BREAK

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

15:30 - 16:00 COFFEE BREAK

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

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

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

17:30 - 18:30 DINNER

19:00 Team Building Activities



www.frascal.fau.eu

PROGRAMME

Saturday, November 18

07:30 - 09:00 BREAKFAST

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

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

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

10:00 - 10:30 COFFEE BREAK

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

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

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

12:00 - 13:00 LUNCH BREAK

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

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

13:40 - 15:00 Poster Session with Coffee

15:00 - 15:10 CLOSING

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5.3 EBM

(Soheil Firooz) The CRC 1540 "Exploring Brain Mechanics" started in January 2023. It represents a cutting-edge collaborative research endeavor that transcends traditional departmental boundaries, bringing together expertise from diverse fields including the mechanics, material science, artificial intelligence, biology, optics, and more. By synergizing insights from multiple disciplines, this project seeks to advance our understanding of the mechanical intricacies underlying brain function and dysfunction. The project is divided into three main subproject and a cross-sectional project.

Focal Research Area A: Brain Development and Malformations: In FRA A, we delve into the intricacies of brain development, with a keen focus on malformations associated with neurological disorders like epilepsy. Sub-project A01 employs computational modeling to systematically decipher the physical mechanisms underpinning brain malformations. This work synergizes with quantitative characterizations of human brain malformations in A02, as well as in vitro and in vivo insights gained from Xenopus (A03/A05) and organoids (A03/A04) using engineered brain tissue-like matrices.

Focal Research Area B: Spinal Mechanics: FRA B zooms in on spinal cord injury and disease, emphasizing mechanically stimulated regeneration of central nervous system (CNS) function. Computational modeling (B01) complements efforts to unravel the mechanical landscape's role in regeneration, disease promotion, and limitation (B02, B03, B04). In addition, in vivo mechanical manipulation is explored in B05 to further advance our understanding of spinal mechanics.

Focal Research Area C: Cellular Mechanics: Cell-matrix interactions take the spotlight in FRA C, where computational modeling in C01 examines the role of mechanics in neuronal plasticity, seizure-like hyperactivity, and cellular differentiation (C02, C03, C04). These investigations draw insights from the versatile experimental platform established in C05, shedding light on mechanosensing and -transduction in cellular processes.

Research Area X: The cross-sectional projects in X form the backbone of our integrative approach. X01 focuses on standardizing and integrating in vivo and ex vivo testing data across scales, while X02 leverages advanced machine learning techniques to explore the transferability of data across different species and experimental methods. Finally, X03 is dedicated to the design of engineered substitute materials for brain tissue, paving the way for innovative solutions in the field.



EBM Kick-Off Meeting

(Soheil Firooz) On March 17th, 2023, EBM held its kick-off meeting at the Fraunhofer Institute for Integrated Systems and Device Technology (IISB) in Erlangen. The event was attended by researchers from the fields of engineering, physics, biology, medicine, and clinics who are involved in the CRC 1540. The goal of the project is to combine the expertise of professionals from Erlangen and Berlin and use mechanics-based approaches to improve our understanding of the central nervous system's function. In the long run, this should lay the foundation for improving the diagnosis and treatment of neurological disorders.



EBM kick-off meeting (image: A. Greiner).







EBM kick-off meeting (discussions).

1st EBM Retreat

(Soheil Firooz) The 1st EBM Retreat took place from September 21st to 22nd, 2023 at the Hotel Arvena Reichsstadt in the small historic town of Bad Windsheim and provided a platform for scientific presentations primarily from doctoral researchers and postdoctoral researchers. The main objective of this conference was to present the current status of the 19 ongoing research projects and stimulate lively and constructive discussions to strengthen and further develop collaboration between various research projects.



EBM first retreat (group photo, image: S. Schmitzer).



EBM first retreat (presentations).

5.4 Capriccio activities

Capriccio Junior Party

(Sebastian Pfaller)

On April 26, the Capriccio group invited their students involved in the group's research activities to the annual "Capriccio Junior Party". It was a great pleasure for all to meet in person and to discuss scientific issues, but also to have individual chats beyond research.

As a good tradition, all participants contributed to a buffet comprising a large variety of salads, side dishes, and desserts and enjoyed freshly grilled bratwursts, steaks, and vegetables. As another good tradition, we were pleased to welcome members of the BRAINIACS group.

We are very much looking forward to future joint activities with our motivated students and will definitely schedule another Capriccio Junior Party for 2024!



Photo: Sebastian Pfaller.

Visit of the Müller-Plathe Group on May 25

(Felix Weber)

On May 25, 2023, the Capriccio group, represented by Sebastian Pfaller and Felix Weber, visited the group of Prof. Dr. Florian Müller-Plathe at the Technische Universität Darmstadt. There, we had a fruitful discussion on fracture simulations using coarse-grained molecular dynamics models. In a first part, the general applicability of (generic) coarse-grained molecular

dynamics models was addressed, which included a summary of important properties these models have to exhibit for a fracture simulation to be physically and chemically sound. After an enjoyable lunch break in the city center of Darmstadt, a second part followed, in which the PULS Group from FAU Erlangen-Nürnberg took part via Zoom. Here, we thematized ways to implement physically motivated bond breaking criteria into the molecular systems. We cordially thank our colleagues in Darmstadt for welcoming us at their institute and look forward to our next meeting.

Maxime Vassaux' visit to Erlangen

(Felix Weber)

From October 2 to 7, 2023, Dr. Maxime Vassaux from France visited the Capriccio group. Maxime is a CNRS Researcher at the Institute of Physics in Rennes and is planning to use the Capriccio method for multiscale FE-MD simulations of silica glass. During the week of his visit, we were able to take the first steps in this direction and have already obtained some very promising results.
On October 6, Maxime gave a special seminar in the research training group FRASCAL on "Probing mechanical properties with chemical specificity using molecular and multiscale simulation". Not only after the seminar, but also during the whole week, many exciting discussions with colleagues from FRASCAL and from the Institute of Applied Mechanics took place. Apart from the scientific program, we still found some time for joint activities: For example, on October 3, which is a public holiday in Germany, Felix and Maxime biked to Nuremberg and met up with Sebastian, who gave a guided tour of the premises of the Fränkische Museums-Eisenbahn e.V. Nürnberg and after this of the city center of Nuremberg. Another highlight was a joint lunch with the PULS group on October 5. In conclusion, the week was a complete success and we are very much looking forward to the upcoming joint activities with Maxime.

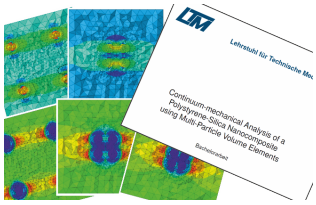


Photo: Sebastian Pfaller.

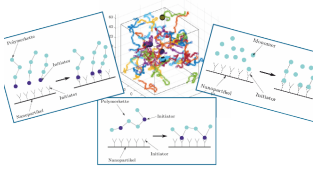
2023 - a year full of graduations for the Capriccio Group

(Maximilian Ries)

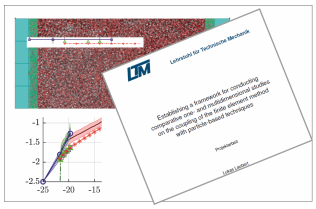
2023 has been a very succesful year for the Capriccio Group in which we could celebrate a plethora of graduations from our doctoral candidates and supervised students. In the following, we briefly recap these highlights and would like to thank everyone who contributed to the success of this year.



Eva Richter, Bachelor thesis. We are pleased to announce the completion and successful defense of Eva Richter's bachelor thesis! She continued the studies within the polystyrene-silica interphase project and implemented an automated generation of representative volume elements (RVEs) with multiple filler inclusions at various sizes and mutual distances. After this, she extensively investigated the impact of filler distribution and content on the overall stiffness and strength of the RVEs. Fortunately, we could win Eva to stay part of the Capriccio group as a student research assistant and to extend her studies in the context of multiscale modelling of polymer nanocomposites. (S. Pfaller)



Sebastian Reber, Project thesis. We congratulate Sebastian Reber who completed and successfully defended his project thesis on polymer nancomposites with grafted nanoparticles. He implemented a numerical tool in LAMMPS to create nanoparticles with surface grafting inspired by the techniques used in polymer synthesis. Based on this, Sebastian generated polymer samples and thoroughly investigated the influence of grafting density, filler size, and filler content on the stiffness and strength of a generic polymer nanocomposite. His work is another important contribution to our research on interphases in polymeric materials at the the nanoscale and extends our capabilities towards filler particles with surface treatment. (S. Pfaller)

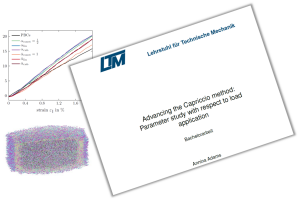


Lukas Laubert, Project thesis. We congratulate Lukas Laubert who completed and successfully defended his project thesis on a comparison between the Capriccio method in 3d with a simplified 1d setting. Lukas set up a one-dimensional representation of a three-dimensional coupled MD-FE system and implemented a smart evaluation scheme to assess the deviation between these two systems. By the highly simplified 1d setting, which mimicks the Capriccio coupling by a chain of particles connected to an "FE system" of linear trusses, he investigated the influence of the coupling parameters and discussed it in view of the 3d setting. Based on Lukas' thesis, subsequent studies will focus on further understanding of the physical meaning of the coupling parameters and on strategies to further reduce deviations. (S. Pfaller)

Maximilian Ries, Doctoral thesis. We are delighted to announce the graduation of Dr.-Ing. Maximilian Ries. In his thesis "Characterization and modeling of polymer nanocomposites across the scales," Maximilian introduces a methodology to derive continuum mechanical models for polymer nanocomposites (PNCs) based on molecular dynamics. He thus combines the advantages of particle-based and continuum approaches. Furthermore, the obtained constitutive descriptions for matrix, filler, and interphase form the prerequisite for analyzing representative volume elements (RVEs). Using these RVEs, he evaluates the influence of filler content and distribution on the polymer nanocomposite's overall stiffness. Consequently, his interdisciplinary work contributes significantly to understanding polymer nanocomposites, especially the crucial matrix-filler interphase, and thus complements experimental insights. Moreover, the transfer of molecular-scale insights into continuum mechanical models forms an essential link between the chemistry and engineering communities for the numerical modeling of polymer nanocomposites. Maximilian will continue his academic career as a postdoctoral researcher in the Capriccio group, where he will switch his research focus to polymer fracture and the mechanical behavior of adhesives. (M. Ries)



Annina Adams, Bachelor thesis. We congratulate Annina Adams on the successful completion of her bachelor thesis titled "Advancing the Capriccio method: Parameter study with respect to load application". In her thesis, Annina complemented a recent study of equilibration simulations of molecular dynamics samples under stochastic boundary conditions using the Capriccio method with respect to the sensitivity to the FE-MD coupling parameters (https://doi.org/10.1016/j.finmec.2022.100159). Particularly, Annina subjected the systems to uniaxial tensile loads and investigated the influence of essential characteristics of the coupling concept. The results obtained in Annina's studies provide important insights into the transmission of deformations between the continuum and the particle domain. (F. Weber)



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



terial behaviour and large strains and gives an outlook to coupled fracture simulations with the vicinity of the crack tip resolved at the molecular level. We wish Wuyang a successful continuation of his research activities and all the best for his future! (S. Pfaller, W. Zhao)

Lukas Laubert, Master thesis. We are very happy to congratulate Lukas Laubert on receiving his master degree and to warmely welcome him as our new group member. His master thesis on "Mechanical Analysis of Bio-Sourced Epoxy: Study of Elastic, Viscous, and Plastic Properties" forms a highly important contribution for the scientific activities of the Capriccio group and lays the foundations for Lukas' succeeding doctoral research project, which is part of the Franco-German project "BIO ART". In his master thesis, Lukas did a literature review on available continuum mechanical material models capable to reproduce the thermo-mechanical behaviour of highly inelastic thermosetting polymers as synthesised from biological reseources by our French colleagues. Furthermore, he specified a numerical representation of the experimental testing set-up used by our collaborators at the Institut de Chimie et des Matériaux Paris-Est (ICMPE) at Thiais. In this course, Lukas revisited, among others, the foundations of Bernoulli's beam theory, of elastic, viscous, and plastic material modelling, of experimental dynamic mechanical thermal analysis (DMTA) and time-temperature superposition as well as various important aspects in the context of applying the Finite Element method for parameter identifications of constitutive laws. To this end, he has been in close interaction with the colleagues at ICMPE, but also with the developers of a highly promising hyperelastic finite-strain viscoelastic-viscoplastic material model at the Université de Liège in Belgium. Eventually, Lukas sucessfully demonstrated the capabilities of the chosen material model and gave a comprehensive overview of aspects requiring careful attention in his further studies. We wish Lukas a good start in the Capriccio group and a successful doctoral project! (S. Pfaller)



5.5 IRTG 2495: Kick-off Meeting in Japan

(Michael Schwarz) From February 27 to March 1, six members of LTM participated in the Kick-off Meeting of IRTG 2495 *Energy Conversion Systems* in Gifu, Japan. On the one hand, the meeting served the annual exchange of all project participants from Japanese and German side. On the other hand, after the first three years of the project, the transition from the first to the second cohort of doctoral researchers was at hand. After the journey via Tokyo, several train rides towards Nagoya (regular customers of Deutsche Bahn highly appreciate the punctuality of Japanese trains) and the onward journey by bus to Gifu, the actual meeting took place in a local hotel.

The first day of the meeting started with an opening by the IRTG and JGGE coordinators Prof. Webber (FAU) and Prof. Kakimoto (Nagoya Institute of Technology, NITech). Since the IRTG consists of twelve subprojects A to L, a presentation was given for each of the projects by the corresponding Principal Investigator (PI), giving the current status and an outlook on the planned future work. The second day continued the missing presentations and gave all doctoral researchers the opportunity to participate in several ring lectures and workshops given by Japanese professors, while the PIs of all projects met separately.
Both days ended with a dinner where everyone could demonstrate their chopstick handling skills and typical Japanese food was served. The Japanese food in general was a great experience. For example, miso soup was served for lunch along with a personalized bento box. While miso soup is a common accompaniment to all sorts of dishes, consisting of a *dashi* stock along with miso paste, bento boxes are a type of Japanese lunch box. With the crucial difference that the individual small bites of fish, meat, vegetables, rice and fruit form a beautifully arranged complete meal.



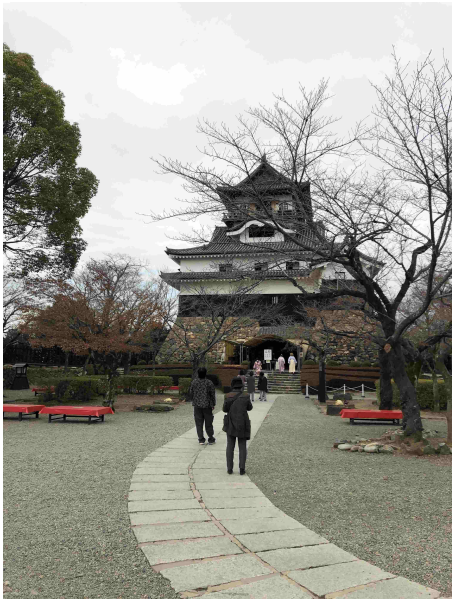
View on Mount Fuji during the approach to Tokyo (left), part of the skyline of Nagoya (middle) and Nagoya city center (right).




Impressions form the meeting venue in Gifu with all participants from Japanese and German side.

On the third and final day, the meeting ended with a small cultural program in the form of an excursion to Inuyama Castle, which has been a national historical site of Japan since 2018 and was built in the 16th century. After arriving by bus, all participants were given a guided tour of the entire complex around the castle. A special highlight was the tour of the castle itself. Access is only permitted without shoes. In case of unintentional non-observance, a friendly but firm warning is immediately given by the surrounding staff (this information was, of course, only communicated to the author by colleagues). The last part of the tour was the walk around the top of the tower with a magnificent view over Gifu and the Kiso River.

Finally, the return bus ride to Nagoya, several train rides towards Tokyo (again all on schedule), and the flight back to Frankfurt formed the conclusion of an intense, but above all interesting trip.




Group photo of all LTM members (right) at the foot of Inuyama Castle (left).

5.6 13th Workshop of Young Researchers in Mechanics in Zell am See

(Nina Reiter) From March 6 to 10, Silvia Budday, Jessica Faber, Alexander Greiner, Jan Hinrichsen and Nina Reiter joined the 13th Workshop of Young Researchers in Mechanics in Zell am See that was organized by the ISD Stuttgart led by Prof. Tim Ricken.
During the day, we went skiing in the Austrian Alps, while the late afternoons and evenings were reserved for presentations and group work. Jan gave a talk on "1) Identifying region-dependent material parameters. 2) Can a multifield computational model help to predict cortical malformations?". Additionally, we used the cozy environment to sit together and discuss strategic aspects regarding the new Institute of Continuum Mechanics and Biomechanics ICM (or LKM in German).
Even though the week ended prematurely for some of us due to a nasty virus, we still had a great time and would happily join the workshop again in the future.





5.7 18th International Symposium on Computer Methods in Biomechanics and Biomedical Engineering (CMBBE)

(Emely Schaller)

In the beginning of May, the "18th International Symposium on Computer Methods in Biomechanics and Biomedical Engineering" took place in Paris (France). Nina Reiter, Emma Griffiths and Saeed Zarzor from LKM and Emely Schaller from LTM attended the Symposium to present their recent research to scientists interested in biomechanics. Silvia Budday (LKM) enriched the Symposium by chairing the session "Exploring brain mechanics". The talks and poster presentations were given in the lecture halls of "Arts et Métiers - Institute of Technology, Institut de Biomécanique Humaine Georges Charpak" that were – to be honest – sometimes hard to find.

Besides the scientific program, Paris has a lot of worth seeing places that we explored during some free time. Especially the conference dinner on the legendary Bateau mouche boat, on which we drove along the Seine, was one of the highlights of this Symposium. During the boat trip we had some wonderful and impressive sights on famous constructions such as the Eiffel Tower by day and night.









5.8 LTM & LKM @ Berg

(Maurice Rohracker with the help of some technology)

The Erlanger Kermis (Berg), a beloved local tradition in the heart of Bavaria, served as the perfect backdrop for a memorable Tuesday afternoon for all the Friends of Mechanics. As the institute members gathered at Berg, they were welcomed by the cheerful strains of brass music, pretzels, and beer. The lively tunes set the tone for an afternoon filled with not only scientific discussions, but also with joy and laughter. Soon, a vibrant party band took the stage, infusing the air with infectious energy. This music, combined with the conviviality of the event, inspired even the scientists to rise from their seats and dance on the benches. It was a day that reminded them that even in the world of science, there's always room for a little joy and togetherness. A big thank you to Lars for his fantastic organisation, let's hope it wasn't the last time!



People from LTM and LKM sitting in the front row of the stage at Erich Keller @ Berg in 2023.

5.9 Summer Party

(Laura Ruhland)

During a very sunny day on June 13 we all gathered for our summer party. The party started at lunchtime with a delicious BBQ. Thanks to our BBQ master Gunnar we had a wonderful choice of beef, lamp and sausages. Additionally, a large variety of salads were contributed as side dishes to our buffet. The lunch was followed by homemade cake and coffee in the afternoon. Later that day we had many lively conversations over some chilled drinks and music which led until the late evening.

The summer party was en enjoyable event to all of us and further strengthened our team. We are pleased to celebrate more parties like this in the upcoming year.









5.10 CISM Course on Nonlinear Electro- and Magneto-Mechanics: Theory, Computations, and Experiments

(Markus Mehnert) In cooperation with Prashant Saxena, Professor Steinmann organized the block lecture on *Nonlinear Electro- and Magneto-Mechanics: Theory, Computations, and Experiments* in the scope of the summer courses of the International Centre for Mechanical Sciences (CISM) in Udine (Italy). Besides the two organizers, the presentations were held by Luis Dorfmann, Daniel Garcia-Gonzales, Costas Danas and Mark-Andre Keip, all of which are well known specialists in the field of electro- and magneto-mechanically coupled problems. In an attempt to hold a presentation that would deliver a unique experience in this high quality field of researchers, similar to Hannibal with his elephants we planned on crossing the alps with a large, heavy and in many aspects impractical surprise: our electro-mechanical testing device (visible in the left of the first picture below). Thus, instead of comfortably flying we chose to rent a car and after an eight hour drive we finally arrived in Udine on the evening before the start of the lectures full of the fear that the sensitive equipment did not survive the strenuous journey. But Fortuna was merciful and apart from a lose PCI-card in the PC that had to be reconnected, the machine worked just fine. So on the first day of the course an electro-mechanical investigation of VHB 4905 could be presented to the interested audience of about twenty people from all around Europe. This served as a welcome change of pace from the other more theoretical presentations. Overall, all talks were excellent and did not contain a lot of redundant information despite their similar research focus. They nicely showed the huge potential and the large variety in research projects and possible applications. All of this with the backdrop of a historic Italian city makes the CISM courses an extraordinary experience and fantastic possibility to receive scientific education.

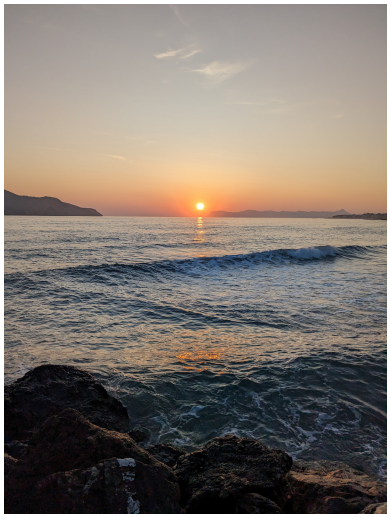


(left) Professor Steinmann starting the lecture on Experimental and Numerical Investigation of the Thermo-Electro-Mechanical Behavior of Dielectric Elastomers. Seen on the left is the testing device shipped safely over the alps. (right) Poster session in the yard of the Piazza Garibaldi with participants and lecturers of the course.

5.11 Science and Sunshine – COUPLED PROBLEMS 2023

(Chaitanya Dev)
What do you get when you combine a conference on "Coupled Problems" with a seaside getaway? A recipe for sun-soaked scientific adventure! Me, Gabriel and Andi, jetted off to International Conference on Computational Methods for Coupled Problems in Science and Engineering (COUPLED PROBLEMS 2023) in the charming Chania, Crete. This beautiful Greek city, perched on the northwest coast, provided the ideal backdrop for our scientific escapade.
While the conference's aim was to tackle complex mathematical models, we decided to add a dash of fun to the mix. Our presentations, delivered with a side of beach time, were a hit. We learned that when it comes to coupled problems, a bit of sunshine and beaches can make all the difference!








5.12 GAMM Juniors Fall Meeting at ETH Zürich

(Text: Nina Reiter, figure arrangement: PowerPoint Designer)
From October 9 to 11, Nina participated at the annual GAMM Juniors Fall Meeting at ETH Zürich. The purpose of this meeting is to expand the Juniors' scientific networks, discuss existing GAMM Juniors projects, and initiate new projects.
This year, we were very happy to have Prof. Claudia Schillings, the GAMM's representative for junior researchers, and Prof. Karsten Urban, the president of the GAMM, as special guests for two Q&A sessions.
During the scientific part of the meeting, Nina gave a talk about "Human Brain Mechanics in Health and Disease", providing an overview of her own research project and its close connection to projects of the new CRC "Exploring Brain Mechanics".
On the last day of the meeting, we went hiking on the Uetliberg and enjoyed the panoramic view of Zürich and the Zürisee from the top of the mountain.



Some impressions from Zürich: Botanical garden in the morning sun. View from the Uetliberg. Mysterious lamp-post animal in the Uetliberg forest. Dozentenfoyer of the ETH (rooftop terrace only for lecturers). The GAMM Juniors who could make it to this year's meeting.

5.13 Advanced Course on Peridynamics in Udine

(Marie Laurien)

From October 22 to 26, the advanced course on "Peridynamic models for material degradation: From fracture/ fragmentation to corrosion; from models to computer codes" took place at the International Centre for Mechanical Sciences (CISM) in Udine (Italy). Two LTM members, Soheil Firooz and Marie Laurien, participated. The four-day program consisted of lectures by four renowned professors in the field of peridynamics, who shared their expertise on various aspects of the peridynamic theory and its application. In the evenings, the authentic and charming town of Udine invited to continue the scientific discussion with the other PhD students from the peridynamic community while enjoying good Italian food.



Group picture of the professors and the participants at CISM.

5.14 Works Outing to Bamberg

(text: Özge Akar, images: Lars Schmelzle, Maximilian Ries)

On October 27th, we organized a works outing to the lovely Franconian town of Bamberg, renowned for its breweries. We opted for a train journey to reach our destination. Upon arrival, our day began with a guided city tour, available in both English and German to cater to everyone's language preferences.





The city tour allowed us to explore Bamberg's historical landmarks, including the Old Town, Bamberg Cathedral, and the Rose Garden, among other points of interest. It was a leisurely walk that provided a deeper understanding of the city's history and charm.





Following the tour, we gathered at the Brudermühle, a traditional Franconian restaurant that complemented the city's historical ambiance. We enjoyed a satisfying lunch with a taste of local specialties, which was a pleasant culinary experience.

The highlight of our day was the brewery tour at Schlenkerla, an informative and entertaining exploration of Bamberg's brewing heritage. We had the chance to learn about the traditional brewing process and sample the distinctive Bamberg Rauchbier, known for its smoky flavor. It was an educational and enjoyable experience that offered insight into the local beer culture.









As the day drew to a close in Bamberg, we departed with a deeper appreciation for the city's history and beer culture. It was a well-rounded excursion that combined history, local cuisine, and the art of brewing, leaving us with meaningful memories of our visit to Bamberg.

