Lehrstuhl für Technische Dynamik
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Report
Institute of Applied Dynamics
2023

Friedrich-Alexander-Universität
Technische Fakultät

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1 Preface

This annual report outlines the scientific and educational endeavors of the Institute of Applied Dynamics (LTD) guided by Prof. Dr.-Ing. habil. Sigrid Leyendecker, the current chairperson of the Department of Mechanical Engineering, at Friedrich-Alexander-Universität Erlangen-Nürnberg throughout 2023. LTD's members are deeply engaged in researching various fields, including multibody dynamics, biomechanics, robotics, motion capture, nonsmooth mechanics, structure-preserving methods, optimal control, and fracture mechanics. Sincere appreciation goes to the technical, scientific, and administrative staff at LTD, along with every student involved, for their contributions toward making this year a success for the Institute of Applied Dynamics. We hope you take pleasure in browsing through our annual report.

2 Team

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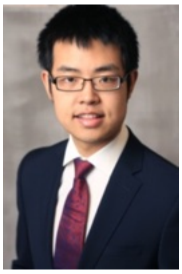
Student assistants are mainly active as tutors for young students in basic and advanced lectures at the Bachelor and Master level. Their contribution to high quality teaching is indispensable, thus financial support from various funding sources is gratefully acknowledged.


G. Capobianco


X. Chen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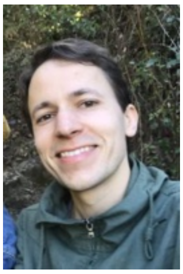
D. Huang


D. Jadhav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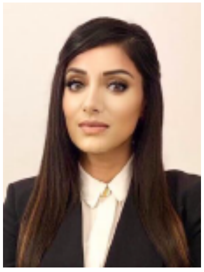
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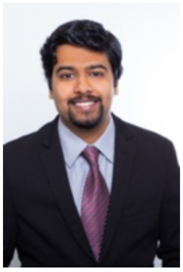
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3 Research

3.1 Research visit from Queensland University of Technology (QUT)

For two weeks in November, Dr. Lavaill from QUT in Brisbane visited LTD in order to collaborate on two following projects: The first project deals with the development of a muscle wrapping algorithm able to accurately predict the path of shoulder muscles before and after shoulder arthroplasties. The second project focuses on the extension of our ligand-receptor model for bone cell population framework published in 2022. The novel feature of the model includes sensitivity to dynamic mechanical stimulus through bone osteocytes. This will improve our understanding of how bone adapts to constant and cyclical mechanical loading. Moreover, Dr. Lavaill held a seminar talk on his most recent research in shoulder musculoskeletal modelling using OpenSim. The talk was public and delivered to researchers from FAU and Empkins. Finally, Dr. Lavaill's visit to Erlangen was utilised to further expand fund seeking strategies in collaboration between FAU, QUT, UKER and THN.

3.2 ETN – THREAD

The Institute of Applied Dynamics takes part in the ETN (European Training Network) project "Joint Training on Numerical Modelling of Highly Flexible Structures for Industrial Applications – THREAD" funded by the European Commission's Marie Skłodowska Curie Programme which is part of Horizon 2020. The project is coordinated by Prof. Dr. Martin Arnold from the Institute of Mathematics at the Martin Luther University Halle-Wittenberg (MLU). Prof. Dr.-Ing. habil. Sigrid Leyendecker is principal investigator and work package leader and M.Sc. Martina Stavole participates as early stage researcher (ESR10) since 2020.
THREAD addresses the mechanical modelling, mathematical formulations and numerical methods for highly flexible slender structures like yarns, cables, hoses or ropes that are essential parts of high-performance engineering systems. The complex response of such structures in real operational conditions is far beyond the capabilities of current virtual prototyping tools.

This year the third deliverables of two of the main work packages (WP2 and WP3, i.e. *Interactions of 1D structures in a 3D world* and *Geometric numerical methods for rod system dynamics* respectively) and the fourth deliverable of WP1, *Advanced constitutive laws of slender structures*, have been successfully submitted. The last project activities, i.e. network-wide training events and industrial workshops, took place. And the project members joined many conferences on-site. Within these events, ECCOMAS *Thematic Conference on Multibody Dynamics* was hosted by the University of Lisbon (Portugal), from 24 to 28 of July 2023. Here, Prof. Dr.-Ing. habil. Sigrid Leyendecker hold a plenary lecture on *Geometric modelling, integration and optimal control of flexible multibody dynamics*. Furthermore, the PIs Prof. Dr.-Ing. habil. Sigrid Leyendecker, Prof. Dr. Martin Arnold and

Prof. Dr. Dejan Zupan organised a minisymposium on *Numerical Modelling of Highly Flexible Structures for Industrial Applications* during the *10th International Congress on Industrial and Applied Mathematics* (ICIAM) in Tokyo (Japan), from 20 to 25 of August 2023. Moreover, the THREAD final meeting occurred in Rijeka (Croatia) between 25 and 29 September 2023, in conjunction with HFSS2023 *International Conference on Highly Flexible Slender Structures*. After the conference, M.Sc. Martina Stavole and the other ESRs joined the European Researchers' Night 2023 where they presented the THREAD project with posters and experiments. More information about the project can be found at https://thread-etn.eu.

3.3 SFB 1483 – EmpkinS

Developing sensor technology and collecting movement data of the human body is the aim of the Collaborative Research Center SFB 1483, which has been approved by the German Research Foundation (DFG) in 2021 for four years. The SFB bears the project title "Empatho-Kinaesthetic Sensor Technology" (EmpkinS) and aims to combine the external observation of body movements, such as movements of the head, torso and limbs, facial expressions with internal processes using body function models to detect several body (dys) functions with non-invasive and in the future easily available sensors. The research team headed by Prof. Dr. Martin Vossiek from the Institute of Microwaves and Photonics and Prof. Dr. Björn Eskofier from the Machine Learning and Data Analytics Lab wants to achieve this by developing methods and technologies that link information from external movements with internal biomedical processes. The external movements are measured with sensory systems, which are also developed within the CRC. EmpkinS focuses on immunology, neurology and palliative medicine as well as mental illnesses such as depression and stress. More information about the SFB can be found on its website https://www.empkins.de.
Subproject C04 "Analysis of Degenerative Movement Restrictions by Embedding Empathokinesthetic Sensor Data in Biomechanical Human Models" is located at the Institute of Applied Dynamics with principal investigator Prof. Dr.-Ing. habil. Sigrid Leyendecker and M.Sc. Simon Heinrich joined in November 2021 as doctoral candidate.
In close collaboration the subproject D01 "Movement Patterns in Hand Motion from Empathokinesthetic Sensor Data as a Diagnostic Parameter for Disease Activity in Patients with Rheumatic Disease" located at the Department of Internal Medicine 3 – Rheumatology and Immunology started in May 2021. PD Dr. sport science Dr. habil. Anna-Maria Liphardt is working as principal investigator in this project and M.Sc. Birte Coppers as doctoral candidate.
There was an *Interdisciplinary Hand Symposium* organized by Prof. Dr.-Ing. habil. Sigrid Leyendecker, PD Dr. sport science Dr. habil. Anna-Maria Liphardt. It gave several international researchers and experts from various backgrounds to present their research and a unique opportunity to discuss common goals and learn about methods, research questions and problems from other fields. The topics covered hand biomechanics, inflammatory arthritis, hand therapy and surgery as well as sensor technology focused on the hand. The symposium also included a young researcher session for doctoral candidates at the beginning of their journey or students to present their theses.
There was a two-day retreat for the general meeting in February. It took place in Prichsenstadt, where all doctoral candidates presented the current state of their subproject and the principial investigators showed their ideas for the second phase of EmpkinS. Additionally, there was a workshop on gender equality for the principal investigators as well as two talks from Prof. Thomas Kaiser and Prof. Elsa Kirchner

Group picture of the researchers presenting their work at the symposium.

about the research areas in the TRR 196 MARIE. Furthermore, the retreat gave all researchers to discuss approaches, potential common goals and new ideas in depth.
EmpkinS also organized a science slam at the E-Werk in Erlangen, where some of the researchers could show their ability to communicate complex research topics to a non-expert audience. Both Birte Coppers and Simon Heinrich — amongst other EmpkinS researchers — used this opportunity to speak about their respective topics. All these science slams can be found on YouTube, in this playlist at the official EmpkinS channel.

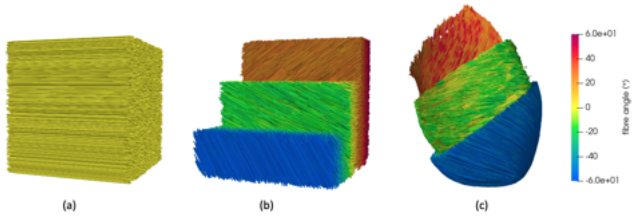
3.4 FRASCAL – Fracture across Scales

The second phase of funding for the DFG research training group FRASCAL GRK 2423 commenced earlier this year in 2023. This interdisciplinary initiative encompasses 12 projects, with project P9 underway at LTD under the guidance of Prof. Dr.-Ing. habil. Sigrid Leyendecker. During the initial FRASCAL cohort, M.Sc. Dhananjay Phansalkar successfully devised a spatially adaptive phase field model of fracture. In the ongoing second cohort, M.Sc. Deepak B. Jadhav is focused on "Temporal Adaptivity in the Phase Field model of Dynamic Fracture" at LTD. This project aims to extend the earlier spatially adaptive phase field model to include temporal adaptivity in dynamic fracture models, utilizing asynchronous variational integrators. This year, LTD held two mini lectures titled "Introduction to Geometric Time Integration" and "Introduction to Numerics" as a part of FRASCAL qualification program. Collaborative efforts involve close partnership with RTG's Mercator fellow Prof. Dr. Michael Ortiz and Prof. Dr.-Ing. Kerstin Weinberg from Universität Siegen. The 3^{rd} RTG Retreat of FRASCAL was hosted at Kloster Banz in Bad Staffelstein from 17 to 18 November. The individual presentations and the poster blitz facilitated highly productive discussions among researchers from all RTG groups.

Doctoral researchers of FRASCAL at the 3^{rd} RTG Retreat (image: Nicole Güthlein).

3.5 Heart project

The heart project is focusing on the modelling of the cardiac function to better understand cardiovascular disease, to be able to early detect or even predict heart failure and develop adequate patient specific therapies and medical devices. We are currently working on a rat as well as a human heart model. In 2023, the project entitled Smoothed finite element method in modelling and simulation of cardiac electromechanics funded by German Research Foundation (DFG) is ongoing. The main goal is to extend an alternative group of numerical techniques, smoothed finite element methods, for cardiac electromechanics to overcome volumetric locking, mesh distortion problem and to decrease simulation time. We are also currently working on a dynamic, viscoelastic, electromechanical shell model to develop an artificial heart muscle to support the cardiac cycle in case of disease.



3.6 SPP 1886

The German Research Foundation (DFG) Priority Programme “Polymorphic uncertainty modelling for the numerical design of structures – SPP 1886”, coordinated by Professor Dr.-Ing. Michael Kaliske from Technische Universität Dresden and Prof. Dr.-Ing. habil. Sigrid Leyendecker, concluded this year with the final meeting in Dresden. The Institute of Applied Dynamics participated with a presentation summarising the work done at the Institute within subproject 14 since 2016. The focus of the program is to develop methods capable of explicitly including polymorphic uncertainty in simulations. In engineering, the sources of uncertainty are many, thus making it a necessary consideration when accurately simulating a system. Within this priority program, the Institute of Applied Dynamics developed the Graph Follower algorithm, which is capable of propagating epistemic uncertainty in the form of fuzzy numbers through complex dynamical multibody systems. As an exemplary structure, a model of carbon fibre spring prosthetic foot was developed and later expanded to include the thigh and shank, resulting in a model of the human leg with a prosthetic foot. To consider polymorphic uncertainty, a further algorithm was developed, based on the Graph Follower algorithm, which is capable of propagating fuzzy random variables.

3.7 Scientific reports

The subsequent pages present a brief overview on the current research projects pursued at the Institute of Applied Dynamics. These are partly financed by third-party funding German Research Foundation (DFG), the European Training Network (ETN) and in addition by the core support of the university.

Research topics

Lobatto-type variational integrators for mechanical systems with frictional contact
Giuseppe Capobianco,Jonas Harsch, Sigrid Leyendecker

Kinematic flexibility analysis of kinases with hydrogen bond identified by machine learning method
Xiyu Chen, Sigrid Leyendecker, Henry van den Bedem

Muscle path kinematic modeling based on the geodesic function
Xiyu Chen, Maxence Lavaill, Simon Heinrich, Sigrid Leyendecker

Identifiying Disease-Characteristic Hand Function Impairments in Patients with Rheumatoid and Psoriatic Arthritis
Birte Coppers, Simon Heinrich, Sara Bayat, Georg Schett, Sigrid Leyendecker, Anna-Maria Liphardt

Data guided optimal control simulations to investigate hand movements
Simon Heinrich, Birte Coppers, Anna-Maria Liphardt, Sigrid Leyendecker

Transmural fibre orientations based on Laplace-Dirichlet-Rule-Based-Methods and their influence on human heart simulations
David Holz, Emely Schaller, Minh Tuan Duong, Muhannad Alkassar, Michael Weyand, Sigrid Leyendecker

Explicit asynchronous variational integrator for linear elastodynamics and numerical illustration of its convergence
Deepak Jadhav, Sigrid Leyendecker

Smoothed finite element methods in modelling and simulation of active cardiac contraction
Denisa Martonová, David Holz, Minh Tuan Duong, Sigrid Leyendecker

High-order variational integrators for continuum mechanics, constrained mechanical systems and optimal control
Rodrigo T. Sato Martín de Almagro, Sigrid Leyendecker

Including polymorphic uncertainty in the form of fuzzy random variables in the homogenisation of a multilayered beam's material parameters
Eduard S. Scheiterer, Sigrid Leyendecker

Variational formulation of the planar elastica in constrained environments
Martina Stavole, Rodrigo T. Sato Martín de Almagro, Giuseppe Capobianco, Olivier Brüls, Sigrid Leyendecker

Symplectic discretizations for optimal control problems in mechanics
Flóra Orsolya Szemenyei, Rodrigo T. Sato Martín de Almagro, Sigrid Leyendecker, Sofya Maslovskaya, Sina Ober-Blöbaum

Lobatto-type variational integrators for mechanical systems with frictional contact

Giuseppe Capobianco, Jonas Harsch[1], Sigrid Leyendecker

Variational integrators are well-suited for the simulation of (bilaterally) constrained mechanical systems due to several key advantages they offer, see [1]. Their good long-term energetic consistency, which bears on their symplecticity, helps to maintain the accuracy and stability of the simulation over long time periods. By their geometric nature, variational integrators are able to accurately preserve bilateral constraints on both position and velocity level. Moreover, variational integrators with high orders of accuracy have been developed. A very prominent example is the family of Lobatto IIIA-IIIB methods, which, depending on the number of stages s, are convergent with order $2s - 2$, see [2, 3].
In this project, we developed a family of Lobatto IIIA-IIIB methods for the simulation of mechanical systems with frictional contact, which we published in [4]. In addition to bilateral constraints, the developed methods can cope with unilateral constraints and set-valued Coulomb friction, which are the two main ingredients for the description of frictional contact. Hence, the developed Lobatto IIIA-IIIB methods are an extension of the existing ones.
The presented family of Lobatto IIIA-IIIB methods have the following two key features:

- **no numerical constraint drift** - the presented schemes numerically satisfy the unilateral and bilateral constraints on position and velocity level. In particular, this implies that the schemes do not exhibit contact penetration due to numerical drift.
- **the discrete contact laws are consistent with the bilateral constraints** - the discretization of the contact laws are such that for sticking contact they correspond to the discretization of the bilateral constraints. This implies that for motions where the contact is always closed and not slipping, e.g., rolling wheels in vehicle dynamics simulations, the convergence rate $2s - 2$ is retrieved.

Many technical systems exhibit high frequency contact patterns, think for example at any system with clearance between components. To showcase the performance of the proposed schemes for mechanical system with high frequency contact patterns, the slider crank mechanism shown in Figure 1 is chosen as an example.

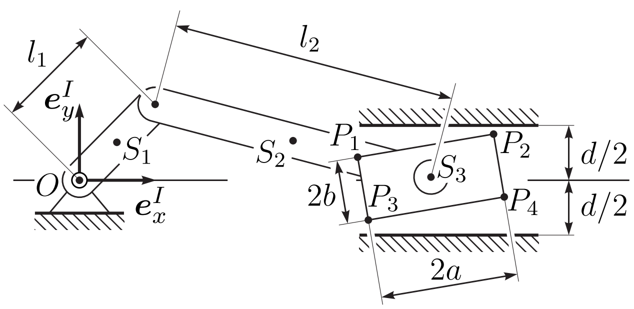


Figure 1: Sketch of the slider-crank mechanism.

The slider crank mechanism consists of three rigid bodies, which are interconnected by revolute joints. The joints are modelled as ideal bilateral constraints. The system is described in redundant coordinates, i.e., each body $i = 1, 2, 3$ is described by the coordinates (x_i, y_i) of its center of mass S_i together with an angle φ_i describing the rotation of the body in the plane. The third body can come into contact with the walls through the points $P_1, \dots, P_4$. The contact distance g_{Nk} of the point P_k

[1]Institute for Nonlinear Mechanics, University of Stuttgart.

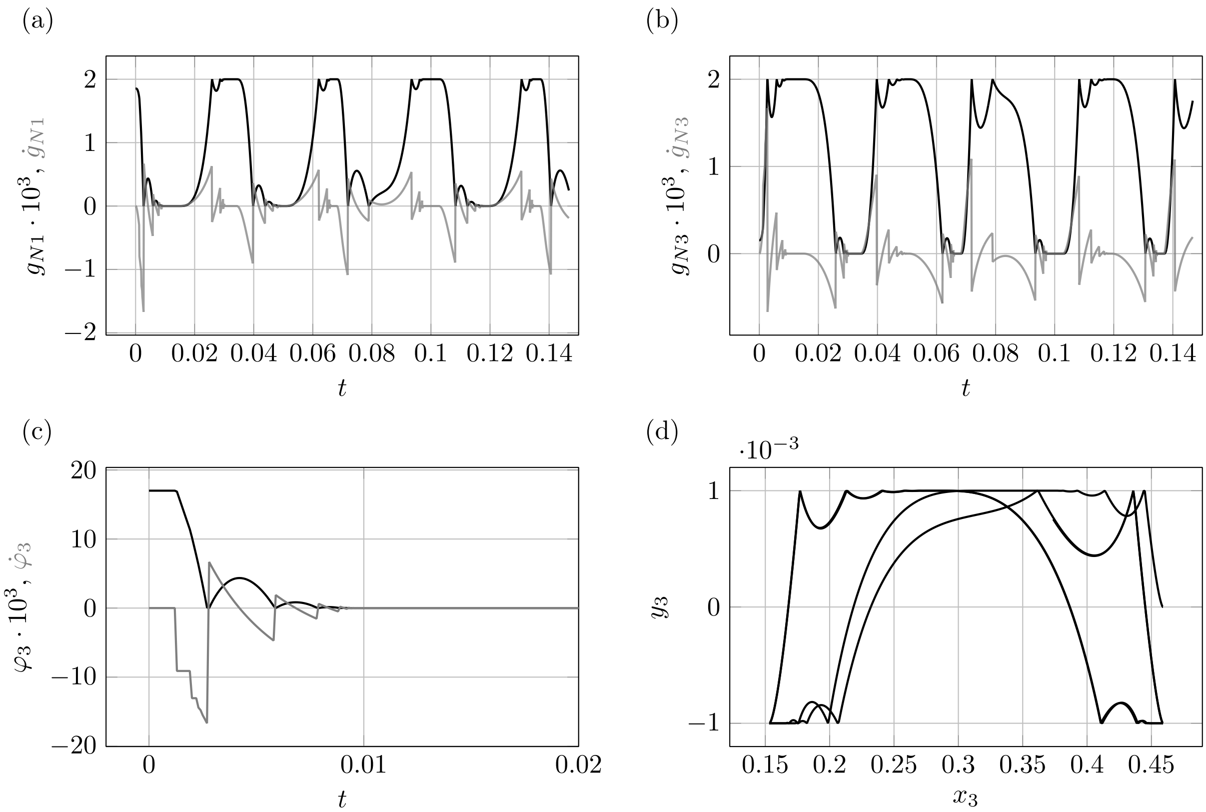


Figure 2: Simulation results for the slider crank mechanism using the presented scheme with three stages.

$(k = 1, 2, 3, 4)$ is defined as the distance of the point P_k with the closest wall. The simulation results using the presented Lobatto IIIA-IIIB scheme with three stages is shown in Figure 2.
Since the simulation started with a small perturbation of the slider's orientation ($\varphi_3 \approx 1°$), it is apparent from Figure 2 (c), that the slider's orientation is stabilized after a short time ($t \approx 0.01$). Moreover, Figures 2 (a) and (b) show the evolution of two contact distances and their time derivatives. As enforced by the scheme, no penetration is present. The spatial trajectory of the center of mass of the third body is shown by (d) of the same figure.

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[4] Giuseppe Capobianco, Jonas Harsch and Sigrid Leyendecker. *Lobatto-Type Variational Integrators for Mechanical Systems with Frictional Contact.* Computer Methods in Applied Mechanics and Engineering, 418:116496, 2024.

Kinematic flexibility analysis of kinases with hydrogen bond identified by machine learning method

Xiyu Chen, Sigrid Leyendecker, Henry van den Bedem[1] [2]

Protein kinases play a pivotal role as vital cellular catalysts, orchestrating the transfer of phosphates from adenosine triphosphate (ATP) to substrates. This intricate process finely tunes various cellular activities. Irregularities in kinase function frequently contribute to the onset of oncogenic conditions. The exploration of kinases stands as a focal point in cancer drug research. Inhibitors target both active and multiple inactive conformations, enhancing the classification of activation and enabling a comprehensive rigidity analysis. Such insights into kinase conformation not only advance drug development but also deepen our overall comprehension of these molecular structures.

In our numerical investigation, we employ kino-geometric sampling (KGS) as a highly effective approach and a framework for modeling. This method enables the comprehensive analysis of functional molecular rigidity and the exploration of transitions, particularly between active and inactive states. KGS represents molecules by depicting them as articulated multi-body complexes, utilizing dihedral angles as revolute degrees of freedom. Additionally, it incorporates selected non-covalent interactions, such as hydrogen bonds, as holonomic constraints. Each hydrogen bond interaction introduces five constraints, restricting the rotation of the hydrogen bond to its axis. The constraint Jacobian matrix is derived from the $5m$ hydrogen bond constraints concerning the cycle dihedral angle d [1, 2]. The nullspace of this constraint Jacobian matrix yields the admissible velocity for the dihedral angle and provides information about rigidified dihedral angle for the flexibility analysis of kinases.

In our previous research, the identification of hydrogen bonds relied on an approach grounded in potential energy, employing a specified cutoff. To refine and expand our methodology, we introduced a machine learning method into the process of identifying hydrogen bonds. Utilizing the HBPLUS software tool [3], we accurately located approximately 60,000 hydrogen bonds, extracting crucial data on parameters such as the D-H-A angle, H-A-AA angle, sp hybridization, distance, donor and acceptor neighbors, and atom names. This substantial dataset underwent partitioning, with 80% allocated to the training set and 20% to the test set. Employing a decision tree model, our system demonstrated an impressive test accuracy score of 0.97, highlighting the effectiveness of the training model.

In the study conducted by V. Modia et al. [4], a novel nomenclature was introduced to categorize kinases, grouping them into eight distinct clusters based on backbone conformations and phenylalanine orientation. Subsequently, we identified 79 kinase crystal structures with structural similarities to 5UG9. These structures were then segregated into five different clusters using V. Modia et al.'s classification method. We applied the trained model to identify hydrogen bonds within these 79 crystal structures and then analyze their flexiblilty and compare the difference between the energy based method and the machine learning method. Figure 1 illustrates the ratio of rigidified Degrees of Freedom (DoFs) to cycle DoFs obtained from both methods. While there are minor discrepancies, the overall trends and values exhibit remarkable similarity. It's noteworthy that the DFGin_BLBtrans group showed a slightly larger difference between the two methods, suggesting that specific hydrogen bonds may generate larger influence on the rigidity of this particular group. Furthermore, Figure 2 depicts the ratio of the size of the largest rigidified cluster to the total number of DoFs. Once again, a comparable pattern emerges between the machine learning and potential energy-based methods.

[1] Atomwise, Inc. 717 Market Street, San Francisco, CA 94103 USA
[2] Department of Bioengineering and Therapeutic Sciences, UCSF, California, USA

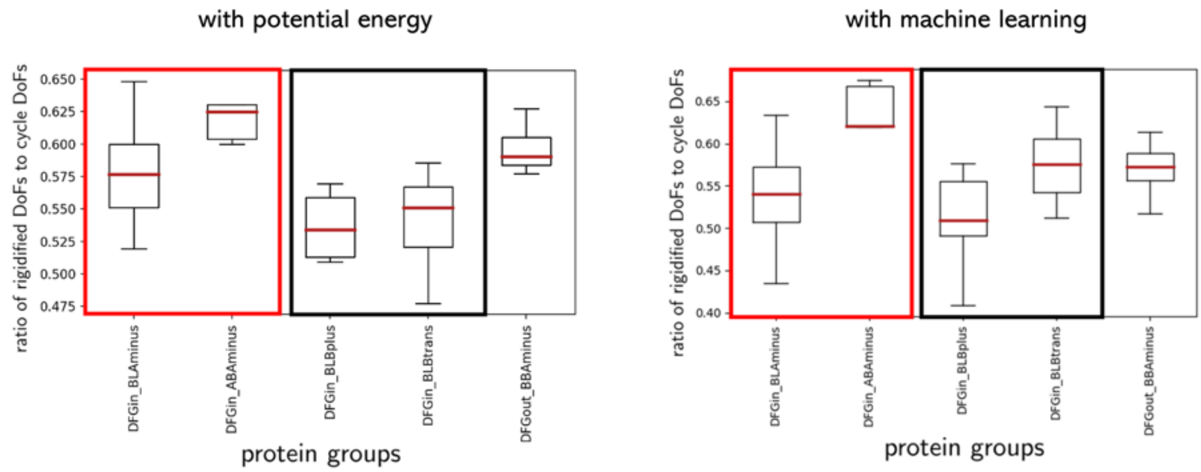

Figure 1: The comparison of the ratio between the number of rigidified DoFs and the number of cycle DoFs for 79 kinases crystal structures with hydrogen bond is identified by using potential energy based method and the machine learning method

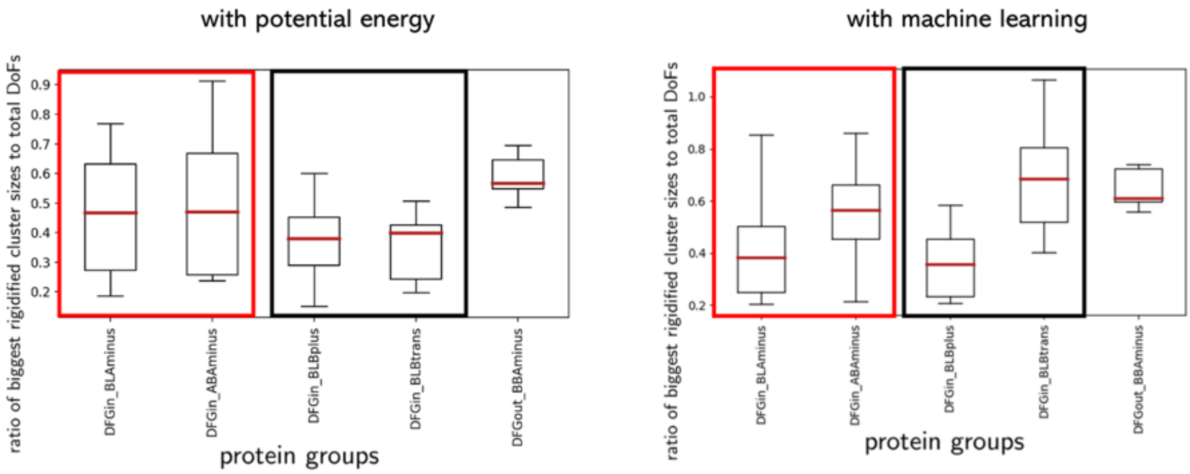

Figure 2: The comparison of ratio of biggest rigidified cluster size to total degree of freedom for 79 kinases crystal structures with hydrogen bond is identified by using potential energy based method and the machine learning method

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Muscle path kinematic modeling based on the geodesic function

Xiyu Chen, Maxence Lavaill[1], Simon Heinrich, Sigrid Leyendecker

Biomechanics plays a crucial role in unraveling the mechanical complexities inherent in biological tissues and musculoskeletal systems. Within the realm of Riemannian geometry, a curve's curvature hinges on the interplay of its normal curvature within a submanifold and its geodesic curvature—measuring the extent to which the curve deviates from being a geodesic. It can be deduced that a geodesic is a curve characterized by a vanishing geodesic curvature and is exclusively dictated by the surface curvature [1, 2, 3]. In this framework, the submanifold's curvature singularly dictates the trajectory of said submanifold. Additionally, geodesics are conventionally expressed through Euler-Lagrange equations, formulated by establishing a geodesic Lagrangian and employing a variational principle. This investigation delves into discrete geodesic Euler-Lagrange equations for the precise calculation of muscle paths [4, 5], contributing significantly to the broader themes of mechanobiology.

A muscle is assumed as a massless, one-dimensional path gliding smoothly and without friction over a surface containing obstacles. The trajectory of this muscle path is represented as a geodesic curve connecting the muscle's origin to its insertion point. For each muscle m, we discretize the geodesic curve in K linear segments. Then Linear interpolation is utilized for the initial approximation of the curve and the muscle path can be represented as $\gamma^m \in \mathbb{R}^{3(K+1)}$ for muscle m with $K+1$ nodes. For all M muscles, we get $\gamma \in \mathbb{R}^{3M(K+1)}$. Examining the implicit definition of a surface through the scalar-valued constraint $\phi(\gamma_k^m) = 0$ and the constraint manifold $\mathcal{G} = \{\gamma \in \mathbb{R}^{3M(K+1)} \mid \mathbf{\Phi}(\gamma) = \mathbf{0} \in \mathbb{R}^{M(K+1)}\}$, this surface constraint depends on the geometry of surface. In this scenario, a smooth curve is compelled to adhere to the imposed constraint and no penetration into the surface. In addition, a geodesic is a locally shortest path between two given points on a curved space, then the geodesic Euler-Lagrange (GEL) is used to find the shortest path for the muscle path, the geodesic Euler-Lagrange equations on the constraint manifold is represented as

$$-\frac{d}{ds}\frac{\partial \mathcal{L}_\gamma(\gamma,\gamma')}{\partial \gamma'} - \frac{\partial \phi^T(\gamma)}{\partial \gamma} \cdot \eta = \mathbf{0}$$

where η serves as a Lagrange contact multiplier and $\mathcal{L}_\gamma(\gamma,\gamma') = \frac{1}{2}\gamma' \cdot \gamma'$ is the Lagrangian of the geodesic. Based on these constraints, the shortest muscle path without penetration can be found.

This method is then applied to an elbow model to study the muscle path, as shown in the Fig 1A. The elbow model, encompassing the upper arm, elbow, and forearm, and it contains two muscles triceps (red) and biceps (green) (Fig 1B and C). The muscle is discretized as 21 nodes. Then we rotate the elbow from -10 to 150 degrees. Figure 2A shows the muscle total length when elbow rotate from -10 to 150 degree. The triceps becomes longer and biceps becomes shorter during elbow rotation, In addition, the total length is a smooth line which indicates not have big jump for the muscles during movement. Figure 2B shows the penetration of muscle triceps, the muscle triceps only has the penetration with magnitude 1e-9, which is belong to numerical result and can be considered as no penetration during the muscle movement.

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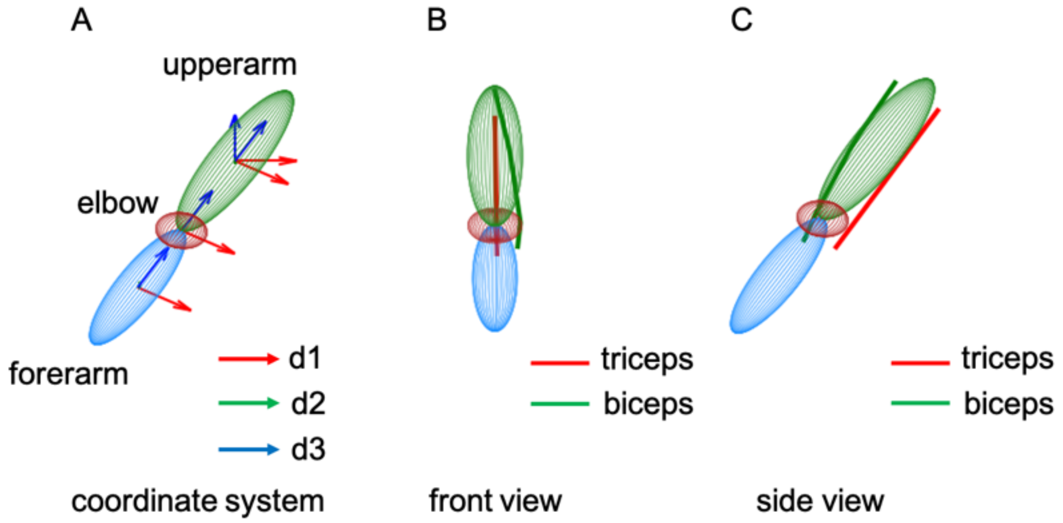

Figure 1: Elbow model (A) elbow model and local coordinate for forearm, elbow and upperarm. (B) front view for elbow model with triceps (red) and biceps(green) (C) side view for elbow model with triceps (red) and biceps(green)

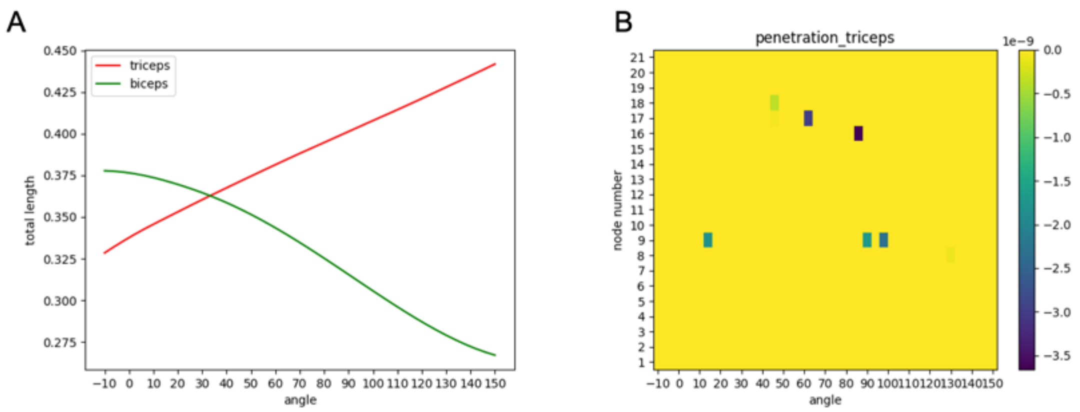

Figure 2: the elbow rotation from -10 degree to 150 degree and the muscle is seperate to 21 nodes. (A) total length change when elbow rotate from -10 degree to 150 degree (B) triceps penetration for 21 nodes when elbow rotate from -10 degree to 150 degree

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Identifiying Disease-Characteristic Hand Function Impairments in Patients with Rheumatoid and Psoriatic Arthritis

Birte Coppers[1], Simon Heinrich, Sara Bayat [1], Georg Schett [1], Sigrid Leyendecker, Anna-Maria Liphardt[1]

The quantification of hand function impairment has the potential to add valuable information on the functional state and disease burden of patients with inflammatory joint disease like Rheumatoid Arthritis (RA) and Psoriatic Arthritis (PsA) [2, 3]. It can further enhance the medical standard assessments to diagnose and monitor the disease and its progression. Yet it remains poorly investigated and is not included in the clinical standard routine. Understanding and addressing sex-specific differences in functional tasks is crucial for optimizing the disease management. This first analysis aimed to compare differences in hand motion tasks that can distinguish between healthy controls (HC) and the two conditions (RA, PsA).

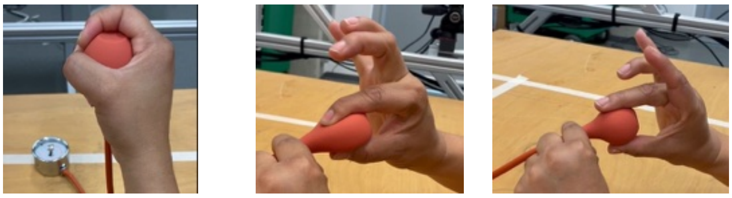

Figure 1: Grip and finger strength test (vigorimeter).

In our study, that was conducted in close cooperation of the Department of Rheumatology and Immunology, Medical Clinic 3, University Hospital Erlangen and the Institute of Applied Dynamics we recruited RA (ACR/EULAR 2010 criteria) and PsA (CASPAR criteria) patients (Internal Medicine 3 outpatient clinics Erlangen, Germany) and HC (Ethics 357 20B, DRKS00032490). Patients were assessed on the day of their quarterly routine clinical appointment and medical scores, including serology, patient reported health status and composite scores for disease activity were evaluated. Hand movements during 20 different functional tasks were recorded using an opto-electronic measurement-system (9 Oqus Series 7+ Cameras, Qualisys Sweden) and a 29-marker setup [1]. Additionally, all participants performed conventional hand function tests: an isometric grip strength test (Dynamometer, Saehan, Korea) (Fig. 2), a dynamic grip and finger strength (Fig. 1)test (Martin Vigorimeter, Germany) and the fine motor skill Moberg Picking-Up Test (MPUT) (Fig. 2).

Figure 2: left: Isometric grip strength test via dynamometer, right: Moberg Picking-Up test (MPUT).

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First analysis of a sub-group focused on the task finger tapping where the participants were asked to tap 10 times as fast and strong as possible on a force sensor placed on the front end of a custom construction (Fig. 3). Performance parameter like the maximum tapping force or tapping frequency were analysed and compared between the three groups. For the conventional hand function tests (grip and finger strength, MPUT) the full data set was analysed using linear mixed-effect models to compare the groups.

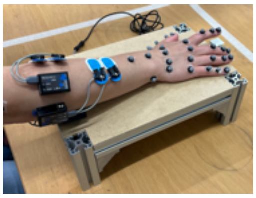

Figure 3: Device setup for the task finger tapping.

Seventy-three RA patients (24 male, 53.9 ± 14.1 years; Disease Activity Score 28: 2.6 ± 0.9), 76 PsA patients (37 male, 52.0 ± 4.3 years; Disease Activity in Psoriatic Arthritis Score: 10.2 ± 7.1), and 77 HC (37 male, 46.0 ± 18.5 years) were included in the study. It was found for the task finger tapping that the time-related parameters like tapping frequency and variation in tapping duration showed higher differences between the groups than the force related variables. Furthermore, the relation between the joint range of motion of the finger might be affected by higher disease activity during this task. The outcomes of the conventional hand function testsindicated that, on average, female patients exhibited lower grip strength with the dynamometer and vigorimeter, reduced strength in the middle finger (PsA), and higher MPUT completion times compared to female HC (all $p < 0.05$). However, in male patients, there were no significant differences in dynamic or isometric grip and finger strength compared to male HC (all $p > 0.05$). Nevertheless, male patients did show significantly higher MPUT completion times in comparison to male HC (all $p < 0.05$).
Our findings suggest that during functional tasks like finger tapping focusing on performance time and joint angle relations might be beneficial for the identification of disease-related functional movement restrictions. Differences between females and males in the outcomes of the conventional hand function tests could be identified. The analysis of grip strength is well suited to distinguish between female patients and HC, whereas the fine-motor MPUT is favourable to separate male patients from HC. The analysis is ongoing and follows the overall aim to identify highly-sensitive functional biomarkers of hand motion which can be associated to clinical disease activity scores and help in monitoring the functional state of the patients.

Acknowledgments This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – SFB 1483 – Project-ID 442419336, EmpkinS.

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Data guided optimal control simulations to investigate hand movements

Simon Heinrich, Birte Coppers[1,2], Anna-Maria Liphardt[1,2], Sigrid Leyendecker

Measurements of human movement are an important tool to investigate and understand movement impairments and the diseases causing these. Inverse simulations to reproduce the measured motion, can be used to additionally investigate immeasurable quantities. This is usually implemented as a minimization between the measured quantity $\boldsymbol{X}(t_i)$ and its representation in the simulation $\overline{\boldsymbol{X}}_i$ for $i \in [0; \ldots; N]$. The simulated quantities $\overline{\boldsymbol{X}}_i$ depend on the control variables $\boldsymbol{u}$ via the model $\boldsymbol{F}$, rendering an optimization problem

$$\min_{\boldsymbol{u}} \sum_{i=0}^{N} \|\boldsymbol{X}(t_i) - \overline{\boldsymbol{X}}_i(\boldsymbol{F}(\boldsymbol{u}))\|^2.$$

These simulations depend strongly on high quality measurements and a well personalized model. Measurements can be affected by various external factors, and accuracy may be limited depending on the type of sensor or the setting in which the measurement takes place. Also, while model personalization is necessary for subject specific simulations and should always be done for such simulations, it is important to note that personalization can improve the model only up to a certain point. Furthermore, some discrepancies between the real world and the model will remain, as a fully realistic model would result in a computational effort that is not feasible. Some phenomena cannot be included in a model with the current state of knowledge, such as soft tissue artifacts (STA) in general. STAs refer to movement of soft tissue (skin, muscle, fat) with respect to the bone, which are a huge source for uncertainty in biomechanical measurements using skin markers. Measurement techniques that would circumvent these STAs would either use bone markers, an invasive measurement technique that places the markers via pins directly in the bone, or medical imaging techniques such as computed tomography or x-ray, which lead to radiation exposure, and the necessary equipment is not easily available [1, 2].

We are investigating an approach for biomechanical simulations, called optimal control simulation, that has the potential compensate for known uncertainties in these measurements (and discrepancies between model and real world) by combining measurement data and knowledge about fundamental principles of human movement. The optimal control problem is posed within the framework of discrete mechancis and optimal control (DMOCC) [3], where a discrete variational principle is used to obtain the discrete equations of motion, leading to a structure-preservering variational integrator. The optimal control problem can be written as a nonlinear constrained optimization problem, like

$$\begin{aligned} \min_{\boldsymbol{q},\boldsymbol{u}} \quad & J(\boldsymbol{q},\boldsymbol{u}) \\ \text{subject to} \quad & \mathrm{DEL}(\boldsymbol{q},\boldsymbol{u}) = \boldsymbol{0} \\ & \boldsymbol{g}(\boldsymbol{q},\boldsymbol{u}) = \boldsymbol{0} \\ & \boldsymbol{h}(\boldsymbol{q},\boldsymbol{u}) \leq \boldsymbol{\varepsilon}. \end{aligned}$$

The objective function $J(\boldsymbol{q},\boldsymbol{u})$, depending on the state variables $\boldsymbol{q}$ and the control variables $\boldsymbol{u}$, is to be minimized. At the same time, the discrete Euler-Lagrange equations $\mathrm{DEL}(\boldsymbol{q},\boldsymbol{u})$ have to be fulfilled exactly, meaning the model adheres to the underlying physics. Additional equality constraints $\boldsymbol{g}(\boldsymbol{q},\boldsymbol{u})$ and inequality constraints $\boldsymbol{h}(\boldsymbol{q},\boldsymbol{u})$ (together with defined tolerances $\boldsymbol{\varepsilon}$) can be prescribed as well.

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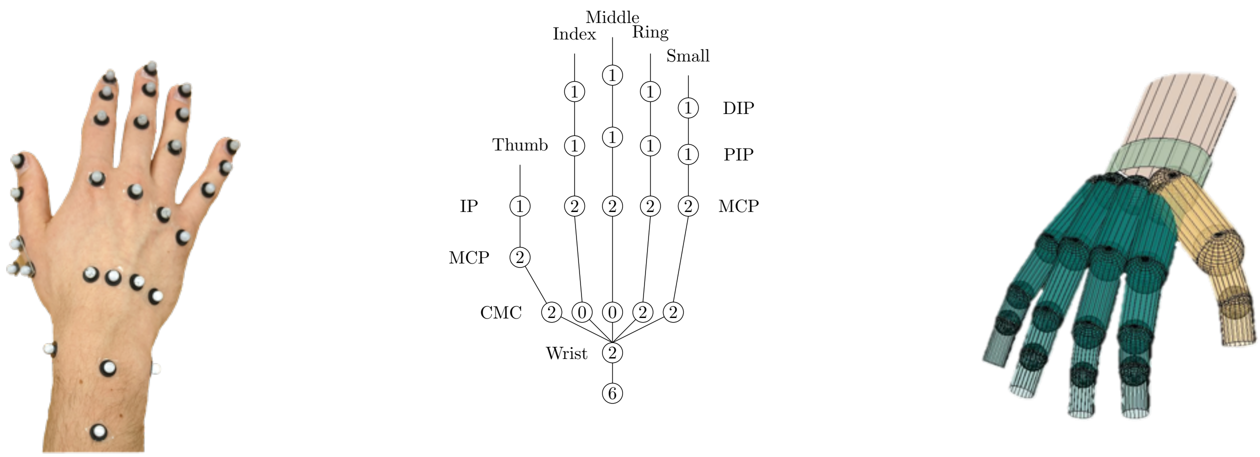
In biomechanical simulations, the objective function $J(\boldsymbol{q}, \boldsymbol{u})$ is usually physiologically motivated and may consist of multiple terms that account for the movement effort, smoothness of muscle forces and torques, energy consumption, endurance or some performance related quantity [4]. The equality constraints $\boldsymbol{g}(\boldsymbol{q}, \boldsymbol{u})$ are often used to define initial and final state while the inequality constraints $\boldsymbol{h}(\boldsymbol{q}, \boldsymbol{u})$ can be used as anatomical limits on the joint angles, limited space for movement or, as we investigate, to include measurement data. In [4], a similar implementation of a data guided optimal control problem was investigated for a steering- and a throwing- motion of the arm. They found that, from a performance standpoint, it was beneficial to include data in the constraints rather than in the objective function. They found that the computational cost decreased substantially when data was included via inequality constraints rather than the objective function.
We are investigating the question of how to optimally choose the tolerance parameter and to implement the marker data for optimal control problem simulations of the human hand, which is a complex system with many degrees of freedom and bodies. Our model of the human hand is a system of rigid bodies, with simplified geometry and constant density. The bodies are connected by ideal joints. The kinematic structure of the model and its visualization can be seen in Fig. 1.



(a) (b) (c)

Figure 1: a) Real hand prepared with skin markers for the measurement, b) kinematic structure and c) visualization of the hand model used for the optimal control problem simulations.

Acknowledgements This work was supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Grant SFB 1483–Project-ID 442419336.

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Transmural fibre orientations based on Laplace-Dirichlet-Rule-Based-Methods and their influence on human heart simulations

David Holz, Denisa Martonová, Emely Schaller, Minh Tuan Duong, Muhannad Alkassar, Michael Weyand, Sigrid Leyendecker

Numerous approaches to compute the orthotropic tissue structure in computational heart models have been developed in the past decades. In this study ([1]), we investigate to what extent the different approaches influence the local orthotropic tissue structure and thus the electromechanical behaviour of the subsequent cardiac simulation. It is well known that the orthotropic tissue structure decisively influences the mechanical and electrical properties. In detail, we are utilising three Laplace-Dirichlet-Rule-Based- Methods ([2],[3],[4]) and compare: i) the local myofibre orientation; ii) important global characteristics (ejection fraction, peak pressure, apex shortening, myocardial volume reduction, fractional wall thickening); iii) local characteristics (active fibre stress, fibre strain). The local characteristics are analysed in various subregions, see Fig. 1. The

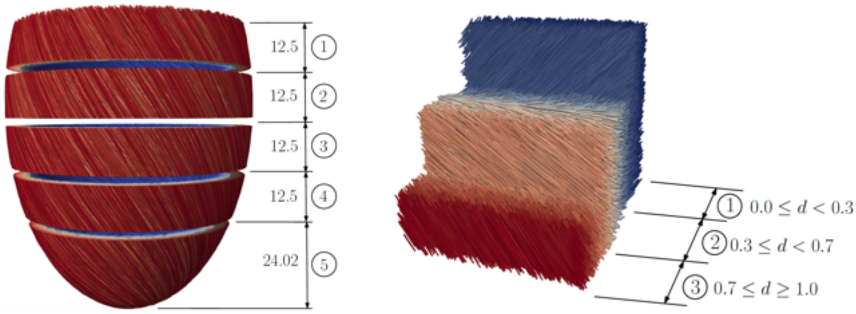

Figure 1: For the comparison of the local fibre orientation and the local cardiac characteristics, 3 transmural and 5 apicobasal subregions are defined.

global characteristics myocardial volume reduction and peak pressure are rather insensitive to a change in local myofibre orientation, while the ejection fraction is moderately influenced by the different LDRBMs. Moreover, the apical shortening and fractional wall thickening exhibit a sensitive behaviour to a change in the local myofibre orientation, see Table 1.

Table 1: Global cardiac characteristics (EF: ejection fraction; p_{max}: peak pressure; a_s: apical shortening; V_{red}: volume reduction of the myocardium; t_f: fractional wall thickening) of the measured subject as well as for the simulations B-RBM, H-RBM and W-RBM. The columns $s_c^{\text{H-RBM}}$ and $s_c^{\text{W-RBM}}$ show the level of sensitivity of each global characteristic. The sensitivity level is coloured (●0.0-0.25: low, ●0.25-0.50: moderate, ●0.50-1.0: high).

	Exp.	B-RBM	H-RBM	$s_c^{\text{H-RBM}}$	W-RBM	$s_c^{\text{W-RBM}}$
EF (%)	58.10	58.19	58.11	0.03	54.48	0.28
Δ^j_{EF} (%)	-	-	0.14	-	6.38	-
p_{max} (mmHg)	110.00	110.00	109.67	0.07	104.91	0.20
$\Delta^j_{p_{max}}$ (%)	-	-	0.30	-	4.63	-
a_s (%)	19.15	18.14	17.76	0.45	21.43	0.80
$\Delta^j_{a_s}$ (%)	-	-	2.09	-	18.14	-
V_{red} (%)	19.43	21.99	21.83	0.16	22.15	0.03
$\Delta^j_{V_{red}}$ (%)	-	-	0.73	-	0.73	-
t_f (%)	29.57	27.15	26.46	0.55	21.47	0.92
$\Delta^j_{t_f}$ (%)	-	-	2.54	-	20.92	-

The highest sensitivity can be observed for the local characteristics fibre stress and fibre strain.

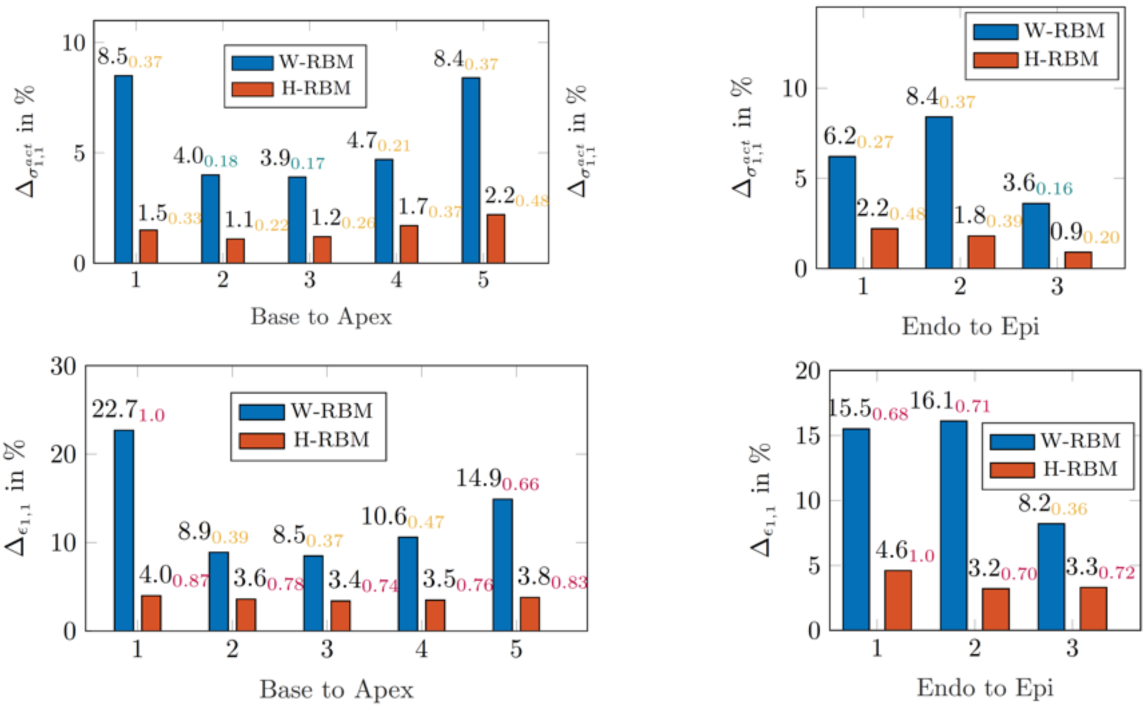

Figure 2: Comparison of the local fibre orientation, stress and strain for B-RBM, H-RBM and W-RBM. The first column represents the apicobasal subregions defined in Fig. 1, left. The second column represents the transmural subregions defined in Fig. 1, right. For more details, we refer to the original publication [1].

The main findings underline the importance of the method-specific orthotropic tissue structure. Therefore, caution is advised when comparing studies with different orthotropic tissue structure models, even if they supposedly have the same transmural orientation. E.g. for the prediction of the myocardial volume reduction, B-RBM, H-RBM and W-RBM predict similar results (i.e. comparison among studies with different orthotropic tissue structure models feasible). For the prediction of e.g. local characteristics like fibre stress or fibre strain, the results seem to be very sensitive (i.e. comparison among studies with different orthotropic tissue structure models not feasible).

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

Deepak Jadhav, Sigrid Leyendecker

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

In this work, an AVI for linear elastodynamic system is developed. The discrete action sum for this integrator is formulated as

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

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

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

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

where, $\boldsymbol{p}_a$ is the momentum of node a, with $\boldsymbol{p}_a^{i+\frac{1}{2}} = m_a \frac{\boldsymbol{x}_a^{i+1} - \boldsymbol{x}_a^i}{t_a^{i+1} - t_a^i}$, and D_a^i is the partial derivative with respect to $\boldsymbol{x}_a^i$. These DELs are then solved asynchronously by using the concept of priority queue to get the flow of the dynamic system. The priority queue holds the triangulated elements, ordered by their impending activation times. The element with the lowest activation time is the highest-priority element in the queue, and thus the first one to be processed. Then, the current nodal velocities are employed to compute the new nodal displacements for this active element. Subsequently, these velocities are adjusted by using the new element configuration. Finally, the next activation time for the element is calculated using the CFL condition, and the element is reinserted into the queue. If the activation time of an element is greater than the final time of the simulation, this element is no longer inserted into the priority queue. This algorithm is iterated until the priority queue is empty [1].

A benchmark case used to investigate the characteristics of AVI is shown in Figure 1. In this case, a 1 mm linear elastic square plate with elasticity modulus $E = 1000$ N/mm^2, Poisson's ratio $\nu = 0.3$ and mass density $\rho = 2$ g/mm^3 is fixed at one side and unrestricted on the other three sides. Initially, the plate is set in a stretched configuration under constant uniform strain and subsequently allowed to vibrate freely after being released from rest. As can be seen from Figure 2 the AVI shows good energy behavior. Figure 4 shows the distribution of elemental updates over the mesh. Coarser elements get updated less frequently than finer elements in the mesh. This leads to a significant reduction in computational cost. Figure 3 shows a nearly 50% reduced computation time with the AVI when compared to its synchronous counterpart. A new numerical convergence framework for the AVI is devised based on the convergence of discrete action sum[2]. As can be seen from Figure 5 the explicit asynchronous variational integrator shows linear convergence when temporal refinement is performed.

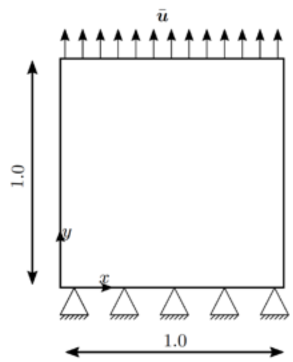

Figure 1: Geometry and boundary conditions of the square plate

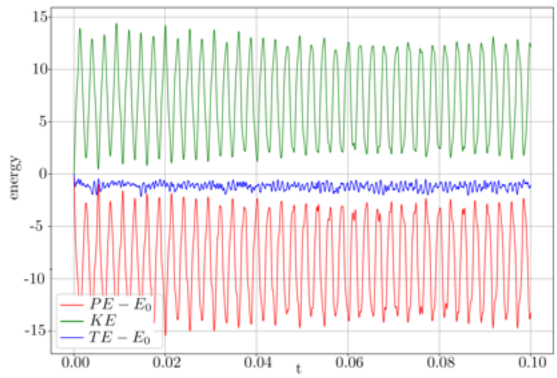

Figure 2: Good energy behavior of AVI.

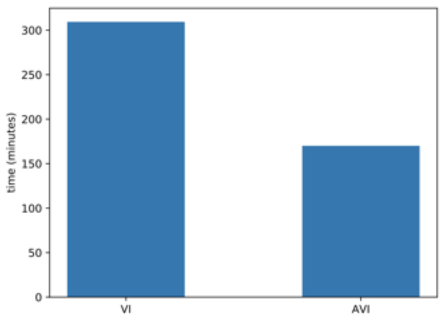

Figure 3: Computational time for VI and AVI.

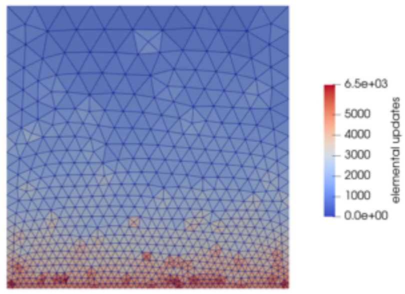

Figure 4: Distribution of elemental updates over mesh.

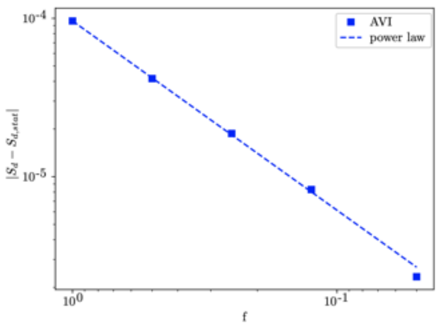

Figure 5: Convergence of the discrete action sum.

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Smoothed finite element methods in modelling and simulation of active cardiac contraction

Denisa Martonová, David Holz, Minh Tuan Duong, Sigrid Leyendecker

Smoothed finite element methods (S-FEMs) combine the finite element method (FEM) with specific meshless techniques, such as strain smoothing across a defined smoothing domain (SD). The benefits and possible applications of S-FEMs are summarised in detail for example in [1]. Briefly, S-FEM models are softer than FEM equivalents utilising the same discretisation, less sensitive to mesh distortion, capable of overcoming volumetric locking issues, and operate well with automatically generated triangular and tetrahedral meshes. Various S-FEMs have been used in biomechanical models for soft tissue, aortic valve opening or passive cardiac mechanics. In our work [2,3], we extend the node-based S-FEM (NS-FEM), face-based S-FEM (FS-FEM) and selective FS/NS-FEM (FS-FEM for the isochoric part and NS-FEM for the volumetric part) towards the modelling and simulation of active cardiac contraction.

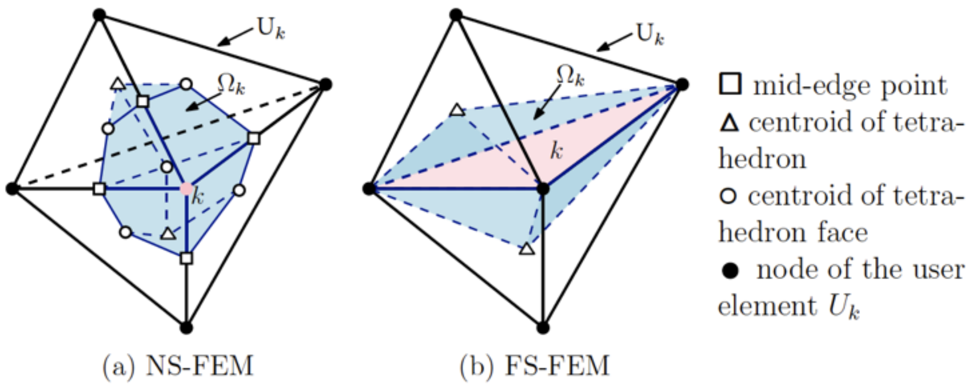

Figure 1: Smoothing domains for FS-FEM (a) and NS-FEM (b).

All mentioned S-FEMs are based on the strain smoothing over a designed SD. First, the computational domain Ω_0 is discretised into non-overlapping tetrahedrons using an automatic meshing algorithm. Second, it is subdivided into a finite number of non-overlapping SDs Ω_k with the boundary Γ_k and the reference volume V_k, i.e. $\Omega_0 = \cup_{k=1}^{n_{sd}} \Omega_k$ and n_{sd} is the number of SDs. We refer to Figure **??**(a) and (b) for the illustration of the SDs in 3D for NS-FEM and FS-FEM, respectively. Further, let $\boldsymbol{X} \in \Omega_0$ be a material point, $\boldsymbol{x}$ a spatial point and $\mathbf{I}$ the identity tensor. The deformation gradient $\mathbf{F}$ is smoothed by convolution with a smoothing function Φ_k, namely

$$\Phi_k(\boldsymbol{X}) = \begin{cases} 1/V_k & \text{if } \boldsymbol{X} \in \Omega_k \\ 0 & \text{else} \end{cases} \quad \text{with } V_k = \int_{\Omega_k} \mathrm{d}\Omega, \tag{1}$$

which satisfies the property $\int_{\Omega_k} \Phi_k(\boldsymbol{X}) \mathrm{d}\Omega = 1$. For tetrahedral discretisations and linear shape functions N_α for the node α on the tetrahedral element e, the smoothed deformation gradient $\bar{\mathbf{F}}^k$ on the SD Ω_k is constant for all $\boldsymbol{X}_k \in \Omega_k$ and takes the form

$$\bar{\mathrm{F}}^k_{iJ}(\boldsymbol{X}_k) = \int_{\Omega_k} \mathrm{F}^e_{iJ}(\boldsymbol{X}) \Phi_k(\boldsymbol{X}) \mathrm{d}\Omega = \frac{1}{V_k} \sum_{e=1}^{n_k^e} \frac{V_e}{4} \sum_{\alpha=1}^{4} \frac{\partial N_\alpha}{\partial X_J} (u^e_\alpha)_i + \delta_{iJ}$$

where u^e_i is the nodal displacement in the element e, V_e is the reference volume of the element e, n^e_k is the set of elements connected to the node k in NS-FEM or face k in FS-FEM and δ_{iJ} is the Kronecker delta.

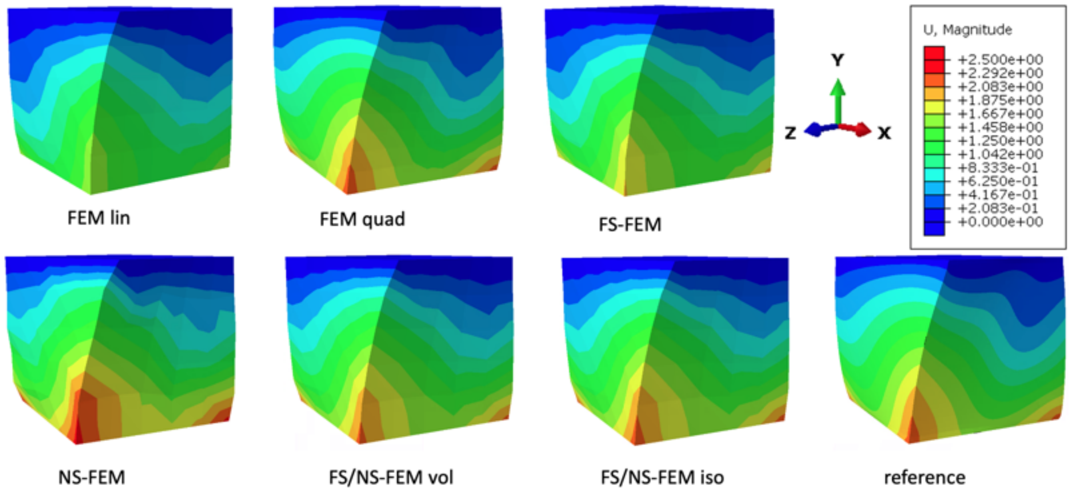

Figure 2: Snapshots at $t = 61$ ms for an active contraction in fibre direction from $-60°$ to $+60°$ on the cube boundaries.

Using different S-FEMs, we simulate an active contraction of a cube with transmurally rotating fibre directions that mimic the fibre architecture in the myocardium. Figure 2 shows the simulation results. The result produced by quadratic FEM on the finest considered mesh (13338 C3D10) serves as the reference solution ($u^{max} = 2.218$mm, $u_R^{max} = 0.314$rad). On the one hand, the known phenomenon of high stiffness due to volumetric locking in linear FEM in combination with nearly-incompressible materials is confirmed. On the other hand, for all S-FEMs, a reduction in volumetric locking is observed. For FS-FEM, it is still present, NS-FEM exhibits a too soft behaviour and the selective methods, FS/NS-FEM iso (active contraction solved on the face-based SD) and FS/NS-FEM vol (active contraction solved on the node-based SD), produce solutions which are close to the reference solution.

Acknowledgments The work is supported by Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) project no. 496647562, LE1841 10-1 which is gratefully acknowledged.

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High-order variational integrators for continuum mechanics, constrained mechanical systems and optimal control

Rodrigo T. Sato Martín de Almagro, Sigrid Leyendecker

Geometric integration involves the numerical solution of differential equations using methods that intend to preserve some or all features or underlying structures that the original problem displays.

At our institute, a particular set of geometric integration methods we are interested in is variational methods [1, 2]. These are numerical methods tailored to systems whose behaviour can be derived from a variational principle, e.g. Hamilton's principle of stationary action, and related systems. These systems display important qualitative features that should ideally be present in the results of a simulation, such as conservation laws due to symmetries in the system (Noether's theorem) or compliance with specified constraints.

Variational methods have been widely applied in the numerical simulation of standard mechanical systems such as systems of particles and rigid bodies, as well as optimal control problems, where the dynamics are governed by ordinary differential equations. But these can also be applied to field theories, where the resulting equations are partial differential equations. These include the equations of finite strain elasticity, perfect fluids, electrodynamics, etc. The study and use of variational methods on fields is still not as extended or well-understood as in mechanics. For that matter, we are trying to understand the basics of these methods.

Currently we are focusing on the following topics:

- **Parallelized variational integrators.** Solving boundary value problems in the context of optimal control of particle systems can be a costly endeavour, particularly for real-time applications. We have analysed the convergence properties of parallelized versions of variational integrators for their implementation in graphics processing units (GPUs) [6]. This has also led us to study very interesting problems in the general theory of discrete Lagrangians. In particular, the discrete Jacobi equation, conjugate points and the pathologies these bring. Joint work with Sebastian J. Ferraro and David Martín de Diego.

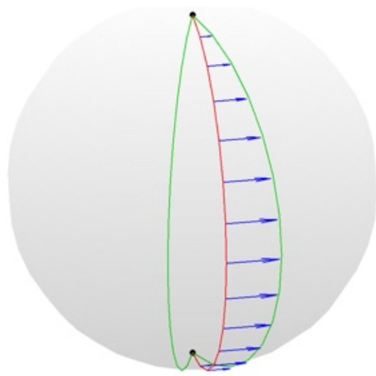

Figure 1: On the sphere and the kinetic Lagrangian, every pair of antipodal points is conjugate, i.e. there are infinitely many minimizing trajectories connecting them related by Jacobi fields.

- **The direct approach in optimal control and its relation with variational integrators.** Optimal control problems can be tackled in two different ways: first discretize, then optimize (direct approach) or first optimize, then discretize (indirect approach). We are trying to understand the relationship between both methods, particularly when applied to mechanical systems and the role of variational integrators [7]. Of particular interest is the role of boundary values of the adjoint system when using variational integrators as dynamical constraints. Joint work with Sofya Maslovskaya, Sina Ober-Blöbaum and Flóra O. Szemenyei.
- **Frequency-dependent damping in multisymplectic methods.** We are also interested in the behaviour of multisymplectic methods [3, 4, 5] in the presence of frequency-dependent dissipative terms. These can be included in the formulation as external forces. We have analyzed their performance as compared to other methods such as the generalized-α method [8], which displays frequency-dependent numerical dissipation, but also other undesired phenomena such as overshoot.

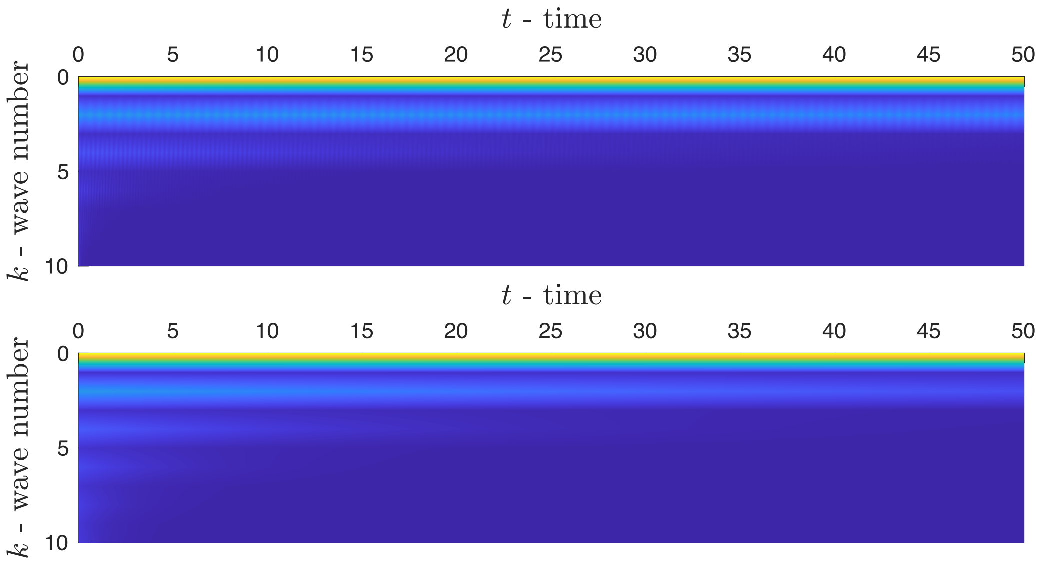

Figure 2: Fourier-space temporal evolution of a sawtooth wave. Generalized-α method (top) and the multisymplectic midpoint rule with frequency dependent damping as forcing (bottom). Overshoot manifests in the high-frequency oscillations of each mode (dark vertical bands) in the generalized-α plot.

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Including polymorphic uncertainty in the form of fuzzy random variables in the homogenisation of a multilayered beam's material parameters

Eduard S. Scheiterer, Sigrid Leyendecker

Modern applications require more and more sophisticated designs and materials. One such high performance material is carbon fibre laminate. As the name implies, it consists of carbon fibres embedded in an resin matrix. This combination performs even better if it is applied in multiple layers which are separated by a lightweight foam, resulting in very stiff yet light structures. This makes the material ideal for use in engineering applications where low weight and high material strength is required, such as aerospace or biomechanics. However, this material imposes many challenges. Due to its more complex structure and production, uncertainty is common when modelling and quantifying the material. This makes it difficult to simulate and predict the performance of designs, an essential step in engineering today. Within this research project, an algorithm is developed that can include polymorphic uncertainty in the material parameters in the form of fuzzy random variables (FRV) and propagate this uncertainty through a model, in this example a prosthetic foot. The prosthesis is modelled as a predeformed geometrically exact beam, based on an existing carbon fibre spring prosthetic foot.

As can be seen in Figure 1, showing a CT scan of the Össur Vari-Flex® prosthesis graciously loaned to the Institute of Applied Dynamics by OrthoPoint in Erlangen, the prosthesis consists of three layers, namely two faces and a core. This structure should be represented in the model to accurately describe the prosthesis' behaviour in the simulation and subsequent calculations. There are a few different options available to do this. The most accurate would be to model each layer individually as well as the interaction between layers at the layer boundary. However, this is computationally very expensive, which poses a problem for the planned uncertainty analysis, which typically require many evaluations of a model. An alternative is to mathematically group the layers into an effective representation. This process is called homogenisation and is the method chosen for this work. The homogenisation can be done in multiple ways, here the method introduced in [1] is used. Of course, this process introduces further uncertainty, again highlighting the importance of explicitly considering uncertainty in simulations.

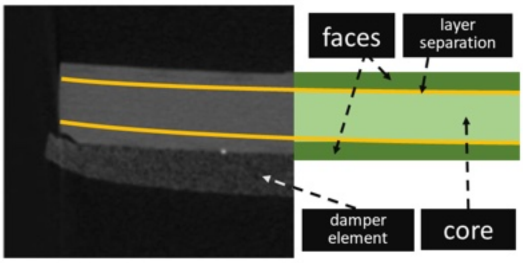

Figure 1: A CT-scan of the cross-section of the prosthetic foot. The prosthesis consists of three layers, two faces and a core, separating the faces. This multilayered structure is accounted for in the simulation via homogenisation of the material parameters.

To consider uncertainty in the simulation, different parameters are modelled as fuzzy random variables. A fuzzy random variable can quantify both uncertainty caused by variability and uncertainty caused by inaccuracy or imprecision. To mathematically describe such a fuzzy random variable, the $l_\alpha r_\alpha$-discretisation from [2] for fuzzy numbers is used. A fuzzy number is a special kind of fuzzy variable, where the membership function is limited to $\mu(x) \in (0, 1]$ and is convex. From the peak point $x_{\alpha_{N_\alpha}}$, with $N_\alpha = 4$ in Figure 2, the subsequent α-level of the fuzzy number is given by the $l_\alpha r_\alpha$-increments $\Delta x_{\alpha_i,l}$ and $\Delta x_{\alpha_i,r}$ as

$$\begin{aligned} x_{\alpha_i,l} &= x_{\alpha_{i+1},l} - \Delta x_{\alpha_i,l} \\ x_{\alpha_i,r} &= x_{\alpha_{i+1},r} + \Delta x_{\alpha_i,r}. \end{aligned} \tag{1}$$

In case of a fuzzy random variable, the peak point $x_{\alpha_{N_\alpha}}$ and the increments $\Delta x_{\alpha_i,l}$ and $\Delta x_{\alpha_i,r}$ are governed by a probability density function. Of course, the convexity condition applies. Using this method, realisations or samples of the fuzzy random variable can be 'drawn', based on the underlying probability density functions (PDFs) for every delta and α-level.

Having created a model of the prosthetic foot and having quantified the uncertainty, it has to be propagated through the model. The newly developed algorithm reduces the uncertainty stepwise, until a deterministic model evaluation is possible. To account for the randomness, the first step is to generate realisations of the fuzzy random variable, which in turn are fuzzy numbers, also called samples. These fuzzy numbers can then be propagated through the model with the Graph Follower algorithm, developed in [3]. This has to be done for all samples, which makes the computation expensive, since stochastic analysis requires the evaluation of many samples. Propagating a sample means, that the fuzzy number is propagated through the system and model with an optimiser which approximates the target output, a scalar quantity of interest of the model. In the case of the prosthesis, this could be the position of a joint or the stored energy in the prosthesis. After all samples have been propagated, the target output fuzzy numbers can then be reassembled into the fuzzy random variable of the target output. The main challenges are how to reduce the computational cost as much as possible, so many samples can be examined and how to efficiently evaluate the results. Due to the stochastic nature of the output, visualisation of the results is also challenging.

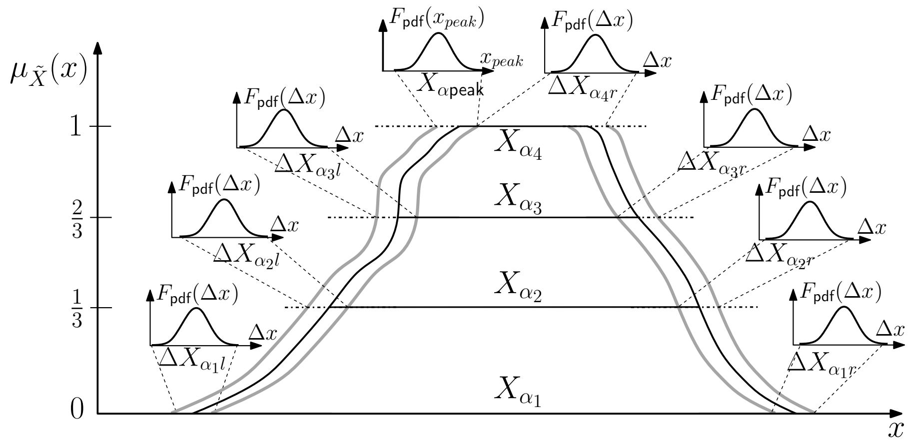

Figure 2: A fuzzy random variable, defined starting from the peak point X_{peak}, which is subject to a probaility distribution $F_{\text{pdf}}(x_{\text{peak}})$. All following α-levels can be calculated via the $\Delta X_{\alpha_i,j}$ with $j =$ l,r for the respective side. The convexity of the realisation of the fuzzy random variable has to be ensured.

With a model of the prosthesis, a quantification method for the uncertain parameters and an algorithm capable of propagating the uncertainty, the remaining step is to decide which parameters to model as uncertain. To demonstrate the algorithms capabilities, the Young's modulus of the faces and core layer are affected with uncertainty. After the simulation, the displacement of the tip of the prosthesis can be examined as an uncertain quantity or the stored energy during the motion can be examined, which is usually linked ot patient comfort with the prosthesis.

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Variational formulation of the planar elastica in constrained environments

Martina Stavole, Rodrigo T. Sato Martín de Almagro, Giuseppe Capobianco, Olivier Brüls, Sigrid Leyendecker

Flexible endoscopes are medical devices that can be modelled as beam-like objects due to their slender geometry. In order to capture the behaviour under large bending deformation, we consider a planar Euler's *elastica* associated to the following second-order Lagrangian $\widehat{\mathcal{L}}\colon T^{(2)}\mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}$ [1, 2]

$$\widehat{\mathcal{L}}\,(q, q', q'', \Lambda) = \frac{1}{2} EI ||q''||^2 + \Lambda \Phi(q, q')\,.$$

Here, $q(s)$ represents the coordinates of the centerline of the beam, $q'(s)$ and $q''(s)$ are its first and second spatial derivatives, respectively, EI is the bending stiffness assumed to be constant along the beam, $\Lambda(s)$ is a Lagrange multiplier that guarantees the inextensibility of the elastica. Via a variational principle, we derive the constrained Euler-Lagrange equations subject to boundary conditions $(q(0), q'(0)) = (q_0, q'_0)$ and $(q(l), q'(l)) = (q_N, q'_N)$.

$$\begin{gathered}\frac{d^2}{ds^2}\left(\frac{\partial \mathcal{L}}{\partial q''}\right) - \frac{d}{ds}\left(\frac{\partial \mathcal{L}}{\partial q'}\right) + \frac{\partial \mathcal{L}}{\partial q} = \frac{d}{ds}\left(\frac{\partial \Phi}{\partial q'}\right)\Lambda + \frac{\partial \Phi}{\partial q'}\Lambda' - \frac{\partial \Phi}{\partial q}\Lambda \\ ||q'||^2 - 1 = 0\,,\end{gathered}$$

Typical usage conditions of endoscopes involves confined environments that strongly constraints their deformation. Then, it is fundamental to study the elastica under contact conditions. In this regard, a further augmented Lagrangian $\widetilde{\mathcal{L}}$ describing the problem of the elastica in contact with a rigid wall is presented in [3].

$$\widetilde{\mathcal{L}} = \widehat{\mathcal{L}} - kg\Lambda_c + \frac{p}{2} g^2 - \frac{1}{2p}\left(dist\left(k\Lambda_c - pg, \mathbb{R}^+\right)\right)^2 \tag{1}$$

Here, k is a scaling factor, $g(s)$ is the gap function w.r.t. the wall, $\Lambda_c(s)$ is a Lagrange multiplier, and p is a positive penalty coefficient. Figure 1 shows the deformed configuration of the elastica in contact with straight and curved rigid walls.

Figure 1: Static equilibria of the planar elastica in contact with a straight narrow tube on the left and an L-shaped wall on the right.

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Symplectic discretizations for optimal control problems in mechanics

Flóra Orsolya Szemenyei, Rodrigo T. Sato Martín de Almagro, Sigrid Leyendecker, Sofya Maslovskaya[1], Sina Ober-Blöbaum[1]

The optimal control of mechanical problems is omnipresent in our technology-reliant society, permeating everyday life. It is also a very rich research subject with many still open questions. Classical applications range from the optimal control of industrial or medical robots, trajectory planning for space missions and aircrafts to motion planning in sports or rehabilitation. As analytical solutions of optimal control problems are not generally available, applications rely on numerical simulations that are robust and accurate, and ready-to-use by engineers.
Direct and indirect numerical methods can be used to obtain an approximate solution [1, 3]. The main difference between the two approaches is the order in which the discretization and the optimization step takes place. By the direct approach one first discretizes, then optimizes, by the indirect approach one first optimizes, then discretizes. This project aims to investigate the connection between these methods for the particular case of mechanical systems, as well as to develop a method to derive symplectic discretizations for optimal control problems. For that aim our first goal was to obtain a new regular Lagrangian which we can discretize.

We have taken the following first steps to reach that goal:
We have investigated an optimal control problem, where the state equation is described by a second order ordinary differential equation (ODE) as a dynamical constraint with fixed initial and free final state, and a running cost term that is quadratic in the control is assumed. More precisely, we consider the problem:

$$\begin{aligned} \min_{u} \quad & J\big(q,u\big) = \phi\big(q(T),\dot{q}(T)\big) + \int_0^T \frac{1}{2}u^2(t)\ dt \\ \text{subject to} \quad & q(0) = q^0, \\ & \dot{q}(0) = \dot{q}^0, \\ & \ddot{q} = f(q) + u, \end{aligned} \tag{1}$$

where $\phi\big(q(T),\dot{q}(T)\big)$ is the terminal cost term, the function $f(q)$ can be interpreted as a force due to a physical potential and the control u as an external force.
For problem (1), we initially considered standard techniques as Pontryagin's maximum principle (PMP) [6] and a variational approach [2, 5] after rewriting the second order ODE as an explicit system of two first-order ODEs [4]:

$$\begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ f(q)+u \end{bmatrix}. \tag{2}$$

Then, we have considered a new approach directly using the second order equation in problem (1) and defined the augmented objective

$$\tilde{\mathcal{J}}^u(q,\lambda,u) = \phi\big(q(T),\dot{q}(T)\big) + \lambda(T)\dot{q}(T) - \lambda(0)\dot{q}(0) + \int_0^T \frac{1}{2}u^2 - \dot{\lambda}^\top\dot{q} - \lambda^\top f(q) - \lambda^\top u\ dt.$$

In order to define a regular Lagrangian, we have introduced a new variable $y = (q,\lambda)$ describing the combined state and adjoint variable. Moreover, via variational principle we have derived that $u = \lambda$. These together lead to a new Lagrangian without dependence on the control

$$\tilde{\mathcal{L}}(y,\dot{y}) = \tilde{\mathcal{L}}(q,\lambda,\dot{q},\dot{\lambda}) = -\dot{\lambda}^\top\dot{q} - \lambda^\top f(q) - \frac{1}{2}\lambda^\top\lambda,$$

which is regular and structurally is of the same form as a mechanical Lagrangian L. Thus, it is possible to derive its Euler-Lagrange equations, and access a Hamiltonian formulation through the Legendre transformation.
We have shown that the Euler-Lagrange equations and the Hamiltonian system for the new, regular Lagrangian $\tilde{\mathcal{L}}$ and Hamiltonian $\tilde{\mathcal{H}}$, respectively, provide the same necessary conditions of the minimization problem (1) as

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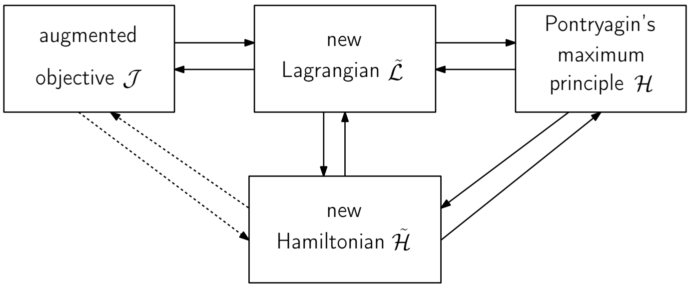
the standard approaches of the PMP for the original Hamiltonian $\mathcal{H}$ and the variational approach regarding the original augmented objective $\mathcal{J}$ with the first order system (2), i.e.,

$$\ddot{\lambda} = \frac{\partial}{\partial q} f(q)^\top \lambda, \qquad \ddot{q} = f(q) + \lambda.$$

Thus, we have commutation in the following diagram.



In our future works our intention is to generalize further the approach to optimal control problems with general second order dynamical constraints and with more general Lagrange term and afterwards to discretize this.

Acknowledgements

This project is funded by the Deutsche Forschungsgemeinschaft (DFG) with the projects: LE 1841/12-1, AOBJ: 692092 and OB 368/5-1, AOBJ: 692093.

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4 Activities

4.1 Collaboration with QUT

In 2023 Prof. Dr.-Ing. habil. Sigrid Leyendecker proudly extends her ongoing collaboration as an adjunct Professor at the Faculty of Engineering, School of Mechanical, Medical and Process Engineering at the Queensland University of Technology in Brisbane, Australia. The enduring partnership has continued to yield significant benefits in terms of both academic and cultural exchange.

Our commitment to fostering a robust academic cooperation remains unwavering, and the ties between our institute and QUT have strengthened, particularly within the dynamic field of biomechanics. This year has seen the continuation of this fruitful collaboration. In particular, we received Prof. Dr.-Ing. habil. Peter Pivonka, whose visit led to interesting and productive discussions; he also offered an insightful talk on "Computational simulation techniques for understanding bone remodeling", later this year with the research visit of Dr. Lavaill further achievements and breakthroughs were envisioned, also in collaboration with the Technische Hochschule Nürnberg (THN) and the Universitätsklinikum Erlangen (UKER); marking another milestone in our shared journey of expanding the horizons and enriching the scope of research at LTD.

4.2 MskLife virtual colloquium
Muskuloskeletal mechanobiology during human life span

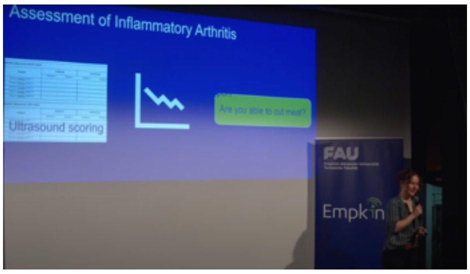
This year heralds the commencement of our virtual colloquium in Musculoskeletal mechanobiology during human life span. The series started with insightful talks by PD Dr. sportwiss. Dr. habil. med. Anna-Maria Liphardt and Prof. Dr. Saulo Martelli.
More engaging presentations are envisioned in the upcoming months with invited speakers from FAU, QUT, THN and UKER. This initiative fosters knowledge exchange and collaboration within our universities and also establishes our institute as a hub for cutting-edge insights in musculoskeletal mechanobiology.

4.3 EmpkinS – Interdisciplinary Hand Symposium

Within the research activities of the Collaborative Research Centre (CRC) 1483 - EmpkinS (funded by the German Research Foundation (DFG)), the Department of Internal Medicine 3 – Rheumatology and Immunology, UKER and the Institute of Applied Dynamics (LTD), organized the Interdisciplinary Hand Symposium on October 4th and 5th 2023. The aim was to reflect the status quo in the areas of clinical and biomechanical research on the human hand and to strengthen interdisciplinary collaboration. Invited speakers addressed the current research in inflammatory arthritis, hand surgery and therapy, biomechanical modelling and simulation, as well as visualising and sensing the hand.

4.4 EmpkinS – Science Slam

On February 10, 2023, in E-Werk, Erlangen, Birte Coppers and Simon Heinrich were invited to participate in the "Zukunftsdiagnose – High-tech meets medicine" science slam, with the aim to make science accessible and interesting to the general public. The short talks challenged the doctoral candidates, as they are required to condense their complex and technical research into a short, engaging presentation that can be understood by a non-expert audience.



4.5 Research stay at Stanford University

As part of development of the DFG-funded project ‚Smoothed finite element methods in modelling and simulation of cardiac electromechanic, M.Sc. Denisa Martonová spent six weeks (September to November 2023) working in Living Matter Lab (Prof. Ellen Kuhl) at Stanford University. The research stay resulted in establishing a collaboration on the heart project, in particular regarding the extension of constitutive neural networks for computational simulation of cardiac tissue

4.6 THREAD – Geometric integration methods for non-linear structural dynamics, Minisymposium

The minisymposium was organized in cooperation by Prof. Dr.-Ing. habil. Sigrid Leyendecker, Prof. Dr.-Ing. Sina Ober-Blöbaum (University of Paderborn), Prof. Dr. Elena Celledoni and Prof. Dr. Brynjulf Owren (National

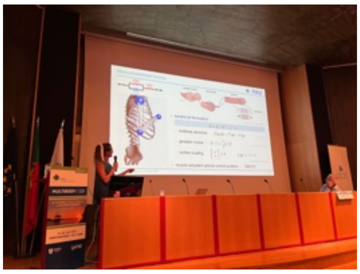
Technical University of Norway) for the International Conference on Highly Flexible Slender Structures (HFSS 2023) from 25-29 September in Rijeka, Croatia.

4.7 ICIAM 2023 – Numerical Modelling of Highly Flexible Structures for Industrial Applications, Minisymposium

The minisymposium was organized in cooperation by Prof. Dr.-Ing. habil. Sigrid Leyendecker, Prof. Dr.-Ing. Martin Arnold (Martin Luther University Halle-Wittenberg) and Prof. Dr. Dejan Zupan (University of Ljubljana) for the International Congress on Industrial and Applied Mathematics (ICIAM 2023) from 20-25 August in Tokio, Japan, where fellows Martina Stavole, Rodrigo Sato and Eduard S. Scheiterer had sucessful talks for a wide international audience.

4.8 ECCOMAS 2023

On 26 July 2023, Prof. Dr.-ing. habil. Sigrid Leyendecker was invited to give a plenary talk at the ECCOMAS Thematic Conference on Multibody Dynamics 2023, her presentation was titled *“Geometric modelling, integration and optimal control of flexible multibody dynamics”*. Additionally, Simon Heinrich and Martina Stavole participate with conference talks showcasing advancements in their respective projects.



4.9 Frascal – Mini Lecture: „Introduction to Geometric Time Integration (IGETI)

As part of the Frascal qualification programme, LTD offered on 10 February 2023 the Mini Lecture *Introduction to Geometric Time Integration (IGETI)*, prepared and given by Dr.-Ing. Giuseppe Capobianco, Dr. Rodrigo T. Sato Martín de Almagro and Prof. Dr.-Ing. habil. Sigrid Leyendecker. Lecture notes were created by the team and published for further distribution within the participants.

4.10 Long Night of Sciences ”Die Lange Nacht der Wissenschaften” (LNdw)

In 2023, we are pleased to highlight our participation in the Long Night of Sciences (LNdw, #NdW23) on October 21, 2023. The Friedrich-Alexander-Universität Erlangen-Nürnberg hosted this event, providing a platform for families, students, politicians, and scientists to explore a diverse range of over 100 activities spanning technology, medicine, natural and engineering sciences, humanities, economics, and social sciences. LTD engaged in the LNdw, showcasing captivating experiments in our Motion Capture Laboratory. Attendees had the opportunity to experience ”Fascination of dynamics” with:

- *Carrera* race – an interactive experiment demonstrating optimal control
- angular momentum conservation and Lagrange gyro
- balancing Lego robot on two wheels
- inverse pendulum – a fascinating human-versus-machine challenge
- motion capture setup – where participants were able to experience motion capturing on their own

Several experiments proved particularly appealing to children. The atmosphere was vibrant, and we received exceptionally positive feedback, reflecting the success of our engaging and educational contributions to the Long Night of Sciences.

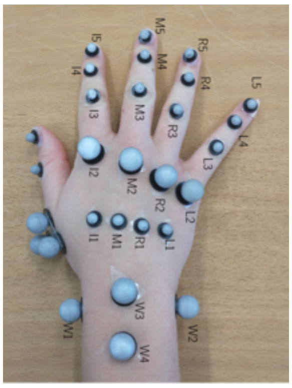
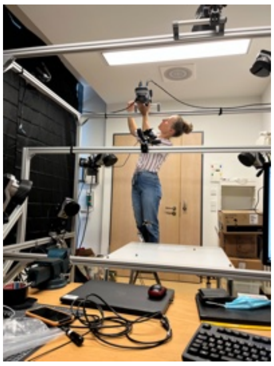
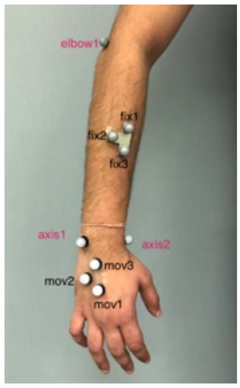
  

4.11 Motion capture laboratory

Our motion analysis lab is equipped with a camera and marker based optical tracking system, including 10 Qualisys MoCap high speed cameras and 2 Qualisys high speed video cameras, as well as Noraxon MyoMotion inertial sensors, Cybergloves III to measure hand joint angle kinematics, force plates, and Noraxon Desktop DTS electromyography sensors.

A frame was constructed to bring the cameras closer to the markers in order to perform motion capturing for small human actions, such as motion of hand digits. With this setup, kinematic parameter identification for joints in the human hand, especially the wrist, the metacarpophalangeal and interpalangeal joints has been performed. This is an essential first step towards formulating a procedure for effective parameter identification to setup subject-specific models. This will enable us to perform biomechanical optimal control simulations with higher levels of confidence and use the results as measures of human performance.

In 2023, the laboratory remains a pivotal hub for advancing motion capture studies. In particular, it plays a significant role in fostering collaboration, like the study with Prof. Dr.-Ing. Ramona Hoffman from Hochschule für Technik und Wirtschaft des Saarlandes. This collaborative study focuses on investigating gender differences in cycling motions through optimal control simulations.

- CyberGlove: The analysis of hand movements can yield useful information and indicators for the detection of rheumatic diseases at an early stage. The CyberGlove project goal is to analyze whether the glove bears potential for this purpose. In a second step, we aim to measure activities of daily life and examine if the use of specific joints has an impact on the development of arthritis.

4.12 Editorial activities

Advisory and editorial board memberships Since January 2014, Prof. Dr.-Ing. habil. Sigrid Leyendecker is a member of the advisory board of the scientific journal Multibody System Dynamics, Springer. She is a member of the Editorial Board of ZAMM – Journal of Applied Mathematics and Mechanics / Zeitschrift für Angewandte Mathematik und Mechanik since January 2016 and since 2017 runs a second term as member of the managing board of the International Association of Applied Mathematics and Mechanics (GAMM), as well as a member of the executive council of the German Association for Computational Mechanics (GACM) and member of the General Council of the International Association for Computational Mechanics (IACM).

Since October 2017, Prof. Dr.-Ing. habil. Sigrid Leyendecker is an elected member of the Faculty Council of the Faculty of Engineering at the Friedrich-Alexander-Universität Erlangen-Nürnberg, and in April 2019 was elected deputy Chair of the Qualification Assessment Committee (Eignungsfeststellungsverfahrens -(EFV-Kommission) of the Bachelor's degree programme Medical Engineering, at the Friedrich-Alexander-Universität Erlangen-Nürnberg.

5 Teaching

Winter semester 2023/2024

Dynamik starrer Körper (MB, ME, WING, IP, BPT, CE, MT)

Vorlesung		S. Leyendecker
Übung + Tutorium		D. Holz, G. Capobianco E.S. Scheiterer

Mehrkörperdynamik (MB, ME, WING, TM, BPT, MT)

Vorlesung		G. Capobianco
Übung		R.T. Sato Martín de Almagro

Laboratory couse Applied Dynamics (MB, ME, WING, ACES)

S. Leyendecker
E.S. Scheiterer, D. Holz, X. Chen
R.T. Sato Martín de Almagro

Laboratory course Matlab (MB, EEI, ACES)

S. Leyendecker
M. Stavole

Summer semester 2023

Biomechanik (MB, MT)

Vorlesung + Übung		G. Capobianco
geprüft	37 + 19 (WS 2022/2023)	

Computational multibody dynamics (MB, MT)

Vorlesung + Übung		G. Capobianco
geprüft	7 + 10 (WS 2022/2023)	

Geometric numerical integration (MB, ME, WING, BPT)

Vorlesung		S. Leyendecker R.T. Sato Martín de Almagro
Übung		F. Szemenyei
geprüft	3 + 1 (WS 2022/2023)	

Statik und Festigkeitslehre (BPT, CE, ME, MWT, MT)

Vorlesung		S. Leyendecker
Tutorium		X. Chen, D. Holz, D. Phansalkar, F. Szemenyei
Übung		D. Holz, D. Phansalkar, G. Capobianco
geprüft	239 + 253 (WS 2022/2023)	

Praktikum Matlab (MB)

Teilnehmer	49	S. Leyendecker X. Chen

Winter semester 2022/2023

Dynamik starrer Körper (MB, ME, WING, IP, BPT, CE, MT)		
Vorlesung		S. Leyendecker
Tutorium		D. Holz, X. Chen, D. Huang
Übung		D. Holz, X. Chen, D. Huang G. Capobianco
geprüft	240 + 74 (SS 2023)	
Mehrkörperdynamik (MB, ME, WING, TM, BPT, MT)		
Vorlesung		S. Leyendecker
Übung		R.T. Sato Martín de Almagro
geprüft	56 + 26 (SS 2023)	
Computational multibody dynamics (MB, MT)		
Vorlesung + Übung		G. Capobianco
geprüft	10	
Praktikum Technische Dynamik – Modellierung, Simulation und Experiment (MB, ME, WING)		
Teilnehmer	3	S. Leyendecker D. Holz, D. Phansalkar, X. Chen R.T. Sato Martín de Almagro
Praktikum Matlab (MB)		
Teilnehmer	66	S. Leyendecker M. Stavole, D. Phansalkar

5.1 Theses

Doctoral theses

- Dr.-Ing. Uday Phutane
  Optimal control simulations of human hand grasping
- Dr.-Ing. Dhananjay Phansalkar
  Phase-field modelling of fracture with a spatially varying length variable and adaptive mesh refinement
- Dr.-Ing. Xiyu Chen
  Kinematic assessment to characterize protein and macromolecular conformations
- Dr.-Ing. David Holz
  On Aspects of Cardiac and Artificial Muscle Modelling – Insights into Orthotropic Tissue Structure and Dielectric Elastomer Actuators
- Dr.-Ing. Denisa Martonová
  Computational modelling and simulation of rat heart electromechanics – from (smoothed) finite element methods towards a ligand-receptor model

Master theses

- Jiandong Zhao
  On the identification of port-Hamiltonian models via machine-learning
- Tim Scharf
  Intra- and inter-subject analysis of kinematic synergies during ball grasping

Project theses

- Hyunjong Park
  Data-driven parameter identification for exergetic port-Hamiltonian systems
- Patrick Buchner
  Time discretization of port-Hamiltonian systems with the Störmer-Verlet method

Bachelor theses

- Laura Alarcón Rueda
  Biomechanical evaluation of cyclic finger tapping analyzing functional movement restrictions in inflammatory arthritis
- Johanna Bloehs
  Homogenisation of the material parameters of a multilayered carbon fiber spring prosthetic foot

5.2 Seminar for mechanics

together with the Chair of Applied Mechanics LTM

15.12.2023 Dr. Michael Konopik
NanoLund: Centre for Nanoscience
Lund University, Sweden
Understanding an artificial motor protein using Langevin equations

20.11.2023 Prof. Dr.-Ing. Robert Seifried
Institute für Mechanik und Meerestechnik
Technische Universität Hamburg
Model inversion by servo-constraints for feedforward control of flexible and soft robots

07.11.2023 Dr. Maxence Lavaill
ARC Training Centre for Joint Biomechanics
Queensland University of Technology
Assessment of shoulder musculoskeletal modelling procedures for clinical applications

18.10.2023 M.Sc. Timo Ströhle
Institute of Mechanics
Karlsruhe Institute of Technology
Controlling nonlinear elastic systems governed by hyperbolic PDEs

24.08.2023 PD Dr. sportwiss. Dr. habil. med. Anna-Maria Liphardt
Internal Medicine 3-Rheumatology and Immunology
Universitätsklinikum Erlangen
MskLife virtual colloquium: Musculoskeletal mechanobiology during human life span
Effects of altered mechanical loading on musculoskeletal tissues

10.07.2023 Prof. Dr. Saulo Martelli
School of Mechanical, Medical and Process Engineering
Queensland University of Technology
MskLife virtual colloquium: Musculoskeletal mechanobiology during human life span
Advances in multiscale experimental mechanics of bones

15.05.2023 Prof. Dr.-Ing. Ramona Hoffmann
Fakultät für Ingenieurwissenschaften
Hochschule für Technik und Wirtschaft des Saarlandes
Towards investigating gender differences in cycling motions using optimal control simulations

22.03.2023 Prof. Dr.-Ing. habil. Peter Pivonka
School of Mechanical, Medical and Process Engineering
ARC Training Centre for Joint Biomechanics
Queensland University of Technology
Computational simulation techniques for understanding bone remodeling

08.03.2023 Prof. Dr. Syn Schmitt
Institute for Modelling and Simulation of Biomechanical Systems
University of Stuttgart
Learning motion in muscle-driven systems – understanding biology and benefits for robotics

08.03.2023 M.Sc. Helena Port
Graduate Programme in Musculoskeletal and Oral Sciences
University of Copenhagen
Understanding extracellular matrix remodeling in axial spondyloarthritis

02.02.2023 Dr. Sara Jiménez Alfaro
Institut Jean Le Rond d'Alembert
Sorbonne Université
Modelling of glass matrix composites by the Coupled Criterion and the Matched Asymptotics Approach. The role of a single platele

5.3 Computational Multibody Dynamics

The course "Computational Multibody Dynamics" has been devised and taught by Dr.-Ing. Giuseppe Capobianco. During this course, the students learn to understand and implement a modular software for the simulation of multibody systems. After a concise treatment of the theory of multibody dynamics, the translation of the theory into a simulation software is discussed. This is complemented with several programming exercises enabling the students to gain practical experience and a profound understanding of the modular software structure. By taking this course, the students will be able to

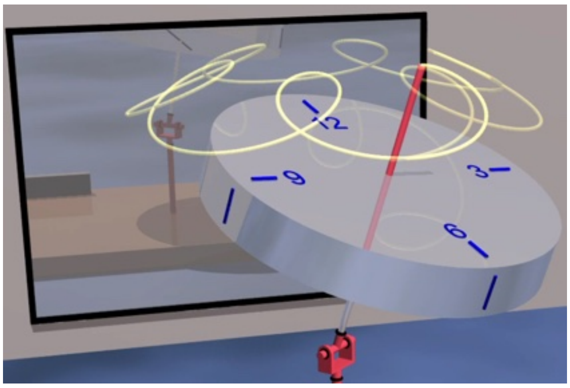
- write their own code for the simulation of complex multibody systems.
- understand what goes on "under the hood" of commercial multibody simulation software.

The course commenced in the winter semester of 2022/2023, and it is currently being offered every subsequent summer semester, consistently attracting a growing number of enrolled students.

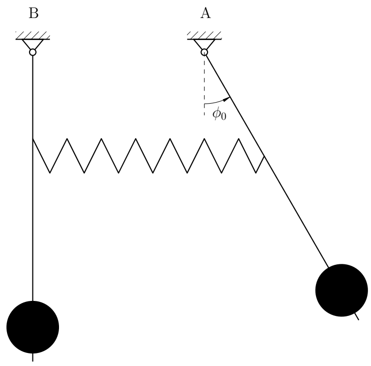
5.4 Laboratory course Applied Dynamics

The laboratory couse Applied Dynamics – modeling, simulation and experiment (Praktikum Technische Dynamik) adresses all students of the Technical Faculty of the Friedrich-Alexander-Universität Erlangen-Nürnberg and it has recently been extended to include master's students specializing in Electromobility. Starting from the winter semester of 2023/2024, the laboratory course is conducted in English. The aim of the practical course is to develop mathematical models of fundamental dynamical systems to simulate them numerically and compare the results to measurements from the real mechanical system. Here, the students learn both the enormous possibilities of computer based modeling and its limitations. The course contains one central programming exercise and six experiments observing various physical phenomena along with corresponding numerical simulations:

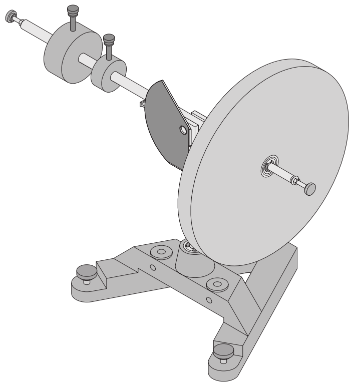
- programming exercise
- beating pendulums
- gyroscope
- ball balancer system
- robot arm
- inverse pendulum
- balancing robot



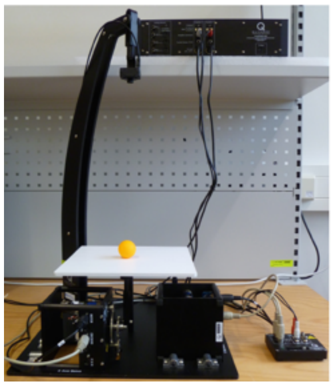
programming exercise



beating pendulums

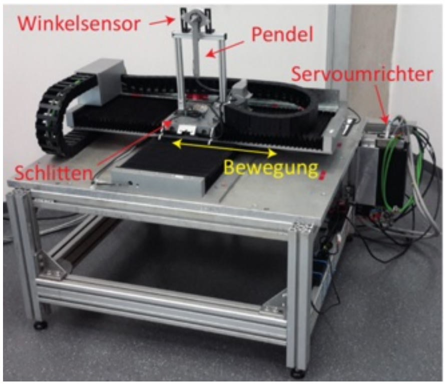


gyroscope



ball balancer system

robot arm



inverse pendulum

balancing robot

5.5 Laboratory course MATLAB

The Laboratory course MATLAB (Praktikum MATLAB) is available to all students at the Technical Faculty of Friedrich-Alexander-Universität Erlangen-Nürnberg, and it has recently been extended to include master's students specializing in Electromobility. Starting from the winter semester of 2023/2024, the laboratory course is conducted in English, which has led to a significant increase in student enrollment. To meet this heightened demand, the course's capacity has been doubled, and we aim to sustain this high level of interest in the upcoming semesters.

The primary objective of the course is to equip participants with essential skills in numerical programming using MATLAB. This collaborative effort involves the Institute of Applied Mechanics (LTM), the Institute of Production Metrology (FMT), and the Institute of Engineering Design (KTmfk).

The course commences with an introductory programming session covering MATLAB fundamentals. Subsequently, each institute introduces a task related to mechanics and engineering. For example, the LTM task involves understanding and simulating the dynamics of a crane. These tasks are presented to students through theory lectures, followed by hands-on programming sessions.

6 Publications

6.1 Reviewed journal publications

1. G. Capobianco, J. Harsch and S. Leyendecker. “Lobatto-type variational integrators for mechanical systems with frictional contact”, *Computer Methods in Applied Mechanics and Engineering*, Vol. 418, Part A, doi.org/10.1016/j.cma.2023.116496, 2023.
2. M. Schubert, R. Sato, K. Nachbagauer, S. Ober-Blöbaum and S. Leyendecker. “Discrete Adjoint Method for Variational Integration of Constrained ODEs and Optimal Control of Geometrically Exact Beam Dynamics”, *Multibody System Dynamics*, pp. 1-28, DOI doi.org/10.1007/s11044-023-09934-4, 2023.
3. J. Schanbhag, A. Wolf, I. Wechsler, S. Fleischmann, J. Winkler, S. Leyendecker, B. Eskofier, A. Koelewijn, S. Wartzack and J. Miehling. “S ”Methods for integrating postural control into biomechanical human simulations: a systematic review”, *Journal of NeuroEngineering and Rehabilitation*, Vol. 20(1), pp. 1-17, DOI doi.org/10.1186/s12984-023-01235-3k, 2023
4. X. Chen, S. Leyendecker and H. van den Bedem. “SARS-CoV-2 main protease mutation analysis via a kinematic method”, *Proteins: Structure, Function, and Bioinformatics*, DOI doi.org/10.1002/prot.26543, 2023
5. D. Martonová, D. Holz, M.T. Duong and S. Leyendecker. “Smoothed finite element methods in simulation of active contraction of myocardial tissue samples”. *Journal of Biomechanics*, Vol. 157:111691, DOI doi.org/10.1016/j.jbiomech.2023.111691, 2023.
6. D. Holz, D. Martonová, E. Schaller, M.T. Duong, M. Alkassar, M. Weyand, and S. Leyendecker. “Transmural fibre orientations based on Laplace-Dirichlet-Rule-Based-Methods and their influence on human heart simulations”, *Journal of Biomechanics*, 11643, DOI 10.1016/j.jbiomech.2023.111643, 2023.
7. M. Nitschke, R. Marzilger, S. Leyendecker, B. Eskofier, A. Koelewijn. “Change the direction: 3D optimal control simulation by directly tracking marker and ground reaction force data”, *PeerJ*, Vol. 11:e14852, DOI doi.org/10.7717/peerj.14852, 2023.
8. D. Martonová, M. Lavaill, M.R. Forwood, A. Robling, D.M.L. Cooper, S. Leyendecker and P. Pivonka. “Effects of PTH glandular and external dosing patterns on bone cell activity using a twostate receptor model — implications for bone disease progression and treatment”. *PLOS ONE*, Vol. 18.3: e0283544, DOI doi.org/10.1371/journal.pone.0283544, 2023.
9. D. Phansalkar, D.B. Jadhav, K. Weinberg, M. Ortiz and S. Leyendecker. “Extension of the spatially adaptive phase-field model to various forms of fracture”. *Forces in Mechanics*, Vol. 10, pp. 100161, DOI 10.1016/j.finmec.2022.100161, 2023.

6.2 Invited lectures

1. S. Leyendecker. “Geometric modelling, integration and optimal control of flexible multibody dynamics”. Plenary lecture, *ECCOMAS - 11th Thematic Conference on Multibody Dynamics*, Lisboa, Portugal, 24-28 July, 2023.
2. S. Leyendecker. “Biomechanical modelling and simulation − Muskuloskeletal, cardiac and protein system”. *Rotary Club*, Nuremberg, Sebald, Germany, 10 March, 2023.

6.3 Conferences and proceedings

1. H. Port, B. Coppers, S. Bayat, E.T. Godonu, L. Valor-Mendez, D. Simon, F. Fagni, G. Corte, A.C. Bay-Jensen, K. Tascilar, A. Hueber, V. Schönau, M. Sticherling, S. Heinrich, D. Bohr, G. Schett, A. Kleyer, S. Leyendecker, S. Holm Nielsen and A.M. Liphardt. “Blood-Based Biomarkers of Inflammation And Tissue Remodeling Can Discriminate Between Rheumatoid Arthritis, Psoriasis, and Psoriatic Arthritis and Are Associated With Hand Function”. *ACR Convergence 2023*, poster, San Diego, California, 10-15 November, 2023.

2. M. Lohmayer and S. Leyendecker. “Exergetic Port-Hamiltonian Systems for Multibody Dynamics”. *4^{th} Workshop of the doctoral college ”Port-Hamiltonian Systems: Modelling, Numerics, and Control”*, Karlsruhe Institute of Technology, Karlsruhe, Germany 11-13 October, 2023
3. B. Coppers, S. Heinrich, S. Leyendecker and A. M. Liphardt. “Monitoring Functional Impairments in Inflammatory Arthritis – Potential and Challenges in Hand Movement Assessment”. *Interdisciplinary Hand Symposium*, Erlangen, Germany, 4-5 October, 2023.
4. S. Heinrich, B. Coppers, A. M. Liphardt and S. Leyendecker. “Why and How to Include Data in Biomechanical Optimal Control Simulations?”. *Interdisciplinary Hand Symposium*, Erlangen, Germany, 4-5 October, 2023.
5. V. Wirth, A.M. Liphardt, B. Coppers, J. Bräunig, S. Heinrich, S. Leyendecker, A. Kleber, G. Schett, M. Vossiek, B. Egger and M. Stämmig. “ShaRPy: Shape Reconstruction and Hand Pose Estimation from RGB-D with Uncertainty”, In: *ICCV CVAMD Workshop 2023*, Paris, France, DOI 10.48550/arXiv.2303.10042, 2 October 2023.
6. M. Stavole, R. T. Sato Martín de Almagro, O. Brüls and S. Leyendecker. “Augmented Lagrangian contact formulation of the 2D Euler elastica”, *ICIAM 2023 - 10^{th} International Congress on Industrial and Applied Mathematics*, Tokyo, Japan, 20-25 August 2023.
7. R. T. Sato Martín de Almagro and S. Leyendecker. “Frequency-dependent damping as forcing on multisymplectic integrators”, *ICIAM 2023 - 10^{th} International Congress on Industrial and Applied Mathematics*, Tokyo, Japan, 20-25 August 2023.
8. E. S. Scheiterer and S. Leyendecker. “Propagation of epistemic uncertainty though a multi-layerd geometrically exact beam”, *ICIAM 2023 - 10^{th} International Congress on Industrial and Applied Mathematics*, Tokyo, Japan, 20-25 August 2023.
9. M. Stavole, R. Sato Martín de Almagro, V. Dörlich and S. Leyendecker. “Propagation of epistemic uncertainty though a multi-layerd geometrically exact beam”. *ECCOMAS - 11^{th} Thematic Conference on Multibody Dynamics*, Lisboa, Portugal, 24-28 July, 2023.
10. S. Heinrich, B. Coppers, A. M. Liphardt and S. Leyendecker. “Inclusion of optical marker position data in optimal control simulations of a rigid body model of the human hand”. *ECCOMAS - 11^{th} Thematic Conference on Multibody Dynamics*, Lisboa, Portugal, 24-28 July, 2023.
11. S. Leyendecker. “Geometric modelling, integration and optimal control of flexible multibody dynamics”. Plenary lecture, *ECCOMAS - 11^{th} Thematic Conference on Multibody Dynamics*, Lisboa, Portugal, 24-28 July, 2023.
12. R.T. Sato Martín de Almagro and S. Leyendecker.“Variational integrators and frequency-dependent damping’. *Foundations of Computational Mathematics*, poster, Paris, France, 12 - 21 June 2023.
13. T. Steigleder, J. Braeunig, J. Penner, M. Klebl, S. Leyendecker, A.M. Liphardt, M. Vossiek, C. Ostgathe. “Radar-based monitoring of movements for objective assessment of health status – a proof-of-technological-concept study for palliative care applicationing”. *European Association for Palliative Care EAPC 2023*, poster, Rotterdam, The Netherlands, 15 - 17 June 2023.
14. M. Stavole and S. Leyendecker. “Endoscopes: from experimental characterisation to modelling”. *Industrial workshop by fleXstructures 2023*, Kaiserslautern, Germany, 25-26 May, 2023.
15. D. Jadhav, D. Phansalkar and S. Leyendecker. “Numerical illustration of *Gamma*-convergence for variational integrators’. *8th FRASCAL seminar*,Erlangen, Germany 28 April 2023.
16. C. Schwöbel, D. Kelkel, S. Leyendecker and R. Hoffmann. “Gender differences in cycling motions: On objective functions for urban cycling”. *GAMM Annual Meeting*, Dresden, Germany, 30 May - 2 June 2023.
17. S. Heinrich, B. Coppers, A.M. Liphardt and S. Leyendecker. “ On the inclusion of motion capture data in optimal control simulations of the human hand”. *18th International Symposium on Computer Methods in Biomechanics and Biomedical Engineering (CMBBE)*, Paris, France, 3 -5 May 2023.

18. D. Martonová, D. Holz, M.T. Duong and S. Leyendecker. "Smoothed finite element methods in modelling and simulation of active cardiac contraction". *18th International Symposium on Computer Methods in Biomechanics and Biomedical Engineering (CMBBE)*, Paris, France, 3 -5 May 2023.

19. A. Koelewijn, M. Nitschke and S. Leyendecker. ""In the Wild' Movement Analysis of Arbitrary Motions. *18th International Symposium on Computer Methods in Biomechanics and Biomedical Engineering (CMBBE)*, Paris, France, 3 -5 May 2023.

20. M. Stavole, R.T. Sato Martín de Almagro, V. Dörlich and S. Leyendecker. "Homogenised stiffness coefficients of unloaded endoscope shafts". *MaGIC 2023*, Øyer, Norway 27 February - 3 March 2023.

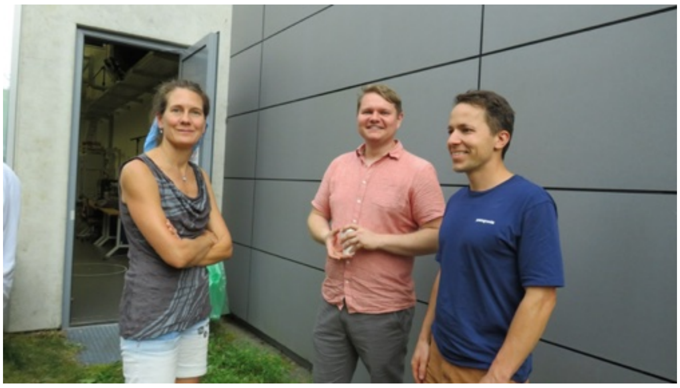
21. S. Leyendecker. "Computational models of geometrically exact beams in multibody dynamics and as smart actuators". *MaGIC 2023*, Øyer, Norway 27 February - 3 March 2023.

22. D. Jadhav, D. Phansalkar, K. Weinberg, M. Ortiz and S. Leyendecker. "Investigation of different forms of fracture using a spatially adaptive phase-field model". *8th GAMM Workshop on Phase-field modeling* , ETH Zurich, Switzerland 6-7 February 2023.

7 Social events

Erlangen Beer Festival "Bergkirchweih"

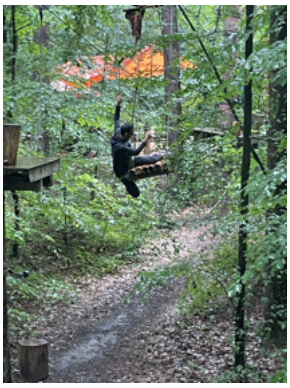
Student summer grill






Summer Trip "Climbing garden"



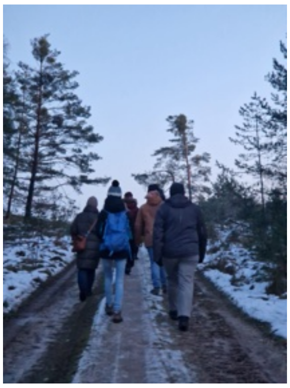
Farewell of team members








Nikolaus hiking



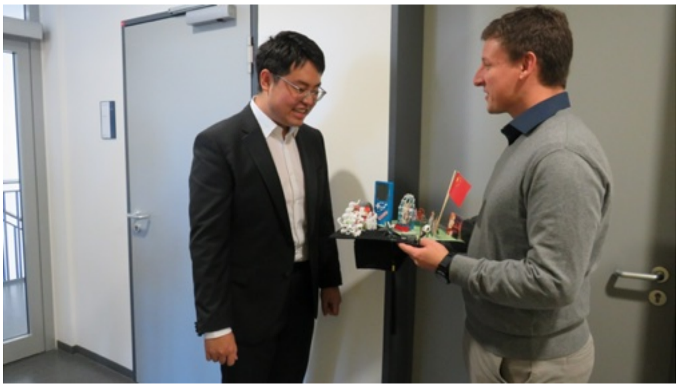
Christmas dinner

Doctoral defenses





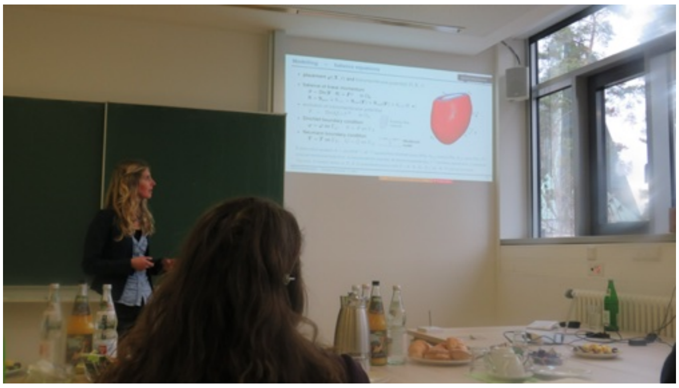







FRASCAL



Elaboration of doctor hats



Ideas: LTD team
3D Printing: Eduard Sebastian Scheiterer and Simon Heinrich
Design, assembly and making it possible: special thanks to Dhananjay Phansalkar.