Lehrstuhl für
Technische Dynamik
Prof. Dr.-Ing. habil. Sigrid Leyendecker

Report
Chair of Applied Dynamics
2018

FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG
TECHNISCHE FAKULTÄT

Prof. Dr.-Ing. habil. S. Leyendecker
Lehrstuhl für Technische Dynamik
Universität Erlangen-Nürnberg
Immerwahrstrasse 1
91058 Erlangen
Tel.: 09131 8561000
Fax.: 09131 8561011
www: http://www.ltd.tf.uni-erlangen.de

Editor: J. Rößler, D. Budday

Contents

1 Preface

This report summarises the activities in research and teaching of the Chair of Applied Dynamics at the Friedrich-Alexander-Universität Erlangen-Nürnberg between January and December 2018. The main directions of research are computational dynamics, optimal control, and biomechanics. While the focus is placed on the methodological development of efficient technologies for dynamical and optimal control simulations, these methods simultaneously provide new insights into the dynamic behavior of biomechanical and biological systems on various scales. The specific problems under investigation originate in contemporary life science and engineering, such as multi-body dynamics of human motion (hand grasping) and robot motion (industrial, spatial and medical) or the electro-mechanical modeling and simulation of muscles (rat heart project, muscle wrapping, artificial muscles). With the advanced motion capturing laboratory at LTD, research comprises experiment, modeling, and simulation of these dynamical systems, as well as their optimisation and optimal control.
At the atomistic level, kinematic and geometric models are developed to obtain insights into protein dynamics and their molecular mechanisms. To bridge the different scales that occur within and across these projects, accurate and efficient simulation techniques are of the essence. Thus, further projects are especially concerned with the development of (variational) integratos for systems with multiscale and multirate dynamics, higher order variational integrators, or Lie group methods, e.g., for use in geometrically exact beam dynamics. The development of numerical methods is likewise important as the modelling of the nonlinear systems, whereby the formulation of variational principles plays an important role on the levels of dynamic modeling, optimal control as well as numerical approximation.

2 Team

chair holder
Prof. Dr.-Ing. habil. Sigrid Leyendecker

technical staff
Beate Hegen
Sven Lässig
Johannes Rößler

academic scientist
Dr. rer. nat. Holger Lang

scientific staff

Dr. Toufik Bentaleb	until 30.09.2018
Dr.-Ing. Dominik Budday	
Dr.-Ing. Minh Tuan Duong	
M.Sc. Markus Eisentraudt	
M.Sc. Verena Hahn	from 15.09.2018 until 31.12.2018
M.Sc. David Holz	from 01.04.2018
Dipl.-Ing. Thomas Leitz	until 30.09.2018
M.Sc. Johann Penner	
M.Sc. Uday Phutane	
Dr.-Ing. Tristan Schlögl	until 31.03.2018
M.Sc. Theresa Wenger	

students

Yusuv Atakan	Pascal Baysal
Verena Hahn	Martin Hoffmann
Thomas Hufnagel	Barakat Ismail
Michael Jäger	Ayse Karabayir
Simon Kaup	Abdul Waseh Khawaja
Marie Laurien	Doan Duy Ky Le
Hanna Martin	Christele Moussi Djeukouva
Arlette Ngnogue	Peter Ostwaldt
Sebastian Penzl	Vijayan Prabhu
Matthias Pschorr	Joab Rajkumar
Mehdi Rezaiepour	Sebastian Scheiterer
Bastian Stahl	Linghui Wang
Jiafeng Wei	Simon Wiesheier
Cikai Yu	Tianhui Zhang
Yu Zou	

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.


B. Hegen

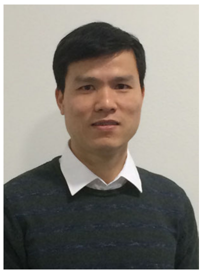

S. Lässig


J. Rößler


H. Lang


T. Bentaleb


D. Budday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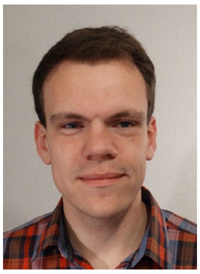
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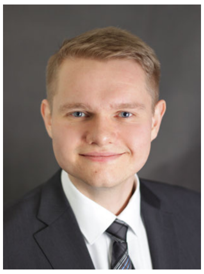
V. Hahn


D. Holz


T. Leitz


J. Penner


U. Phutane


T. Schlögl


T. Wenger


S. Leyendecker

3 Research

3.1 Biomechanics Workshop

On the 13th and 14th of November, 2018, the Chair of Applied Dynamics (LTD) hosted a workshop on Biomechanics from participants affiliated to the LTD, lead by Prof. Dr.-Ing. habil. Sigrid Leyendecker, Fraunhofer Institute for Industrial Mathematics (ITWM), headed by Dr. Michael Roller and Fraunhofer-Chalmers Centre, represented by Staffan Björkenstam. On the first day, the workshop began with a talk from Björkenstam presenting his work on “Discrete mechanics and optimal control of digital humans” and followed by a talk by Uday Phutane (LTD) on the topic “The scope for measurements to improve biomechanical simulations”. The last talk of the day was on the topic “Optimal control via reinforcement learning” by Simon Gottschalk (LTD). This was followed by a discussion and then a nice dinner at ZEN Bar. On the second day, there were more talk on the topics “Comparison of different actuation modes of a biomechanical human arm model in an optimal control framework” by Marius Obentheuer, “Optimal control simulations for human precision grasping” by Uday Phutane and “Biomechanical simulations with dynamic muscle paths” by Johann Penner. The day concluded with a discussion and lunch.

3.2 Rat heart project

The rat heart project is a research cooperation between the Chair of Applied Dynamics and the Pediatric Cardiology at University of Erlangen-Nürnberg and is funded by the Klaus Tschira Stiftung. The goal of the project is to explore the heart function on pathological and normal conditions by developing a computational model of a rat heart which will be validated with realistic experiments at the Pediatric Cardiology. Consequently, a support heart system, for example, vascular assist system and/or artificial muscles can be properly designed and attached to and/or inserted into the rat heart for improving heart functionality. In the framework of the project, a research team is hence established to develop a computational heart model. Two master theses and one project thesis were completed with significant contributions. There are three ongoing master theses on the right tracks and the rat heart project still offers two more master topics concerning enhanced electrophysiological and excitation-contraction models for further investigations, such as influence of multiscale modelling on the heart function (from the microscale with cells and drugs to macroscale-tissue behaviour).

3.3 FRASCAL - Fracture across Scales

In 2018, the research training group FRASCAL – Fracture across Scales (GRK 2423) Prof. Dr.-Ing. habil. Paul Steinmann from the Chair of Applied Mechanics at FAU as spokesperson, was successfully granted and will start at the beginning of 2019. Within FRASCAL, the P9 project – Adaptive Dynamic Fracture Simulation – is advised by Prof. Dr.-Ing. habil. Sigrid Leyendecker. The project is concerned with the kinetics of heterogeneous, e.g. cracked materials, and their effective computational resolution and simulation through suitable combinations of spatial and temporal mesh adaption strategies. It will be carried out at LTD by Dhananjay Phansalkar, who will join the team early next year.

3.4 BMBF 05M2016 - DYMARA

The Federal Ministry of Education and Research (BMBF) promotes cooperation between universities and companies in the new funding priority “Mathematics for Innovation”. “Healthy Life” is the motto of the current promotional campaign. The joint project 05M2016 – DYMARA is coordinated by Prof. Dr. rer. nat. habil. Bernd Simeon from Technische Universität Kaiserslautern (UNIKL) and has a thematic relation to ergonomics and health promotion at work. The aim of the project is to develop an innovative digital human model with detailed skeletal muscle modelling and fast numerical algorithms for fundamental research. As part of the collaborative project, the LTD investigates muscle paths in the biomechanical simulation of human motion and the integration of new fiber-based muscle models to multi body dynamics while the UNIKL is developing a continuum mechanical muscle model. The project partner Dr. Michael Burger from the Fraunhofer-Institut für Techno- und Wirtschaftsmathematik (ITWM) is focusing on the optimal control of the complete digital human model. Industrial partners are MaRhyThe-Systems GmbH & Co. KG. and flexstructures GmbH.

3.5 Scientific reports

The following pages present a short overview on ongoing research projects pursued at the Chair of Applied Dynamics. These are partly financed by third-party funding (German Research Foundation (DFG), The Federal Ministry of Education and Research (BMBF), Bavarian Environment Agency (LfU), Deutsche Telekom Stiftung) and in addition by the core support of the university.

Research topics

Kino-geometric modeling of proteins and molecular mechanisms
Dominik Budday, Sigrid Leyendecker, Henry van den Bedem

Computational modelling of cardiac muscles of a rat heart
Minh Tuan Duong, David Holz, Sigrid Leyendecker, Muhannad Alkassar, Sven Dittrich

The nonlinear fibre distribution and a fluid-cavity model of a rat heart
David Holz, Minh Tuan Duong, Sigrid Leyendecker, Muhannad Alkassar, Sven Dittrich

A Hill muscle actuated arm model with dynamic muscle paths
Johann Penner, Sigrid Leyendecker

Optimal control simulations of two-finger precision grasps
Uday D. Phutane, Michael Roller, Sigrid Leyendecker

Linear stability of variational integrators of mixed order
Theresa Wenger, Sina Ober-Blöbaum, Sigrid Leyendecker

Kino-geometric modeling of proteins and molecular mechanisms

Dominik Budday, Sigrid Leyendecker, Henry van den Bedem[1]

Proteins are dynamic macromolecules that perform a tremendous variety of biological and cellular functions crucial to life on our planet. Their motions occur on a wide range of spatial and temporal scales, often out of reach for traditional approaches, demanding an efficient, yet detailed computational tool to obtain insights across scales. We have developed kinematic and geometric modeling techniques that aim to fill this gap and provide information on conformational dynamics and molecular mechanisms of proteins on various levels.

At the core of our method lies a kino-geometric protein model, which encodes the molecules as kinematic spanning trees, with d dihedral angles as degrees of freedom $\mathbf{q} \in \mathbb{T}^d$ and non-covalent interactions such as hydrogen bonds or hydrophobics as holonomic constraints $\mathbf{\Phi}(\mathbf{q})$, imposing cycle-closure conditions. Thus, geometrically the conformation space of proteins can be described as an algebraic constraint variety or manifold $\mathcal{Q}$, where admissible velocities $\dot{\mathbf{q}}$ are restricted to the tangent space $\mathcal{T}_q\mathcal{Q}$ onto the variety at the current conformation $\mathbf{q}$. A singular value decomposition (SVD) $\mathbf{JV} = \mathbf{U\Sigma}$ of the constraint Jacobian $\mathbf{J} = \partial\mathbf{\Phi}/\partial\mathbf{q}$ provides a basis for these admissible velocities, which lie in the nullspace of $\mathbf{J}$. Here, $\mathbf{U}$ and $\mathbf{V}$ are orthonormal matrices, while $\mathbf{\Sigma} = \mathrm{diag}(\boldsymbol{\sigma})$ contains the singular values $\boldsymbol{\sigma}$ on its diagonal in decreasing order. Thus, the SVD automatically sorts kinematic motions, i.e., the columns $\mathbf{v}_i$ of $\mathbf{V}$, by their norm of constraint violation, as given by the singular value σ_i.

We display our results on the example of Adenylate Kinase (ADK), an abundant enzyme associated with maintaining energy levels in our cell (Fig. 1). On an instantaneous level, motions in the nullspace fully observe the velocity constraints and inform on remaining flexibility between larger, rigidified substructures (individually colored) in the protein (Fig. 1, top left), solely based on a single input structure (Fig. 1, top center). Thus, geometric rigidity analysis identifies conformationally coupled regimes in the protein in a matter of seconds, with identical results to existing rigidity analysis software via pebble game algorithms (FIRST, CNA, KINARI) [2].

As opposed to these tools, however, our approach is geometry based and provides a natural extension to motions that increasingly violate constraints. This hierarchy of protein motions, as encoded by dihedral degrees of freedom and non-covalent constraints, is highly conserved across the protein universe and simultaneously reveals fold-specific dynamics [3]. It further allows us to couple enthalpic contributions – given the (energetic) perturbation of non-covalent interactions approximated by σ_i of mode i – with entropic terms computed via the Shannon entropy $s_i = 1/d \exp\left[-\sum_{j=1}^{d} \kappa_{i,j}\log(\kappa_{i,j})\right]$, where $\kappa_{i,j} = v_{i,j}^2/\sum_{j=1}^{d} v_{i,j}^2$. For normalized singular values, we arrive at a mode-specific change in free energy $\Delta F_i = \sigma_i - c_T s_i$, where $\Delta F_i \in [-1, 1]$ for a dimensionless temperature factor $c_T = 1$. Estimating flexibility and sampling protein motions via kinematic motion modes from the emerging plateau of lowest free energy (Fig. 1, top right) results in conformational ensembles that show increased correlations to motions observed in MD simulations or experimental temperature factors [3].

Building on these instantaneous insights, the transition toolbox extends analysis to study conformational pathways between different substates, as indicated by the two input states (Fig. 1, top/bottom center). Our toolbox is capable to approximate transition pathways (Fig. 1, lower left) that closely pass known intermediates, and simultaneously informs on important residue networks that drive the transition through steric interaction (Fig. 1, lower right). At the heart of the sampling suite is our motion planner dCC-RRT [1], which integrates the principle of minimal frustration via dynamic Clash-avoiding Constraints (dCC) into a bidirectional rapidly exploring random tree (RRT). RRTs have in inherent drive towards open areas in conformation space and are suitable to reveal transition pathways between separated substates. The dCC are formulated in such a way that whenever two atoms are in steric contact, a dynamic constraint is formed which allows them to slide past each other, but prevents

[1]Division of Biosciences, SLAC National Accelerator Laboratory, Stanford University, California, Menlo Park, USA

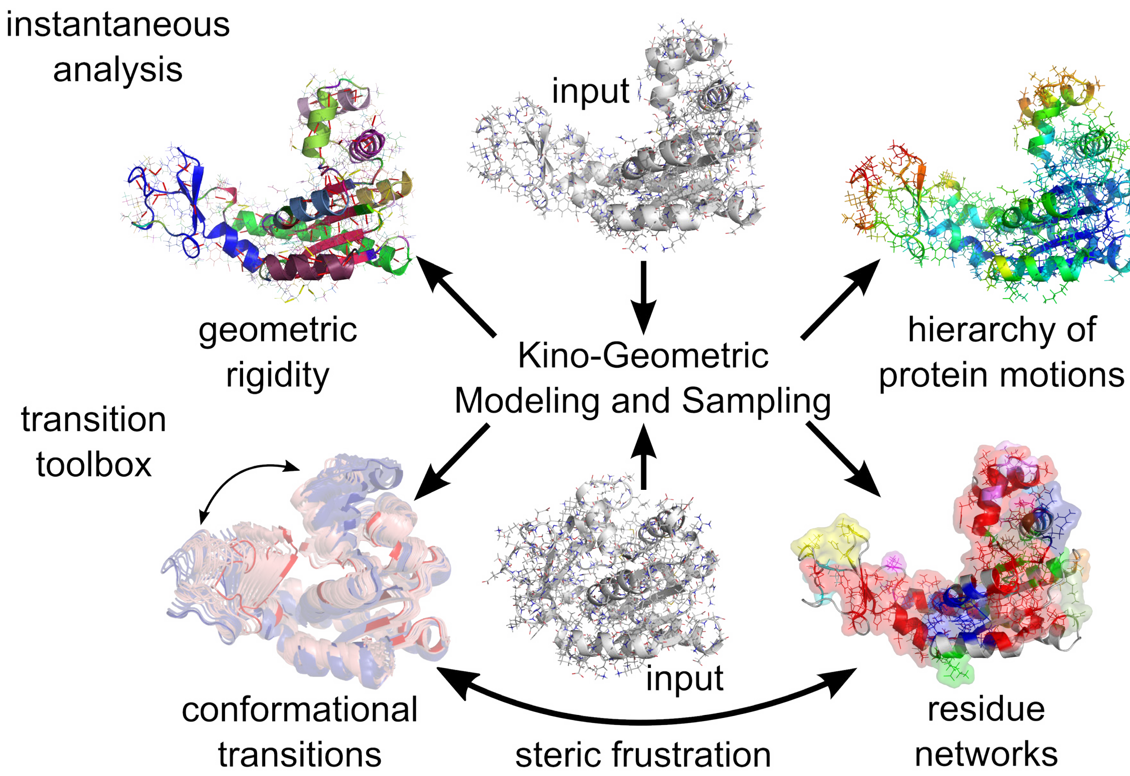


Figure 1: Kino-geometric modeling provides insights into protein dynamics on various levels.

them from moving closer towards each other. This way, dCC simultaneously enhance acceptance rates for new conformations by projecting exploration onto lower-dimensional, clash-free submanifolds, and inform on important non-native contacts that guide the transition. The algorithm identifies disjoint residue networks that interact via dCC along the pathway, thereby providing a basis for allosteric communication across the entire protein. The largest dCC network in ADK (red) spans all protein domains and may constitute the main avenue for the protein to efficiently open and close throughout its catalytic cycle (Fig. 1, lower right).
Overall, our versatile software tools reveals protein dynamics and molecular mechanisms across scales. It is implemented in the open-source Kino-Geometric Sampling (KGS) suite and freely available via `https://github.com/ExcitedStates/KGS`.

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Computational modelling of cardiac muscles of a rat heart

Minh Tuan Duong, David Holz, Sigrid Leyendecker, Muhannad Alkassar, Sven Dittrich

This work presents a computational model for the electromechanics of rat cardiac muscles taking into account the mechanoelectrical feedback (MEF) and a generalized Hill-type model for active muscle contraction (active stress-strain approach). The excitable and deformable model e.g. the left ventricle (LV) can be described by two primary field variables, placement $\boldsymbol{\varphi}(\boldsymbol{X}, t)$ and action potential $\Phi(\boldsymbol{X}, t)$. Thus, two field equations, which govern the state of the material points $\boldsymbol{X}$ at time t, can be formulated. By ignoring the inertial force, we can write the local reference equilibrium equation for the mechanical field as $\boldsymbol{0} = \mathrm{Div}[\mathbf{F} \cdot \mathbf{S}] + \boldsymbol{F}^{\varphi}$ in Ω_0. The other differential equation describes the spatio-temporal evolution of the transmembrane AP Φ and can be written as $\dot{\Phi} = \mathrm{Div}[\boldsymbol{Q}] + F^{\Phi}(\Phi, r)$ in Ω_0.

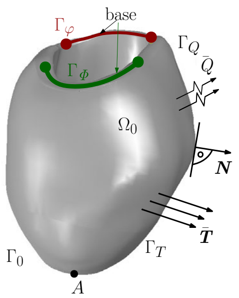

Figure 1: A rat left ventricle (LV, depicted in Figure) and a biventricular model (BV) are constructed from the 3D geometry of a rat provided by the Pediatric Cardiology in Erlangen. The boundary conditions for the solution of the two governing equations can be seen in Figure 1 (left). Boundary surface Γ_0 decomposed in Γ_φ and Γ_T for mechanical model and Γ_Φ and Γ_Q for electrical model

Herein, $\mathbf{F}$ is the deformation gradient and $\boldsymbol{F}^{\varphi}$ is the body force. To model the electrical wave propagating in the heart, we use the Aliev-Panfilov model for the cardiac muscle cells based on the monodomain formulation [1].

The mechanical model of the coupled problem for the cardiac muscle contraction simulation can be transversely isotropic or orthotropic and compressible or incompressible. We use different passive mechanical models to decribe the behavior of the muscle as follows: a transversely isotropic (TIC model), a incompressible model and the Holzapfel-Ogden orthotropic model (HO model), see [3]. All equations and parameters and the invariants of the the right Cauchy-Green tensor $\mathbf{C} = \mathbf{F}^T \cdot \mathbf{F}$ can be found in literature. Therefore, the fully coupled model for the electromechanics of the LV and BV are developed by employing the active stress and active stress-strain approach. The fully coupled model is developed for the LV and BV, in which an electrical stimulation induces a mechanical contraction, and a deformation in turn can result in an excitation (MEF). The excitation-contraction model is based on the active stress approach as $\mathbf{P} = \mathbf{P}^{pas} + \mathbf{P}^{act}(\boldsymbol{\varphi}, T^{act})$ where the passive stress is $\mathbf{P}^{pas}$ and its active counterpart is $\mathbf{P}^{act}$ as a function of the placement $\boldsymbol{\varphi}$ and the active muscle traction T^{act} defined by $\dot{T}^{act} = \epsilon(\phi)[k_\sigma(\phi - \phi_r) - T^{act}]$, in which $\epsilon(\phi)$ determines a smooth activation, k_σ and ϕ_r control the maximum active force and resting potential, respectively. The active stress is introduced as a result of electrical stimulation $\mathbf{P}^{act} = T^{act}[\nu_{ff}\boldsymbol{f_0} \otimes \boldsymbol{f_0} + \nu_{ss}\boldsymbol{s_0} \otimes \boldsymbol{s_0}]$ where ν_{ff} and ν_{ss} are the weighting factors for active stress generation. Further, the active stress-strain approach is also utilized to simulate the healthy and diseased BV model. This approach splits the deformation gradient into two parts, one is the elastic passive deformation $\mathbf{F}^e$ and the other is the active deformation tensor $\mathbf{F}^a$ such that $\mathbf{F} = \mathbf{F}^e \cdot \mathbf{F}^a$. This formulation is also in combination with the additive term of the total stress as $\mathbf{P} = \mathbf{P}^e + \mathbf{P}^a$, where $\mathbf{P}^e$ is the elastic passive term and the active stress part $\mathbf{P}^a$. Herein, we consider the cases in which the MEF can be omitted to have the partially coupled problem and the MEF is active resulting in the fully coupled problem for cardiac muscles of the left ventricle model. The results of the impact of the MEF using the above electromechanical model with the active stress approach can be seen in Figure 2. On the one hand, the responses of the three models in combination with the MEF are also depicted in Figure 2 (left). The potential and displacement curve of the apex by the HO

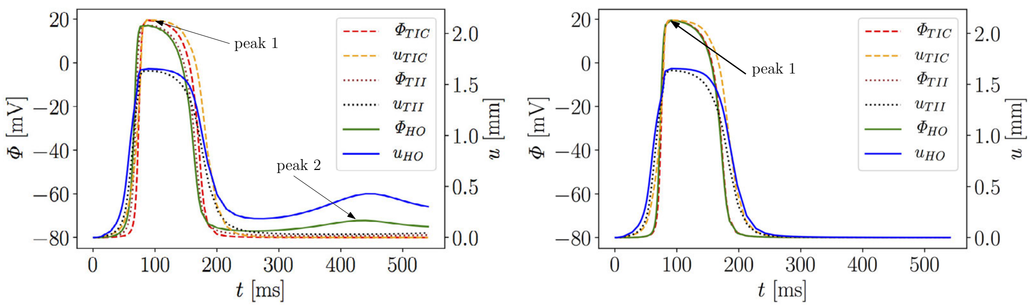

Figure 2: Evolution of AP Φ and displacement u of apical node A in a rat left ventricle for three models, without (right) and with MEF using $G_s = 10$ (left).

model show not only the normal peak (peak 1) but also a second peak (peak 2) after the repolarization, whereas the curves for the TIC and TII model exhibit no second peak, see Figure 2 (right). On the other hand, when MEF is deactivated, all reponses of the LV for the three models show normal behavior with no residual deformation. Obviously, the result by the HO model gives rise to some residual deformation. The LV is incapable of retrieving its resting potential and the initial shape and persistently contracts slightly with the residual deformation. To solve this, we propose a simple method to get rid of the residual deformation of the LV model by modifying the original form of the active stress (linear form) as $\mathbf{S}^{act}(\boldsymbol{f}_0, \Phi) = T^{act}(\Phi)\boldsymbol{f}_0 \otimes \boldsymbol{f}_0$ with $T^{act}(\Phi) = \frac{1}{1+\Delta t\, v(\Phi)} \left[T_n^{act} + \Delta t\, v(\Phi) \left[k_T\left(\Phi - \Phi_r\right)\right]\right]$. All parameters can be found in [1]. A simple modified model can be a polynomial model as $T_{poly}^{act}(\Phi) = \frac{1}{1+\Delta t\, v(\Phi)} \left[T_n^{act} + \Delta t\, v(\Phi) \left[k_T \frac{1}{\Phi_d^2} \left(\Phi - \Phi_r\right)^3\right]\right]$. The simulation result using this model can be seen in Figure 3 (left) with no residual deformation.

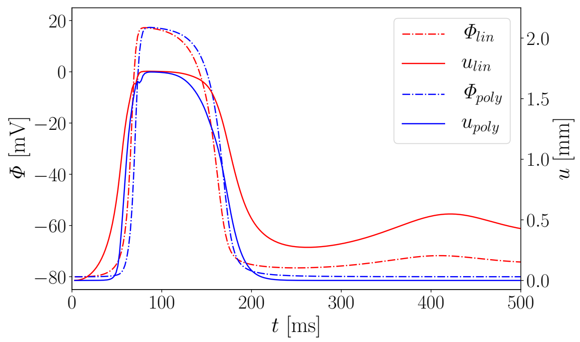

Figure 3: Evolution of AP Φ and displacement magnitude u of node A in a rat left ventricle with orthotropic HO model, with MEF. The polynomial active stress model ($poly$) results in good behavior (no second peak) with a slightly smaller plateau region compared with the original (lin). Excitation by setting seven nodes at the base to $\Phi = -20$mV for $t = 40$ms

References

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The nonlinear fibre distribution and a fluid-cavity model of a rat heart

David Holz, Minh Tuan Duong, Sigrid Leyendecker,Muhannad Alkassar[2], Sven Dittrich[2]

Computational modelling is essential to better understand the function of rat hearts under pathological and normal conditions. In this work, the nonlinear fibre distribution as well as a lumped parameter model, representing the fluid cavity, are addressed for a rat left ventricle (LV) and biventricular model (BV). A 3D geometry of a rat LV and a BV is first constructed from MRI images provided by the Pediatric Cardiology in Erlangen. Fibre orientation maps are then computed approximately for the LV and BV to account for cardiac muscle directions which are important for their orthotropic mechanical and electrical properties. Cardiac muscles are commonly aligned on sheet planes and helically distributed in the ventricular wall with respect to the longitudinal axis. Furthermore, the fibre angle with respect to the local circumferential direction varies from the endocardium to the epicardium, so-called boundary surfaces $\partial\mathfrak{B}_\theta$ (80° to -70° for rat). Consequently, the components of

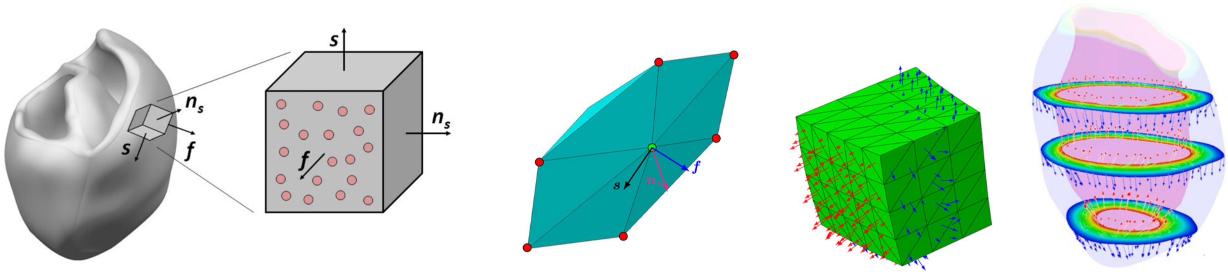

Figure 1: Rat left ventricle with fibre orientations (very right); the linear distribution of fibre angles in colors, fibres (streamlines) on the endocardium and the epicardium, fibres on different layers. General fibre structure (very left); the two figures in the middle are representing the orthotropic material directions for a single node and a simple cube.

the fibre vector $\boldsymbol{f}_0$ and the sheet vector $\boldsymbol{s}_0$ can be interplolated through the ventricular wall-thickness by solving the Laplace equation for each scalar-component value θ of these vectors; $\Delta\theta = 0$ in $\mathfrak{B}$ with the Dirichlet boundary conditions $\theta = \bar{\theta}$ on $\partial\mathfrak{B}_\theta$ [2]. Fibre orientation maps are then generated approximately for the LV and BV to account for the transmural cardiac muscle directions. Herein, we are able to take into account arbitrary continous functions for the transmural fibre direction, see Figure 1 (right) and Figure 2. However, different fibre distributions can be used to represent the microstrucuture of the heart which are important for capturing accurately their orthotropic mechanical and electrical properties.

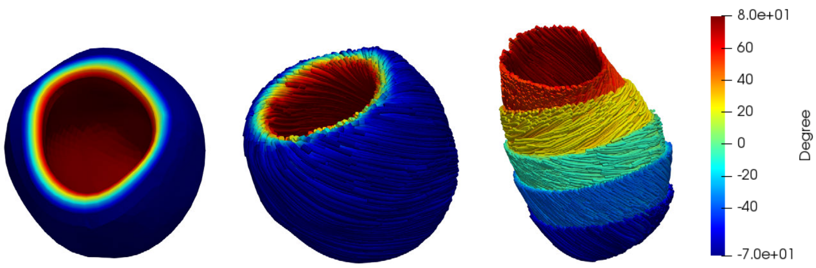

Figure 2: Rat left ventricle with fibre orientations; the nonlinear distribution of fiber angles in colors, fibres (streamlines) on the endocardium and the epicardium, fibres on different layers.

[2]Pediatric Cardiology, University of Erlangen Nuremberg, Loschgestrasse 15, 91054 Erlangen, Germany

A structurally based passive material law (Holzapfel-Ogden) for the LV and BV is described as

$$W = \frac{a}{2b} e^{b(I_3 - 3)} + \sum_{i=f,s} \frac{a_i}{2b_i} \left[e^{b_i (I_{4i}-1)^2} - 1 \right] + \frac{a_{fs}}{2b_{fs}} \left[e^{b_{fs} \left(I_{8fs} \right)^2} - 1 \right], \tag{1}$$

where a, b, a_i, b_i, for $i = s, f$ and a_{fs}, b_{fs} are material constants; I_3, I_{4i}, and I_{8fs} are the invariants of the right Cauchy-Green tensor, see [3].

Furthermore, the pressure-volume curve (p-V-loop) of the LV and BV is created by using a fluid cavity model with a 3-element Windkessel model in combination with active stress model for the muscle contraction [5]. Figure 3 (left) shows the output of the fluid-cavity model in combination with the fully coupled electromechanical model of a left ventricle (LV). The plot contains the pressure, volume and action potential (AP) over time during one cycle. Figure 3 (right) shows the reasonable behavior of the LV with an ejection fraction of about 30%. With the above mentioned active stess-strain approach, the ejection fraction can be further improved to over 50%. The right figure shows three different cases for different afterloads, imitating pathalogical conditions [4]. The computational model is a good reference to design an external support system for the diseased rat heart.

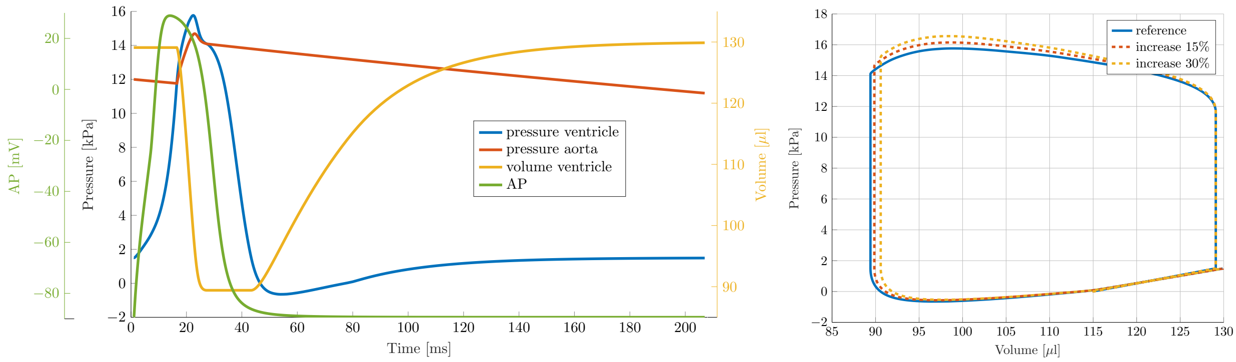

Figure 3: Evolution of AP, pressure in ventricle and aorta, volume of the left ventricle during one cardiac cycle (left). Imitating pathalogical conditions of the heart by applying different afterloads leading to a change in p-V-curve (right).

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A Hill muscle actuated arm model with dynamic muscle paths

Johann Penner, Sigrid Leyendecker

Within this work, we consider a arm model that must be steered from a given initial state to a predefined final state. In particular, the musculoskeletal motion is modelled as a multibody system representing bones and joints with Hill-type muscle actuation. Therein, the muscle force is characterised by the muscle path, which represents the interaction between muscle and multibody system. In our work, we assume that the muscle path is a locally length minimising curve that wraps smoothly over adjacent obstacles representing bones [1]. The major contribution lies in the use of discrete variational calculus [2] to describe the entire musculoskeletal system, including the muscle path in a holistic way [3]. A key advantage of this formulation is that the structure preserving properties of the integrator enable the simulation to account for large, rapid changes in muscle paths at relativity moderate computation coasts. In particular, the derived muscle wrapping formulation does not rely on special case solutions, has no nested loops, a modular structure, and works for an arbitrary number of obstacles. An example shows the application of the given method to an optimal control problem with smooth surfaces.

Biomechanical model

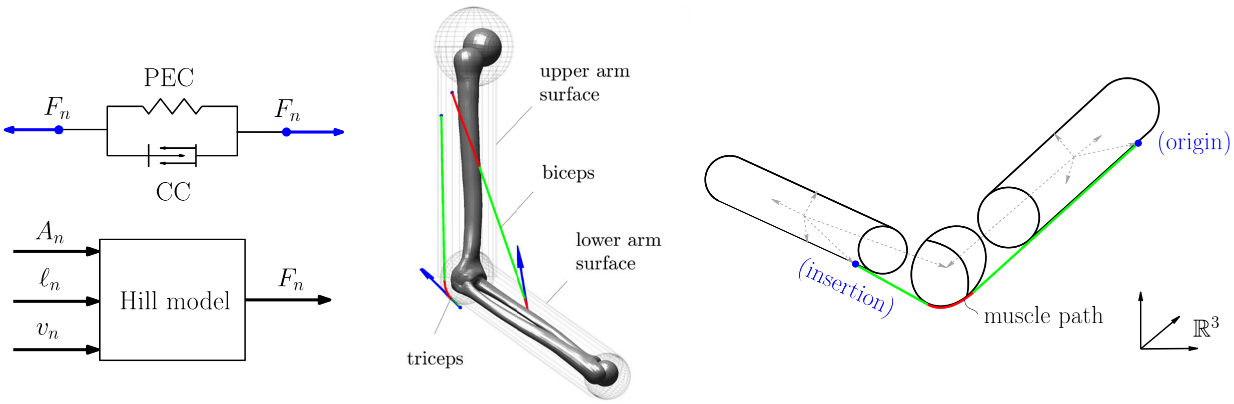

Figure 1: Hill type muscle model, muscle paths around the elbow and force directions acting on the lower arm

The multibody system in Figure 1 consists of two rigid bodies that represent the upper and lower arm, with a fixed shoulder and a revolute joint that represents the elbow. Muscle origin and insertion points according to [4] are used for the musculus triceps and biceps. Moreover, the muscle path of the triceps is modelled around an ellipsoid which represents the elbow joint, and the biceps wraps over two cylinders representing the upper and lower arm. As illustrative test scenario, the lifting of the arm from an outstretched initial configuration to a flexed elbow is examined.
The essential task of the Hill muscle model is to represent the force-length and force-velocity relations of the real muscle. The Hill model in this work consists of a contractile component (CC) and a parallel elastic component (PEC). Here, the scalar muscle force amount F_n of a single muscle is calculated as a function of activity of the muscle A_n, the muscle length ℓ_n and the contraction velocity v_n – both defined by the shortest path problem – at the n-th time step, see [4]. The muscle's action (3 dimensional force) is then characterised by the scalar muscle force value F_n and the muscle path's tangent direction at the muscle origin and insertion point.

Numerical example

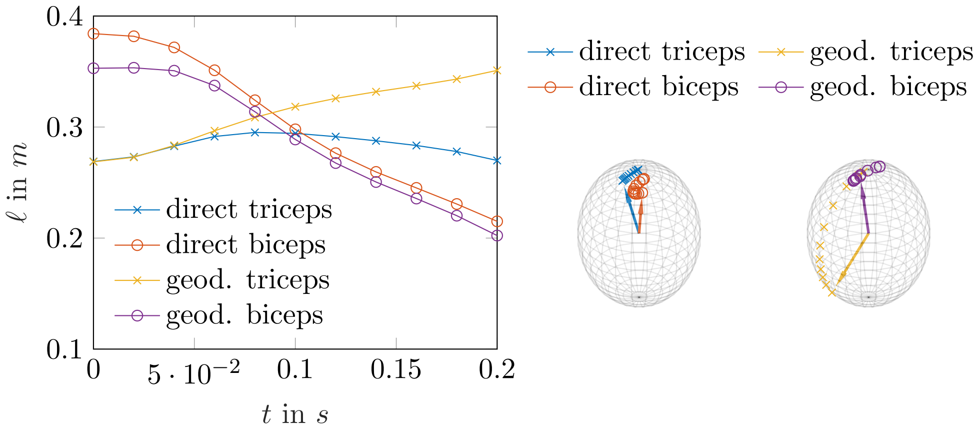

Figure 2: Comparison of muscle length and force direction (on a unit sphere) during flexion of the elbow with a direct line connection and the geodesic muscle path formulation

The simulation performs a rest-to-rest manoeuvre from a outstretched configuration to a flexed configuration. Figure 2 shows the evolution of the muscle lengths and force directions with different approaches to represent the muscle path. A direct line connection between the muscle origin and insertion points is compared to the geodesic muscle path formulation. In this comparison, the muscle path of the straight line formulation can intersect bodies, resulting in different results for the two formulations. In particular, this leads to differences in the muscle length, where the geodesic approach takes the stretching of the muscles while wrapping around obstacles into account. Consequently, when comparing the muscle length of the triceps, one sees larger values for the wrapping formulation. The contrary holds for the biceps, which is closer to the surface, resulting in smaller muscle length. Another major difference between both formulations becomes clear when investigating muscle force directions on the right side of Figure 2. Again, we see the sliding of the muscles around obstacles that results in a large and rapid change in force directions. While the straight line approach leads to nearly constant force direction, the force direction of the wrapping approach rotates by over 100 degrees.

Acknowledgments This work is funded by the Federal Ministry of Education and Research (BMBF) as part of the project 05M16WEB - DYMARA.

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Optimal control simulations of two-finger precision grasps

Uday D. Phutane, Michael Roller[3], Sigrid Leyendecker

Introduction Grasping is a complex human activity which is performed with high dexterity and coordination. It is possible due to the complicated kinematic and dynamic nature of the hand. Grasping research has major implications in areas such as ergonomic tool development, industrial robotics, and assembly planning etc. Here, we solve optimal control problems, see [1], to reproduce human-like grasping of an object with a three-dimensional, rigid multibody two-finger hand model, as shown in Figure 1. The model is constructed with a variety of joints, such as revolute, cardan, fixed, and nino (non-intersecting and non-orthogonal axes, see [3]), and is actuated by joint torques.

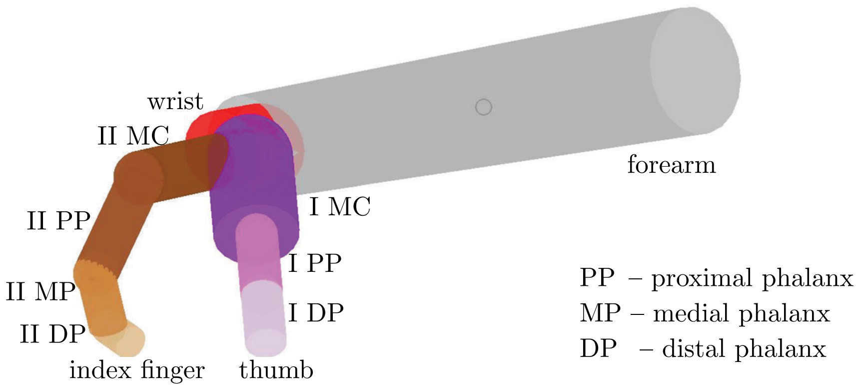

Figure 1: The two-finger model, where the thumb and index finger are denoted with roman numerals I and II.

Grasping optimal control problem During the grasping motion when the fingers close around the object, the multibody system changes from a kinematic tree structure to a closed loop contact problem. The contact between the finger digits and the object surface(s) is first closed through gap functions to locate the object and then through spherical joints, while performing the grasping action. This results in a hybrid dynamical system to describe two sequential phases with distinct discrete Euler-Lagrange equations of motion, see [4]. As mentioned in the introduction, we solve an optimal control problem (ocp) to generate time evolutions for hand and object configurations, control torques and contact forces for a grasping motion. We also determine the contact points on the finger digits and the object, and optimum time duration for the two phases. The ocp is formulated using a direct transcription method to transform it into a constrained optimisation problem. This method minimises a discrete objective function subject to the discrete Euler-Lagrange equations of motion, initial and final boundary conditions on configuration and momentum, and path constraints. The objective functions that we employ to solve the grasping ocp can be broadly divided into two perspectives. Firstly, we consider a kinematic perspective concerning the contact points. For example, we evaluate the centroid of the polygon formed by the contact points and minimise the distance of the polygon centroid to the object centre of mass. Secondly, we can choose objectives from a biomechanical perspective which either minimises the rate of change of control torques or strives toward a good hand posture while performing the grasp. We also perform optimal control simulations with a combination of multiple objective functions, as a weighted sum.

Result In [4], we have shown the ocp to perform tip and lateral pinch grasps. Here, we present a simulation result for a two-finger palmar pinch grasp with a cube. The grasp is performed with two

[3]Fraunhofer Institute for Industrial Mathematics, Kaiserslautern, Germany

contact points on each of the distal phalanges of the thumb and the finger, which are fixed to the phalanx surfaces. The boundary condition is to a perform rest-to-rest manoeuvre and place the cube on a plane. The objective is the weighted sum of the two objective functions, namely the minimise contact polygon centroid distance, see [2], and the minimise control torque change, see [4],, which satisfies a kinematic and a biomechanical perspective, respectively. The minimise distance objective seeks to have a better spread of the contact points on the object and is evaluated only at the contact closing time node, while the minimise change of control torques objective works towards ensuring a smoother motion of the fingers in both the phases. To choose the weights, we solve the ocp with the individual functions and determine the order of the function values from the NLP solver. The weights are then chosen to bring the individual objectives at a common order, so as to minimise both objectives. The configuration trajectories for the finger and the object are shown with different snapshots in Figure 2.

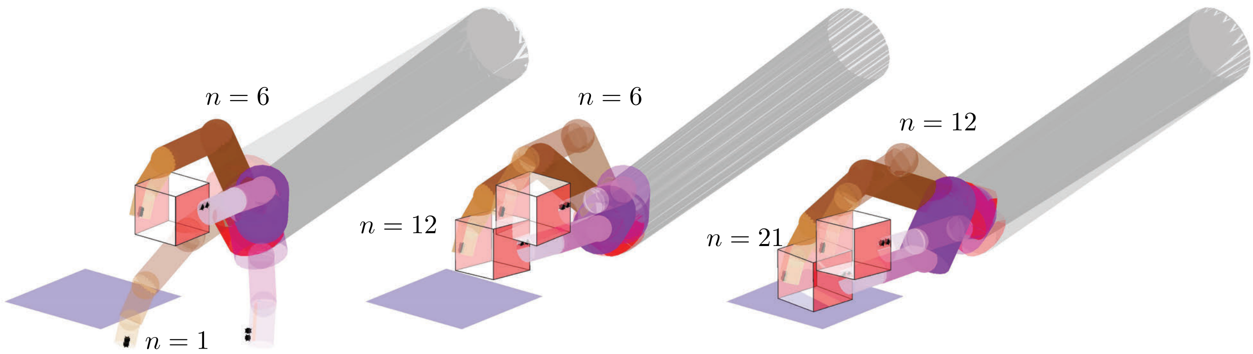

Figure 2: The palmar pinch configuration snapshots at time nodes $n = 1, 6, 12, 21$ for minimisation of contact-polygon centroid distance for a grasp and lay motion. The contact is closed at $n = 6$. Here, the shaded surfaces on a box are defined as the areas for the grasp.

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Linear stability of variational integrators of mixed order

Theresa Wenger, Sina Ober-BlÃ¶baum, Sigrid Leyendecker

The simulation of mechanical systems that act on multiple time scales, caused e.g. by different types or stiffnesses in potentials, is challenging. For resolving the fast motion a tiny time step is required, whereas for the slow motion a coarser approximation is accurate enough, pointing out the conflict of highly accurate results on the one hand and low computational costs on the other hand. Typical examples of systems comprising dynamics on different time scales can be found in astrophysics, molecular dynamics, and vehicle dynamics, to mention just a few.

Let $q(t) \in Q$ be the configuration vector defined on the n-dimensional vector space Q. It is assumed that the potential of the mechanical system is composed of different parts with strongly varying dynamics acting on different time scales, and thus, is separable into a slow potential V and a fast potential W. Furthermore, the configuration q might be split into n^s slow variables q^s and n^f fast variables q^f, $n = n^s + n^f$. The variational integrators (VIs) of mixed order build up on the higher order Galerkin variational integrators in [2] that are derived via Hamilton's variational principle with a polynomial to approximate the configuration and an appropriate quadrature rule for the approximation of the integral of the Lagrangian. To take the motions on different time scales into account two approaches are pursued. One idea is to use different quadrature rules for the integrals of the slow and fast potential, in particular a quadrature rule of order o^V for V and of order o^W for W, with $o^V \leq o^W$, reducing the number of possibly costly evaluations of $V(q)$. Secondly, the fast variables are approximated via a polynomial of degree f and a polynomial of degree s, $s < f$, is used to approximate the slow variables, reducing the number of unknowns in the discrete Euler-Lagrange equations. Both approximations can be applied solely or combined, providing the generating function of the VIs of mixed order, see [1] for more details on the construction of the integrators. Due to their variational derivation, the integrators preserve the underlying geometric structure of the dynamical system as momentum maps and symplecticity. The linear stability of the VIs of mixed order is investigated. First only systems with split potentials are considered and then systems with split potentials and split variables.
To analyse the linear stability of VIs of mixed order for split potentials, a harmonic oscillator with eigenfrequency $\sqrt{\omega^2+1}$ serves as a test system. The corresponding Lagrangian reads

$$L(q,\dot{q}) = \frac{1}{2}\dot{q}^2 - \frac{1}{2}q^2 - \frac{1}{2}\omega^2 q^2$$

with slow potential $V = \frac{1}{2}q^2$ and fast potential $W = \frac{1}{2}\omega^2 q^2$. The derivation of the linear stability conditions is based on the eigenvalue analysis of the propagation matrix P of the integrator. As the integration scheme is symplectic, it is stable, if $|\mathrm{tr}(P)| < 2$, i.e. if the following conditions are fulfilled

$$p_1 = +\mathrm{tr}(P) + 2 > 0 \qquad p_2 = -\mathrm{tr}(P) + 2 > 0 \tag{1}$$

The analysis of the linear stability of VIs of mixed order for split potentials and split variables follows next. The linear test system is a two-mass oscillator, both masses equal to 1, connected by a stiff linear spring with spring constant ω^2. Each mass is connected to a fixed point via a soft linear spring with spring constant $c = 0.5$, respectively $c = 1.5$. The Lagrangian reads

$$L((q^s,q^f),(\dot{q}^s,\dot{q}^f)) = \frac{1}{2}(\dot{q}^s)^2 + \frac{1}{2}(\dot{q}^f)^2 - \underbrace{\frac{1}{2}(q^s q^f + (q^s)^2)}_{=V(q^s,q^f)} - \underbrace{\frac{1}{2}(\omega^2+1)(q^f)^2}_{=W(q^f)}$$

The length of the stiff spring, assigned to the fast variable q^f, and the center of the stiff spring, assigned to the slow variable q^s, are used as coordinates. Analysis of the eigenvalues of the $[4 \times 4]$

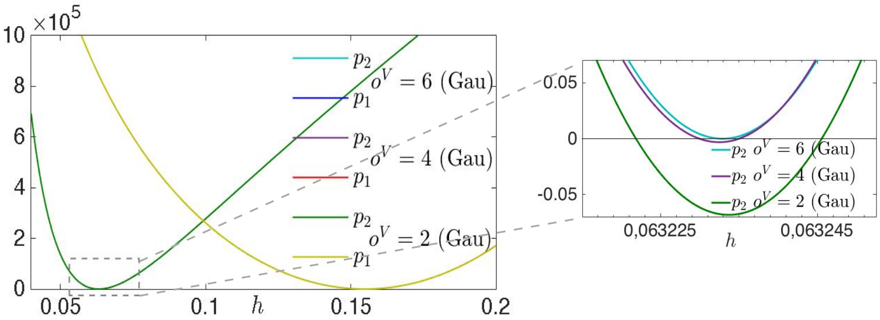

Figure 1: Linearly stable if $p_1 > 0$, $p_2 > 0$ in (1)

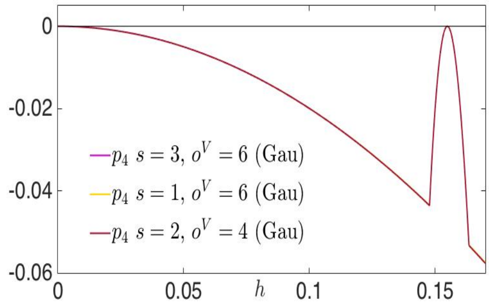

Figure 2: Linearly stable if $p_4 < 0$ in (2)

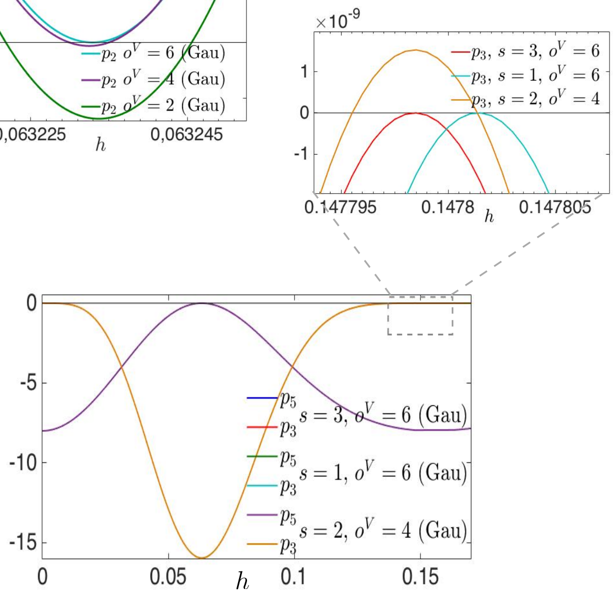

Figure 3: Linearly stable if $p_3 < 0$, $p_5 < 0$ in (2)

propagation matrix P yields three conditions, that guarantee linear stability of the integration scheme

$$p_3 = -2\mathrm{tr}(P^2) + \mathrm{tr}(P)^2 - 8 < 0 \qquad \begin{aligned} p_4 &= +\mathrm{tr}(P) + \sqrt{2\mathrm{tr}(P^2) - \mathrm{tr}(P)^2 + 8} - 4 \quad < 0 \\ p_5 &= -\mathrm{tr}(P) + \sqrt{2\mathrm{tr}(P^2) - \mathrm{tr}(P)^2 + 8} - 4 \quad < 0 \end{aligned} \tag{2}$$

The conditions in (1) and (2) depend on the time step size h and the spring constant ω. In Fig. 1 - 3, ω is set to 50, while h is plotted on the abscissa. In Fig. 1, the conditions given in (1) are depicted for the parameters $s = 3$, $o^W = 6$ (Gauss), whereas o^V (Gauss) varies from 6 to 2. The evolution of the graphs looks quite similiar. However, if we zoom in, slightly increased instability regions by decreasing o^V can be observed. Fig. 2 - 3 show the conditions given in (2) for the parameters $f = 3$, $o^W = 6$ (Gauss), while s is reduced from 3 to 1, o^V (Gauss) from 6 to 4. The instability regions, $p_3 \geq 0$, $p_4 \geq 0$, $p_5 \geq 0$, differ not or only slightly, as can be seen in the zoom of p_3. Note that for $s = f = 3$, $o^V = o^W = 6$ (Gauss) the integration scheme is equivalent to the Gauss collocation method with $s = 3$ collocation points and therefore unconditionally linearly stable. Reducing s comes along with linear instabilities. The effect of increased instability regions is more visible when the order o^V is reduced. In [1], it is shown that reducing o^V and/or s saves run-time, while the accuracy of the results stays nearly the same. However, the linear stability analysis reveals that the run-time savings come at the cost of slightly increased instability regions.

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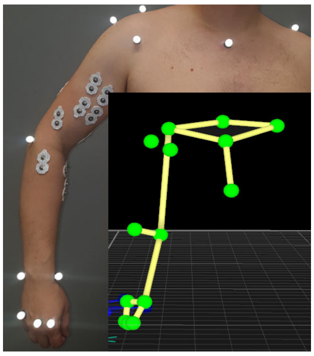
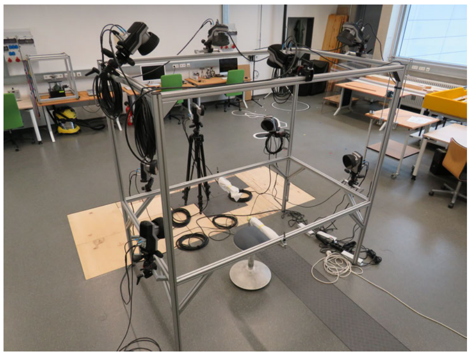
4 Activities

4.1 Motion capture laboratory

Our motion analysis lab (DFG proposal for major instrumentation INST 90/985-1) is equipped with a camera and marker based optical tracking system (10 Qualisys MoCap high speed cameras Typ Oqus 700+, 12 MP at 300 fps, 3 MP at 1100 fps, 2 Qualisys high speed video cameras 4 MP at 180 Hz, 1 MP at 360 Hz), inertial sensors (Noraxon MyoMotion Research Pro 16 Inertial Sensors, up to 200 Hz, 30 m range), Cyberglove III (Cyberglove systems LLC, 22 angle measurement sensors, sensor resolution ¡ 1 degree at 120 fps, 30 m operating range), 3 force plates (Bertec FP4060-08-2000, 400x600x83 mm, Fz max 10 kN, Fx/y max 5 kN, eigenfrequency Fz 340 Hz, Fx/y 550 Hz), and electromyography (Noraxon Desktop DTS 12 Kanal EMG System).

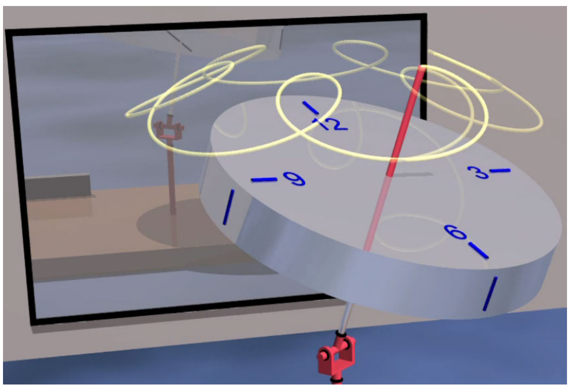




For example, several flexion tests of the elbow joint with different weights and forearm positions (neutral and supinated) at three different shoulder angles were performed in the motion analysis laboratory. Kinematic data for the upper and lower arm as well as EMG data for the m. biceps, m. brachialis, m. triceps, m. pronator teres, m. flexor carpi radialis and m. flexor carpi ulnaris were collected. This test scenario was developed and recorded in cooperation with Marius Obentheuer (ITWM).

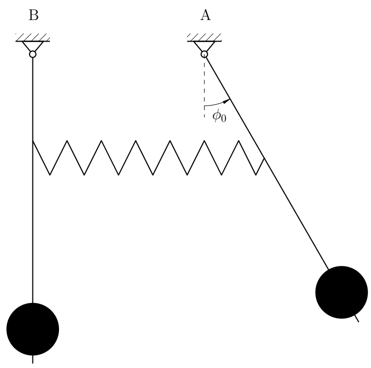
4.2 Dynamic laboratory

The dynamic laboratory – modeling, simulation and experiment (Praktikum Technische Dynamik) adresses all students of the Technical Faculty of the Friedrich-Alexander-Universität Erlangen-Nürnberg. 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 experiment and six experiments at the real existing objects, including the corresponding numerical simulation:

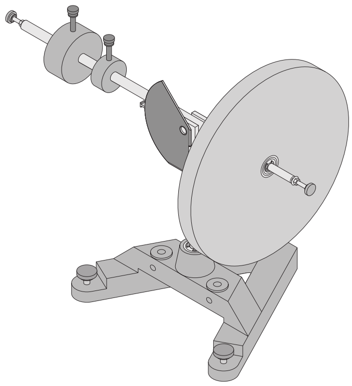
- programming training
- beating pendulums
- gyroscope
- ball balancer
- robot arm
- inverse pendulum
- balancing robot



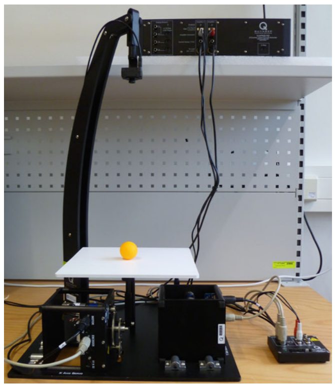
programming training



beating pendulums

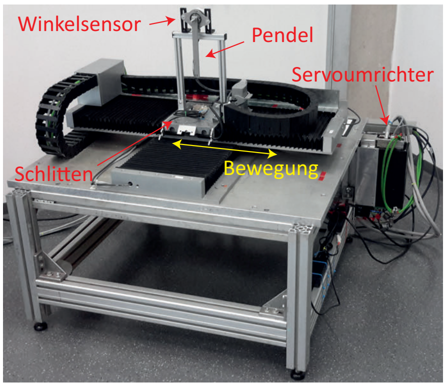


gyroscope



ball balancer

robot arm



inverse pendulum

balancing robot

4.3 MATLAB laboratory

The MATLAB laboratory (Praktikum MATLAB) attends to all the students of the Technical Faculty of the Friedrich-Alexander-Universität Erlangen-Nürnberg. The course aims to develop amongst the participants the necessary skills of mathematical programming. The course is offered in conjunction with the Chair of Applied Mechanics (LTM), the Chair of Production Metrology (FMT) and the Chair of Engineering Design (KTmfk). The first lecture is an introductory programming session for MATLAB fundamentals. Thereafter, every chair presents a task related to mechanics and engineering, for example, the LTD task is to understand and program, the modelling and numerical methodology to describe the dynamics of a crane. The task is introduced to the students through a theory lecture, which is then followed by two programming sessions in the successive weeks, for two groups of students.

4.4 Teaching

Wintersemester 2018/2019

Dynamik starrer Körper (MB, ME, WING, IP, BPT, CE, MT)		
Vorlesung		S. Leyendecker
Übung + Tutorium		D. Budday, D. Holz J. Penner, U. Phutane T. Wenger
Mehrkörperdynamik (MB, ME, WING, TM, BPT, MT)		
Vorlesung		S. Leyendecker
Übung		T. Wenger
Praktikum Technische Dynamik – Modellierung, Simulation und Experiment (MB, ME, WING, IP, BPT)		
		S. Leyendecker D. Budday, D. Holz U. Phutane, T. Wenger
Praktikum Matlab (MB)		
		U. Phutane

Sommersemester 2018

Biomechanik (MT)		
Vorlesung + Übung		S. Budday
geprüft	33 + 20 (WS 2017/2018)	
Dynamik nichtlinearer Balken (MB, M, Ph, CE, ME, WING, IP, BPT)		
Vorlesung		H. Lang
Übung		T. Leitz
entfallen im SS 2018		
geprüft	0 + 1 (WS 2017/2018)	
Geometrische numerische Integration (MB, ME, WING, BPT)		
Vorlesung		S. Leyendecker
Übung		T. Wenger
geprüft	10 + 0 (WS 2017/2018)	
Statik und Festigkeitslehre (BPT, CE, ME, MWT, MT)		
Vorlesung		S. Leyendecker
Übung + Tutorium		T. Bentaleb, D. Budday
geprüft	432 + 0 (WS 2017/2018)	M. Eisentraudt, T. Leitz J. Penner, U. Phutane T. Wenger

Theoretische Dynamik (TM, MB, ME, BPT, WING)

Vorlesung		H. Lang
Übung		J. Penner
entfallen im SS 2018		
geprüft	0 + 4 (WS 2017/2018)	

Praktikum Matlab (MB)

Teilnehmer	41	T. Wenger, U. Phutane

Wintersemester 2017/2018

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

Vorlesung		S. Leyendecker, T. Wenger
Übung + Tutorium		T. Bentaleb, D. Budday
geprüft	360 + 100 (SS 2018)	T. Gail, T. Leitz
		J. Penner, U. Phutane

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

Vorlesung + Übung		T. Wenger
geprüft	11 + 5 (SS 2018)	S. Leyendecker
entfallen im WS2017/2018		

Praktikum Technische Dynamik – Modellierung, Simulation und Experiment (MB, ME, WING, IP, BPT)

Teilnehmer	6	S. Leyendecker
		T. Bentaleb, D. Budday
		M. T. Duong, T. Gail
		T. Leitz, U. Phutane
		T. Schlögl, T. Wenger

Praktikum Matlab (MB)

Teilnehmer	52	M. Eisentraudt, T. Schlögl

4.5 Theses

Doctoral theses

- Dr.-Ing. Tristan Schlögl
  Modelling, simulation and optimal control of dielectric elastomer actuated systems

- Dr.-Ing. Dominik Budday
  High-Dimensional Robotics at the Nanoscale – Kino-Geometric Modeling of Proteins and Molecular Mechanisms

Master theses

- Thomas Hufnagel
  Modelling a surface-based fluid cavity of a rat left ventricle using finite element method

- Daria Frolova (mit Dr. M. Alkassar, FAU)
  Investigation of the heart function under normal and patological conditions using finite element sumulation

- Verena Hahn (mit Prof. J. Forst, FAU)
  Modelling and Dynamic Simulation of a Prosthetic Foot – Variational Integrators and Optimal Control

- Kevin Lösch
  A decoupled approach to the simulation of cardiac electromechanics in a rat heart

- Alexander Leberle
  A fourth-order explicit one-step Taylor Maclaurin series based integration scheme for Lagrangian Cosserat beams

Project theses

- Jiafeng Wei
  Model-based control for a ball-balancer system

- Linghui Wang
  Kinematische Analyse von Protein-Konformationen mit Hilfe des Rouché-Capelli-Theorem

- Tianhui Zhang
  Geometrische Modellierung hydrophober Wechselwirkungen zur Steifigkeitsanalyse von Proteinen

- Nils Mößner
  Automatisierte Ausgleichsrechnung zur Modellparameterbestimmung einer spurgebundenen Autorennbahn

- Alexander Leberle
  Higher-order dervatives of Lagrangian Cosserat beam model for Taylor Maclaurin series based integration scheme

- E. Sebastian Scheiterer
  Autonomous point to point navigation for a balancing Lego NXT robot with external camera-based state detection

Bachelor theses

- Tim Heinzmann (mit Dr. V. Vierow, FAU)
  Dynamische Füllstandmessung flüssigkeitsgefüllter Gebinde in der medizinischen Anwendung

- Fabian Bengl
  Ein spieltheoretischer Ansatz zur variationellen Integration der Multiratendynamik von Massenpunktsystemen

4.6 Seminar for mechanics

together with the Chair of Applied Mechanics LTM

17.01.2018 Theresa Ach
Master thesis, Chair of Applied Dynamics, University of Erlangen-Nuremberg
Computational modelling of the cardiac electromechanical coupling and Purkinje networks in a rat heart using FEM

30.01.2018 Yunfeng Mao
Tongji University / Technische Universität Darmstadt
Simulating gas transport by Finite Volume Method and Lattice Boltzmann Method

28.02.2018 Sebastian Scheiterer
Project thesis, Chair of Applied Dynamics, University of Erlangen-Nuremberg
Autonomous point to point navigation for a balancing Lego NXT robot with external camera-based state detection

14.03.2018 Nils Mößner
Project thesis, Chair of Applied Dynamics, University of Erlangen-Nuremberg
Automatisierte Ausgleichsrechnung zur Modellparameterbestimmung einer spurgebundenen Autorennbahn

16.05.2018 Dr. Daniel Arndt
Interdisciplinary Center for Scientific Computing (IWR), Universität Heidelberg
Ideas on Schwarz Smoothers in Efficient Multigrid Solvers

30.05.2018 Alexander Leberle
Project thesis, Chair of Applied Dynamics, University of Erlangen-Nuremberg
Higher-order dervatives of Lagrangian Cosserat beam model for Taylor Maclaurin series based integration scheme

30.05.2018 Alexander Leberle
Master thesis, Chair of Applied Dynamics, University of Erlangen-Nuremberg
A fourth-order explicit one-step Taylor Maclaurin series based integration scheme for Lagrangian Cosserat beams

18.07.2018 Linghui Wang
Project thesis, Chair of Applied Dynamics, University of Erlangen-Nuremberg

Kinematische Analyse von Protein-Konformationen mit Hilfe des Rouché-Cpaelli-Theorem

18.07.2018 Tianhui Zhang
Project thesis, Chair of Applied Dynamics, University of Erlangen-Nuremberg
Geometrische Modellierung hydrophober Wechselwirkungen zur Steifigkeitsanalyse von Proteinen

18.07.2018 Daria Frolova
Master thesis, Chair of Applied Dynamics, University of Erlangen-Nuremberg
Investigation of the heart function under normal and patological conditions using finite element simulation

18.07.2018 Kevin Lösch
Master thesis, Chair of Applied Dynamics, University of Erlangen-Nuremberg
A decoupled approach to the simulation of cardiac electromechanics in a rat heart

24.07.2018 Prof. Karin Nachbagauer
University of Applied Sciences Upper Austria, Campus Wels Josef Ressel Center for Advanced Multibody Dynamics
Optimal Control based on the Adjoint Method for Multibody Systems including ANCF for Flexible Bodies

25.07.2018 Verena Hahn
Master thesis, Chair of Applied Dynamics, University of Erlangen-Nuremberg
Modelling and Dynamic Simulation of a Prosthetic Foot - Variational Integrators and Optimal Control

25.07.2018 Thomas Hufnagel
Master thesis, Chair of Applied Dynamics, University of Erlangen-Nuremberg
Modelling a surface-based fluid cavity of a rat left ventricle using finite element method

12.10.2018 Juan Esteban Alvarez Naranjo
Chair of Applied Dynamics, University of Erlangen-Nuremberg
Bridging multiscale dynamic analysis of heterogeneous materials

30.10.2018 Tim Heinzmann
Bachelor thesis, Chair of Applied Dynamics, University of Erlangen-Nuremberg
Dynamische Füllstandmessung flüssigkeitsgefüllter Gebinde in der medizinischen Anwendung

30.10.2018 Michael Klebl
Chair of Applied Dynamics, University of Erlangen-Nuremberg
Herleitung und Implementierung der Bewegungsgleichungen eines Roboter-Testsystems zum Einsatz in der biomedizinischen Technik

30.10.2018 Annalisa Baronetto
Chair of Applied Dynamics, University of Erlangen-Nuremberg
The use of robotics in biomedical engineering: developing an artificial arm

06.11.2018 Denisa Martonová
Chair of Applied Dynamics, University of Erlangen-Nuremberg
Multiplikative Zerlegung des Verformungsgradienten in biologischen Wachstumsprozessen

05.12.2018 Jiafeng Wei
Project thesis, Chair of Applied Dynamics, University of Erlangen-Nuremberg
Model-based control for a ball-balancer system

18.12.2018 Prof. Dr.-Ing. habil. Ellen Kuhl
Mechanical Engineering, Living Matter Lab, Stanford University
The multiphysics of Alzheimer?s disease

4.7 Editorial activities

Advisory and editorial board memberships Since January 2014, 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.

5 Publications

5.1 Reviewed journal publications

1. M. Eisentraudt, S. Leyendecker. *Epistemic uncertainty in optimal control simulation.* Mechanical Systems and Signal Processing, 121, 876-889, DOI: 10.1016/j.ymssp.2018.12.001, 2018.

2. D. Budday, S. Leyendecker, and H. van den Bedem. *Kinematic Flexibility Analysis: Hydrogen Bonding Patterns Impart a Spatial Hierarchy of Protein Motion.* Journal of Chemical Information and Modeling, Vol. 58(10), pp. 2108-2122, DOI: 10.1021/acs.jcim.8b00267, 2018.

3. R. Fonseca, D. Budday, and H. van den Bedem. *Collision-free poisson motion planning in ultra high-dimensional molecular conformation spaces.* Journal of Computational Chemistry, DOI: 10.1002/jcc.25138, 2018.

4. D. Glaas, S. Leyendecker. *Variational integrator based optimal feedback control for constrained mechanical systems.* Z Angew Math Mech., DOI:10.1002/zamm.201700221, 2018.

5. S. Björkenstam, S.J. Carlson, J. Linn, S. Leyendecker and B. Lennartson. *Inverse Dynamics for Discrete Geometric Mechanics of Multibody Systems with Application to Direct Optimal Control.* Journal of Computational and Nonlinear Dynamics, accepted for publication, 2018.

6. T. Leitz, and S. Leyendecker. *Galerkin Lie-group variational integrators based on unit quaternion interpolation.* Comput. Methods Appl. Mech. Engrg., Vol. 338, pp. 333-361, DOI:10.1016/j.cma.2018.04.022, 2018.

7. O.T. Kosmas, and S. Leyendecker. *Variational integrators for orbital problems using frequency estimation.* Advances in Computational Mathematics, DOI: 10.1007/s10444-018-9603-y, 2018.

5.2 Invited lectures

1. S. Leyendecker. *Ein dynamisches Manikin mit faserbasierter Modellierung der Skelettmuskulatur.* Biomechanik Workshop Arbeitstreffen Verbundprojekt DYMARA, Erlangen, Germany, 05-06 September 2018.

2. S. Leyendecker. *Optimal control of human motion - biological and artificial muscles.* EMMA-CC, Digitale Menschmodellierung für ergonomische Arbeitsplätze, Kaiserslautern, Germany, 12 April 2018.

3. D. Budday, R. Fonseca, A. Héliou, S. Leyendecker, and H. van den Bedem. *Functional Insights from Kino-Geometric Modeling of Macromolecules.* Invited lecture, 9. Workshop junger Nachwuchswissenschaftler in der Mechanik, Zell am See, Austria, 18-22 February 2018.

5.3 Conferences and proceedings

1. D. Budday, S. Leyendecker, and H. van den Bedem. *Bridging protein rigidity theory and normal modes using kino-geometric analysis with hierarchical constraint relaxation.* PAMM, Vol. 18, GAMM Annual Meeting, Munich, Germany, 19-23 March 2018.

2. T. Wenger, S. Ober-Blöbaum, and S. Leyendecker. *Numerical properties of mixed order variational integrators applied to dynamical multirate systems.* Conference on the Numerical Solution of Differential and Differential-Algebraic Equations (NUMDIFF-15), Halle, Germany, 3-7 September 2018.

3. J. Penner, and S. Leyendecker. *Multi-obstacle muscle wrapping based on a discrete variational principle.* European Consortium for Mathematics in Industry (ECMI) Conference, Budapest, Hungary, 18-22 June 2018.

4. U. Phutane, M. Roller and S. Leyendecker. *Optimal control simulations of tip pinch and lateral pinch grasping.* European Consortium for Mathematics in Industry (ECMI) Conference, Budapest, Hungary, 18-22 June 2018.

5. M. T. Duong, T. Ach, M. Alkassar, S. Dittrich and S. Leyendecker. *Numerical simulation of cardiac muscles in a rat biventricular model.* 6th European Conference on Computational Mechanics (ECCM 6) and 7th European Conference on Computational Fluid Dynamics (ECFD 7), Glasgow, UK, 11-15 June 2018.

6. M. T. Duong, D. Holz, T. Ach, S. V. Binnewitt, H. Stegmann, S. Dittrich, M. Alkassar and S. Leyendecker. *Simulation of cardiac electromechanics of a rat left ventricle.* GAMM Annual Meeting, Munich, Germany, 19-23 March 2018.

7. U. Phutane, M. Roller and S. Leyendecker. *Optimal control simulations of two finger grasping.* GAMM Annual Meeting, Munich, Germany, 19-23 March 2018.

8. D. Budday, S. Leyendecker, and H. van den Bedem. *Bridging protein rigidity theory and normal modes using kino-geometric analysis.* GAMM Annual Meeting, Munich, Germany, 19-23 March 2018.

9. M. Eisentraudt and S. Leyendecker. *Fuzzy uncertainty in forward dynamics simulation using variational integrators.* GAMM Annual Meeting, Munich, Germany, 19-23 March 2018.

10. J. Penner, and S. Leyendecker. *Optimization based muscle wrapping in biomechanical multibody simulations.* GAMM Annual Meeting, Munich, Germany, 19-23 March 2018.

11. D. Budday, R. Fonseca, S. Leyendecker, and H. van den Bedem. *Bridging Rigidity Theory and Normal Modes.* Second Lecture Award, 32nd Molecular Modelling Workshop Erlangen, Germany, 12-14 March 2018.

6 Social events

Visit of the Bergkirchweih 22.05.2018

Visit of escape Rooms Nürnberg 29.08.2018

Christmas party together with LTM 20.12.2018

Doctoral defense celebrations

Defense Dr.-Ing. Tristan Schlögl (26.02.2018)

Defense Dr.-Ing. Dominik Budday (18.12.2018)