Mathematics of Thin Structures
(Modeling, Analysis and Simulation)

Technische Universität Dresden
Faculty of Mathematics
September 26 – 28, 2018

Organizers: Stefan Neukamm, Oliver Sander and Axel Voigt

Contents

1 General Information

Objectives

Many models in mechanics, physics and biology invoke thin structures and physical processes in such structures. With this workshop we intend to bring together mathematicians and physicists working on the modeling, mathematical analysis and numerics of such models. In particular, topics of interest include variational models for thin films (e.g., featuring wrinkling, prestrain and microstructure) and vector- and tensor-valued partial differential equations on surface (e.g., models for surface liquid crystals and surface fluids).

Organizers

Stefan Neukamm, Oliver Sander, and Axel Voigt (Technische Universität Dresden).

Location of the Lectures

The workshop will be hosted at TU Dresden. All lectures take place at

Faculty of Mathematics
Willers-Bau (Zellescher Weg 12–14)
Room C207

Dinner

The conference dinner will take place on Sept. 26 during a boat round trip on the Elbe river on the boat MS Bad Schandau.

Support

The organizers gratefully acknowledge financial support by the DFG in the context of TU Dresden's Institutional Strategy "The Synergetic University". The workshop is supported by "Förderverein für Mathematik zu Dresden e.V."

Website

`https://tu-dresden.de/mn/math/wir/neukamm/die-professur/workshops/Workshop2018`

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2 Program

Wednesday, Sept. 26, 2018

8:30 – 9:00		**Registration**
9:00 – 9.50	Alain Goriely (University of Oxford)	Brain wrinkling
9:50 – 10:15	Sebastian Aland (HTW Dresden)	Swimming by buckling instability: simulations and experiments of thin shell microswimmers
10:15 – 10:45		**Coffee break**
10:45 – 11:35	Peter Hansbo (Jönköping University)	Finite element modelling of thin structures using tangential differential calculus
11:35 – 12:00	Michael Nestler (TU Dresden)	A finite element approach for vector- and tensor-valued surface PDEs
12:00 – 12:25	Thomas-Peter Fries (TU Graz)	Higher-order surface FEM for incompressible flows on curved manifolds
12:25 – 14:00		**Lunch break**
14:00 – 14:50	Peter Bella (Universität Leipzig)	Wrinkling of a thin elastic sheet on a compliant sphere
14:50 – 15:15	Matthias Ruf (Université libre de Bruxelles)	Hemihelical local minimizers in prestrained elastic bi-strips
15:15 – 15:40		**Coffee break**
15:40 – 16:30	Andreas Fery (IPF Dresden)	Wrinkling: From flower leaves to nanotechnology
17:45 – 21:15		*Free discussions & Social dinner (during a boat roundtrip)*

Thursday, Sept. 27, 2018

9:00 – 9.50	John Ball (University of Oxford and Heriot-Watt University)	Liquid crystal thin films
9:50 – 10:15	Len Pismen (Technion – Israel Institute of Technology)	Design and morphology of nematic elastomers
10:15 – 10:45		**Coffee break**
10:45 – 11:35	Gaetano Napoli (Università del Salento)	Curvature effects in two-dimensional nematic films
11:35 – 12:00	Alejandro Torres-Sánchez (Universitat Politècnica de Catalunya)	Modeling and simulating fluid surfaces: from Onsager's principle to numerical methods
12:00 – 12:25	Michele Ruggeri (TU Wien)	Finite element methods for the simulation of chiral magnetic Skyrmion dynamics
12:25 – 14:00		**Lunch break**
14:00 – 14:50	Patrizio Neff (Universität Duisburg-Essen)	Cosserat modeling of thin shells
14:50 – 15:15	Hanne Hardering (TU Dresden)	Discretization error estimates for a geometrically nonlinear Cosserat shell model
15:15 – 15:40	Daniel Schöllhammer (TU Graz)	Classical shell theory based on tangential differential calculus
15:40 – 16:10		**Coffee break**
16:10 – 17:00	Sören Bartels (Universität Freiburg)	Approximating gradient flow evolutions of self-avoiding inextensible curves and elastic knots
17:00 – 18:00		*Poster session & Free discussions*

Friday, Sept. 28, 2018

9:00 – 9.50	Marta Lewicka (University of Pittsburgh)	Dimension reduction for thin films with transversally varying prestrain
9:50 – 10:15	Mathias Schäffner (TU Dresden)	Derivation of a homogenized bending–torsion theory for rods with microstructural prestrain
10:15 – 10:45		**Coffee break**
10:45 – 11:35	Amin Doostmohammadi (University of Oxford)	Active thin structures
11:35 – 12:00	Thomas Ranner (University of Leeds)	A finite element method for simulating three dimensional nematode locomotion
12:00 – 12:25	Daniel Matoz Fernandez (University of Dundee)	Wrinkle formation in developing bacterial biofilms
12:25 – 14:00		**Lunch break**
14:00 – 14:25	Sebastian Hensel (IST Austria)	Weak-strong uniqueness for Navier–Stokes two-phase flow with surface tension
14:25 – 14:50	Igor Velčić (University of Zagreb)	Sharp operator-norm asymptotics for linearised elastic plates with rapidly oscillating periodic properties
14:50 – 15:40	Paul Plucinsky (California Institute of Technology)	The deformations of thin nematic elastomer sheets

3 Abstracts

Swimming by buckling instability: simulations and experiments of thin shell microswimmers

Sebastian Aland, *HTW Dresden*

We consider the surprisingly complex dynamics of an air-filled, spherical, thin shell immersed in a fluid. The interplay of in-plane surface elasticity and bending stiffness leads to a violent buckling instability when the fluid pressure is increased. Pressure oscillations can be used to trigger periodic buckling/unbuckling to propel the shell, suggesting the application as a novel microswimmer driven by ultrasound.
We present an efficient numerical model to describe this system of deformable elastic surface, inner gas and outer fluid. Simulations are compared to recent experiments and show the intense interaction of fluid pressure, shape deformations and hydrodynamics.

Liquid crystal thin films

John Ball, *University of Oxford and Heriot-Watt University*

Usually in director-based theories of liquid crystals, the director, which represents the mean orientation of the rod-like molecules, is assumed to belong to a Sobolev space, and is thus not allowed to have jump discontinuities across surfaces. However at very small length scales such wall singularities may be energetically favoured, and can be modelled with a theory in which the director belongs to SBV. The talk will explore this approach and its application to nematic and smectic thin films. This is joint work with Stephen Bedford and with Giacomo Canevari & Bianca Stroffolini.

Approximating gradient flow evolutions of self-avoiding inextensible curves and elastic knots

Sören Bartels, *Universität Freiburg*

We discuss a semi-implicit numerical scheme that allows for minimizing the bending energy of curves within certain isotopy classes. To this end we consider a weighted sum of the bending energy B and the tangent-point functional TP, i.e.,

$$E(u) = \kappa \mathrm{B}(u) + \varrho \mathrm{TP}(u) = \frac{\kappa}{2}\int_I |u''(x)|^2 \,\mathrm{d}x + \varrho \iint_{I\times I} \frac{\mathrm{d}x\,\mathrm{d}y}{r(u(y),u(x))^q}$$

with the tangent-point radius $r(u(y), u(x))$ which is the radius of the circle that is tangent to the curve u at the point $u(y)$ and that intersects with u in $u(x)$.
We define evolutions via the gradient flow for E within a class of arclength parametrized curves, i.e., given an initial curve $u^0 \in H^2(I;\mathbb{R}^3)$ we look for a family $u : [0,T] \to H^2(I;\mathbb{R}^3)$ such that, with an appropriate inner product $(\cdot,\cdot)_X$ on $H^2(I;\mathbb{R}^3)$,

$$(\partial_t u, v)_X = -\,\delta E(u)[v], \quad u(0) = u^0,$$

subject to the linearized arclength constraints

$$[\partial_t u]' \cdot u' = 0, \quad v' \cdot u' = 0.$$

Our numerical approximation scheme for the evolution problem is specified via a semi-implicit discretization, i.e., for a step-size $\tau > 0$ and the associated backward difference quotient operator d_t, we compute iterates $(u^k)_{k=0,1,\dots} \subset H^2(I;\mathbb{R}^3)$ via the recursion

$$(d_t u^k, v)_X + \kappa([u^k]'', v'') = -\varrho\delta\mathrm{TP}(u^{k-1})[v]$$

with the constraints

$$[d_t u^k]' \cdot [u^{k-1}]' = 0, \quad v \cdot [u^{k-1}]' = 0.$$

The scheme leads to sparse systems of linear equations in the time steps for cubic C^1 splines and a nodal treatment of the constraints. The explicit treatment of the nonlocal tangent-point functional avoids working with fully populated matrices and furthermore allows for a straightforward parallelization of its computation.
Based on estimates for the second derivative of the tangent-point functional and a uniform bi-Lipschitz radius, we prove a stability result implying energy decay during the evolution as well as maintenance of arclength parametrization.
We present some numerical experiments exploring the energy landscape, targeted to the question how to obtain global minimizers of the bending energy in knot classes, so-called elastic knots. This is joint work with Philipp Reiter (University of Georgia).

Wrinkling of a thin elastic sheet on a compliant sphere

Peter Bella, *Universität Leipzig*

Wrinkling of thin elastic sheets can be viewed as a way how to avoid compressive stresses. While the question of where the wrinkles appear is (mostly) well-understood, understanding properties of wrinkling is not trivial. Considering a variational viewpoint, the problem amounts to minimization of an elastic energy, which can be viewed as a non-convex membrane energy singularly perturbed by a higher-order bending term. To understand the global minimizer (ground state), the first step is to identify its energy, in particular how it depends on the small physical parameter (thickness).
I will focus on one specific example – a disk-shaped thin elastic sheet bonded to a compliant sphere. There the leading-order behavior of the energy determines the macroscopic deformation of the sheet and provides insight about the length scale of the wrinkling. The next-order correction then provide insight about how the wrinkling pattern should vary across the film, and is in particular related to the form of transition between different wrinkling patterns.

Active thin structures

Amin Doostmohammadi, *The Rudolf Peierls Centre for Theoretical Physics, University of Oxford, UK*

Monolayers of cells in tissue and bacterial colonies growing on substrates are ample examples of thin structures that are continuously driven out of equilibrium by the activity of their constituent elements. One generic property of these active layers is the spontaneous emergence of collective flows which often leads to chaotic flow patterns characterised by swirls, jets, and topological defects in their orientation field [1]. In this talk I will discuss recent works on cell monolayers and growing bacterial colonies, where we find interesting correlations between liquid crystal-like features of these active systems and their biological functionality.

I will explain our recent finding on the role of topological defects in regulating the morphology of growing cell colonies [2] and represent evidence on spontaneous formation of singularities in cellular alignment in the form of nematic topological defects, as a previously unidentified cause of cell apoptosis and extrusion, suggesting that such defects govern cell fate in epithelial tissues [3]. In addition, I will use theory of active liquid crystals to explain how motility of Pseudomonas aeruginosa bacteria leads to a slower invasion of bacteria colonies, which are individually faster. Moreover, the ability to achieve structured flows and ordered disclinations is of particular importance in the design and control of active systems [4]. By confining an active nematic fluid within a channel, we find a regular motion of disclinations, in conjunction with a well defined and dynamic flow structure. As pairs of moving disclinations travel through the channel, they continually exchange partners producing a dynamic ordered state, reminiscent of Ceilidh dancing [5]. I will show that this state is an intermediate state governing the transition to meso-scale turbulence in living fluids and that the transition belongs to the directed percolation universality class [6].

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Wrinkle formation in developing bacterial biofilms

Daniel Matoz Fernandez, *University of Dundee*

Bacterial biofilms are one of the most widespread forms of living communities on Earth capable of colonising almost any environment from humans to metals. They are defined as self-organised multicellular aggregates in which the resident cells are embedded in a self-produced extracellular polymeric matrix. Production of the matrix fulfils a variety of functions from nutrient acquisition to protection, signalling and mechanical structure, thereby allowing microorganisms to disperse and thrive, in diverse, hostile habitats.
Biofilm morphology as exhibited in laboratory conditions is commonly used as a measure of genetic mutation: the paradigm is that the architecture of the biofilm is a proxy for an underlying genotype. A typical example is the appearance of wrinkles exhibited by many biofilms formed at a substrate-air interface, with apparently reproducible patterns. Broader significance has been associated with these structures, which have variously been described as being evolutionarily advantageous for the transport of nutrients and water. However, a simple change to the environment, e.g. to the density of the substratum significantly alters this “characteristic” morphology.

This brings into question the validity and/or utility of a simple relationship between form and function.
Using experimental and a model of biofilm described by an active elastic sheet, I will explore the formation of wrinkles and the interplay between biochemical signalling in developing and mature biofilms. I will show the exact manifestation of the wrinkles apparent in lab assays can be radically altered by changes in the environmental conditions and should more appropriately be viewed as a read-out of the functional consequences of the underlying microstructure rather than a direct read-out of the genetic changes.

Wrinkling: From flower leaves to nanotechnology

Andreas Fery, *Leibniz Institut für Polymerforschung Dresden and TU Dresden*

Wrinkling is a mundane phenomenon: Wrinkles of cloth or paper are frequently encountered in everyday life and many biological systems such as skin or plant surfaces are wrinkled [1]. In spite of its ubiquity, wrinkling has only recently found applications in material science. This is mainly due to the fact that the buckling process underlying wrinkle formation is highly nonlinear in nature and, therefore, reproducibility is often low and wrinkle formation suffers in many situations from defects. The control over wrinkle morphology is increased, if the thin membrane is not free-standing but rather coupled to an elastomeric substrate much thicker than the membrane thickness.
We have investigated wrinkling under these conditions both as a metrology method [2,3] for quantifying the mechanical properties of thin films and as a means for topographical patterning [4-6]. In the first case, thin films of unknown mechanical properties are wrinkled while in adhesive contact with a substrate of know elastic properties. Under these conditions, the elastic constants of the thin film can be derived from the observed wrinkling wavelength. This method is particularly powerful for molecularly thin layers, where classical methods like (nano-)indentation fail. In the second case, wrinkles are used as templates for assembly of particles, as molds or as stamps for micro-contact printing. These approaches are particularly successful for creating optically functional surfaces such as plasmonic metamaterials [5,6].

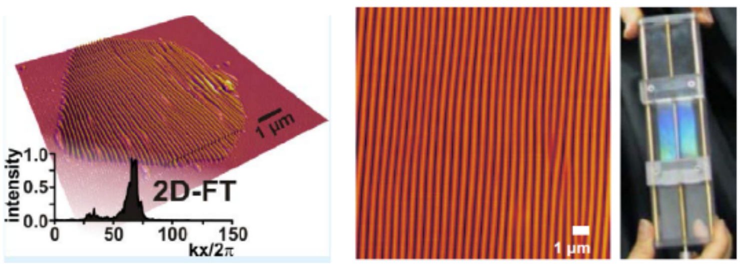

Figure 1: Mechanical properties of 2D Materials can be derived by wrinkling (right)[2,3]; wrinkles can be created with well defined wavelength in the sub.micron range for topographical patterning (left)

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Higher-order surface FEM for incompressible flows on curved manifolds

Thomas-Peter Fries, *TU Graz*

For the modeling of transport processes on interfaces, e.g., in foams, biomembranes and bubble surfaces, Stokes and Navier-Stokes flows on two-dimensional manifolds have to be considered. Models for fixed or moving curved surfaces in three dimensions are available [1]. Herein, the focus is on the approximation of stationary and instationary (Navier-)Stokes flows based on the surface finite element method as outlined in [2]. Individual orders for the geometry, velocities, pressure and Lagrange multiplier to enforce tangential velocities are chosen [3]. Stabilization is employed for flows at high Reynolds numbers. Applications are presented which extend classical benchmark test cases from flat domains to general manifolds. Highly accurate solutions are presented and higher-order convergence rates confirmed.

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Brain wrinkling

Alain Goriely, *University of Oxford*

The fascinating convolutions of the human brain are believed to be caused by mechanical forces generated in the rapid expansion of the cortex with respect to the subcortical areas of the brain. An ideal version of this problem is the wrinkling of a growing elastic film bounded to an elastic substrate. In this talk, we will discuss the validity of such a model for the brain and revisit the wrinkling problem in the nonlinear regime by using both a variational approach and methods from dynamical systems.

Finite element modelling of thin structures using tangential differential calculus

Peter Hansbo, *Department of Mechanical Engineering, Jönköping University, Sweden*

Tangential differential calculus was first used in the context of elasticity by Gurtin and Murdoch [1] for the modelling of surface tension, but was not used for models of thin structures until the work of Delfour and Zolésio, e.g., [2]. Finite element models of surface differential equations using tangential differential calculus was introduced by Dziuk [3] for the Laplace–Beltrami operator. His approach was later generalized and applied to membrane problems, beams, and plates in [4]–[8], using triangulated surfaces. Cut finite element methods were considered in [9]–[11].
We give an overview of this recent work on finite element methods for the simulation of thin structures. A background on tangential differential calculus in general and as applied to elasticity problems is given.

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Discretization error estimates for a geometrically nonlinear Cosserat shell model

Hanne Hardering, *Faculty of Mathematics, TU Dresden*

We analyze the discretization of a geometrically nonlinear elastic planar Cosserat shell by geodesic finite elements. The model is formulated as an energy minimization problem that has been obtained by dimensional reduction from a full-threedimensional Cosserat continuum model. Its degrees of freedom are the displacement of the midsurface together with an orientation field. Thus, the continuous Ansatz space $W^{1,2}(\omega, \mathbb{R}^3 \times SO(3))$ is defined over a two-dimensional Euclidean parameter domain $\omega \subset \mathbb{R}^2$, and takes values in a nonlinear Riemannian manifold. Geodesic finite elements provide an intrinsic method of discretization that has been used to obtain numerical approximations. We discuss how a priori error estimates can be obtained.

Weak-strong uniqueness for Navier–Stokes two-phase flow with surface tension

Sebastian Hensel, *IST Austria*

We establish a weak-strong uniqueness principle for the flow of two immiscible, incompressible and viscous fluids with surface tension under the assumption of identical viscosities. As long as there exists a strong solution to the system, every varifold solution originating from the same initial condition has to coincide with it. Our result covers the regime of phase-dependent densities and holds true in two and three spatial dimensions. The global-in-time existence of varifold solutions was established by H. Abels (Interfaces Free Bound. 9, 2007). The key ingredient of our result is the construction of a relative entropy functional which is capable of controlling the interface error. This is joint work with Julian Fischer.

Dimension reduction for thin films with transversally varying prestrain

Marta Lewicka, *University of Pittsburgh*

We compute the Gamma-limit of the non-Euclidean elasticity on thin films, with prestrain that varies across the specimen in both the midplate and the thin (transversal) directions. We also cover the case of the oscillatory prestrain and exhibit its relation to the non-oscillatory case via identifying the effective metric. Our analysis pertains to the Kirchhoff and the von-Karman energetical regimes.

Curvature effects in two-dimensional nematic films

Gaetano Napoli, *Dipartimento di Matematica e Fisica "E. De Giorgi", Università del Salento, Lecce, Italy*

Nematic films are thin fluid structures, ideally two dimensional, endowed with an in-plane degenerate nematic order. In this talk, I illustrate an effective two-dimensional model obtained as a reduction of the three-dimensional Frank's energy. At equilibrium, the shape of the nematic film results from a competition between surface tension, which favors the minimization of the film area, and the nematic elasticity, that instead brings up the role of curvature [2].
As an application, I consider a generalization of the classical Plateau problem to an axisymmetric nematic film bounded by two coaxial parallel rings. In particular, I revise the problem studied in [1] in the light of the correction to the two-dimensional nematic free energy proposed in [2]. This correction includes terms accounting for the extrinsic curvature of the film which are instead neglected in [1]. Two classes of equilibrium solutions have been found, where the nematic director is aligned along the meridians or parallels. Depending on two parameters, one related to the geometry and the other to the constitutive moduli, the Gaussian curvature of the film shape may be negative, vanishing or positive [3].
This is joint work with Luigi Vergori (Università di Perugia).

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Cosserat modeling of thin shells

Patrizio Neff, *Universität Duisburg-Essen*

In this talk we consider the so-called six parameter resultant shell model which allows for membrane and bending, transverse shear and drill. The kinematic degrees of freedom are the deformation and the rotation (an attached orthogonal triad at the shell surface). This model is successfully used quite often in the engineering community. The derivation of this model is usually obtained from equilibrium considerations for thickness averaged quantities. The constitutive parameters are then calibrated to some standard tests. In contrast to this approach we obtain the same model by dimension reduction from a three dimensional Cosserat model. The dimension reduction may follow two paths: an engineering path with an ansatz over the thickness of the shell or by Γ-convergence. Both methods nearly coincide: the only difference occurs in the expression for the transverse shear; in the variational context we are able to provide the first existence proof based on the direct methods. In joint work with Oliver Sander (TU Dresden) the model has been numerically implemented to calculate the mechanical response of a thin polyurethane sheet in wrinkling.
We also present preliminary results of the same approach for curved shells including an expression of the energy up to order h^5. Interestingly, the h^5-contribution vanishes for initially planar shells. Depending on the initial curvature of the shell the higher order terms may stabilize or destabilize the response. Nevertheless, an existence proof might be possible.
This is joint work with Mircea Birsan (Universität Duisburg-Essen).

A finite element approach for vector- and tensor-valued surface PDEs

Michael Nestler, *Faculty of Mathematics, TU Dresden*

We derive a Cartesian componentwise description of the covariant derivative of tangential tensor fields of any degree on general manifolds. This allows to reformulate any vector- and tensor-valued surface PDE in a form suitable to be solved by established tools for scalar-valued surface PDEs. We consider piecewise linear Lagrange surface finite elements on triangulated surfaces and validate the approach by a vector- and a tensor-valued surface Helmholtz problem on an ellipsoid. We experimentally show optimal (linear) order of convergence for these problems. The full functionality is demonstrated by solving a surface Landau–de Gennes problem on the Stanford bunny. All tools required to apply this approach to other vector- and tensor-valued surface PDEs are provided.

The deformations of thin nematic elastomer sheets

Paul Plucinsky, *California Institute of Technology*

Thin structures exhibit a broad range of mechanical responses as the competition between stretching and bending in these structures can result in buckling and localized deformations like folding and tension wrinkling. Active materials also exhibit a broad range of mechanical responses as features that manifest themselves at the microscale in these materials result in mechanical couplings at the engineering scale (thermal/electrical/dissipative) and novel function (e.g., the shape memory effect and piezoelectricity in select metal alloys and the immense fracture toughness of hydrogels). Given this richness in behaviors, my research broadly aims to address the following questions: What happens when active materials are incorporated into thin structures? Do phenomena inherent to these materials compete with or enhance those inherent to thin structures? Does this interplay result in entirely new and unexpected phenomena? And can all this be exploited to design new functions in engineering systems?

In this talk, we explore these questions in the context of nematic liquid crystal elastomers. These materials are active rubbery solids made of cross-linked polymer chains that have liquid crystals either incorporated into the main chain or pendent from them. Their structure enables a coupling between the mechanical elasticity of the polymer network and the ordering of the liquid crystals, and this in turn results in fairly complex mechanical behavior including large spontaneous distortion due to temperature change, soft-elasticity, and fine-scale microstructure. We study thin sheets of nematic elastomer. First, we show that thin of sheets of a particular class of nematic elastomer can resist wrinkling when stretched. Second, we show that thin sheets of another class of nematic elastomer can be actuated into a multitude of complex shapes.

A finite element method for simulating three dimensional nematode locomotion

Thomas Ranner, *University of Leeds*

We are motivated by understanding the locomotion of the microscopic nematode Caenorhabditis elegans. C elegans is a 1mm long, transparent round worm whose behaviour has only very recently been characterised in three dimensions. The talk will present a new numerical method for a three dimensional inextensible, viscoelastic curve model. The model is based on a driving a curve through muscle forces which are specified through a material frame which must be solved for as part of the problem. I will detail the numerical method and some preliminary numerical analysis and show how the model can be effectively used to provide insight into recent experiments.

Hemihelical local minimizers in prestrained elastic bi-strips

Matthias Ruf, *Université libre de Bruxelles*

We study the stable configurations of a thin three-dimensional weakly prestrained rod subject to a terminal load as the thickness of the section vanishes. We derive a one-dimensional limit theory and show that isolated local minimizers of the limit model can be approached by local minimizers of the three-dimensional model. Motivated by recent experiments we then focus on isotropic materials and a two-layer prestrained three-dimensional model for which the limit energy further simplifies to that of a Kirchhoff rod-model of an intrinsically curved beam. In this case we study the stability of the straight configuration. We show that at a critical load the intrinsic curvature makes the straight configuration unstable and hemihelical local minimizers emerge.

Finite element methods for the simulation of chiral magnetic Skyrmion dynamics

Michele Ruggeri, *University of Vienna*

We consider the numerical approximation of the Landau–Lifshitz–Gilbert equation, which describes the dynamics of the magnetization in ferromagnetic materials. In addition to the classical micromagnetic contributions, the energy comprises the Dzyaloshinskii–Moriya interaction, which is the most important ingredient for the enucleation and the stabilization of chiral magnetic skyrmions. We discuss a family of schemes, for which we prove (unconditional) convergence of the finite element solutions towards a weak solution of the problem. Numerical experiments demonstrate the applicability of the methods for the simulation of practically relevant problem sizes.

Derivation of a homogenized bending-torsion theory for rods with microstructural prestrain

Mathias Schäffner, *Faculty of Mathematics, TU Dresden*

We consider a nonlinear elastic composite material with ε-periodic microstructure that occupies a thin cylindrical domain (in $\mathbb{R}^3$) with small thickness h. We are interested in the situation when the different phases of the composite are prestrained (i.e. the reference configuration is not a stress-free state for the individual phases). As a consequence the rod will show a non-flat equilibrium shape that depends in a nonlinear and nonlocal way on the heterogeneity of the material and the distribution of the prestrain. By combining homogenization and dimension reduction, we derive a one-dimensional nonlinear bending-torsion theory for rods that invokes a spontaneous curvature/torsion tensor that captures the macroscopic effect of the microstructural prestrain. The spontaneous curvature/torsion tensor characterizes the equilibrium shape in the asymptotic limit $(h, \varepsilon) \downarrow 0$. It can be computed by solving linear elliptic systems. This is joint work with Robert Bauer and Stefan Neukamm.

Classical shell theory based on tangential differential calculus

Daniel Schöllhammer, *TU Graz*

The classical approach of modelling shells is to introduce a local coordinate system [1]. This concept requires the introduction of co- and contra-variant base vectors and Christoffel symbols, which makes the approach less intuitive and more complex. Yet it has been the standard approach to simulate shells for the last decades. We propose a new formulation of the linear shell theory without the explicit introduction of curvilinear coordinates. In particular, we recast the shell equations for the Kirchhoff-Love shell and Reissner-Mindlin shell in the frame of tangential operators using a global Cartesian coordinate system, which leads to a more compact and intuitive implementation. Moreover, the resulting shell equations are a generalization compared to the classical expressions, because the obtained PDEs do not hinge on a parametrization of the middle surface [2, 3]. For the numerical simulation, the derived equations are discretized with surface finite element techniques [4] using higher-order shape functions implied by Lagrange elements or NURBS patches. The boundary conditions are weakly enforced with Nitsche's method. The approach is equivalent compared to the classical theory for curved shells with arbitrary shape. Furthermore, convergence studies for numerous test cases are performed. The numerical results show that our proposed approach is equivalent to the classical theory, yet from a different viewpoint. Higher-order convergence rates are achieved.

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Modeling and simulating fluid surfaces: from Onsager's principle to numerical methods

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Fluid surfaces are a common motif in cell and tissue biology, with examples including lipid bilayers, the actomyosin cortex, or epithelial monolayers. These surfaces exhibit a non-linear coupling between elasticity, hydrodynamics and chemistry, which plays a key role in important biological processes such as cell division, migration or tissue morphogenesis. For these reasons, there is a growing interest in modeling and simulating fluid interfaces. Here, we develop a novel framework for the three-dimensional modeling and simulation of fluid surfaces from a continuum mechanics viewpoint. We show that Onsager's variational principle provides a transparent way to derive the governing equations of fluid surfaces, involving complex couplings between chemistry, elasticity and hydrodynamics. The three-dimensional simulation of fluid surfaces requires unconventional numerical methods since the resulting equations involve higher-order derivatives of the parametrization, lead to a mixed system of elliptic and hyperbolic partial differential equation, are stiff and difficult to integrate in time, and often involve discretizing tensor fields on the surface. Here, we develop a numerical framework based on subdivision finite elements, a variational time integrator rooted in Onsager's principle, and a novel method to discretize general tensor fields on smooth discrete surfaces. We show the application of our theoretical and computational methodology in examples involving lipid bilayers and the cell cortex.

Sharp operator-norm asymptotics for linearised elastic plates with rapidly oscillating periodic properties

Igor Velčić, *University of Zagreb*

In this talk we analyse a system of partial differential equations describing the behaviour of an elastic plate with periodic moduli in the two planar directions. We assume that the displacement gradients of the points of the plate are small enough for the equations of linearised elasticity to be a suitable approximation of the material response. Following the application of an appropriate version of the Floquet transform, we analyse the operator-norm resolvent behaviour of the operators in each fibre of the resulting direct integral, as the period and the plate thickness go to zero simultaneously. The convergence estimates we obtain are uniform with respect to both the Floquet parameter and the plate thickness, which yields order-sharp resolvent estimates for the convergence of the original plate problems as the plate thickness goes to zero. We use the approach of Cherednichenko, Cooper (ARMA 219, 1061-1086 (2016)) where they analyzed high-contrast elliptic equation. This is a joint work with Kirill Cherednichenko (University of Bath).

Design and morphology of nematic elastomers

Len Pismen, *Technion – Israel Institute of Technology*

Reshaping of nemato-elastic sheets or shells opens ways of creating a variety of forms that can be manipulated by boundary anchoring, positioning of defects, and topological changes. Besides static reshaping, the forms can be actuated dynamically, thereby creating crawling and swimming micro robots. Firstly, we consider three-dimensional reshaping of thin nemato-elastic sheets containing half-charged defects upon nematic-isotropic transition and show representative cases: a vicinity of isolated defects, an elliptic sheet and a sheet with two holes. Then we demonstrate a novel strategy of patterning nematic elastomers that does not require inscribing the texture directly and is based on varying the dopant concentration that, beside shifting the phase transition point, affects the nematic director field via coupling between the gradients of concentration and nematic order parameter. Next, we consider reshaping of nematoelastic films upon imbibing an isotropic solvent under conditions when isotropic and nematic phases coexist and demonstrate that the folding patterns emerging due to differential extension or contraction can be compared with folding and wrinkling patterns of different physical origin in soft materials, but their distinguished feature is, on the one hand, anisotropy specific to soft nematic solids, and on the other hand, spatial inhomogeneity that allows one to manipulate them by external inputs. Functionality and some applications of active elastomers are discussed as well. We consider the motion of the various configurations of nematoelastic crawlers made of slender rods and thin stripes with both uniform and splayed nematic order in cross-section and detect the dependence of the gait and speed on flexural rigidity and substrate friction. Also we demonstrate the motion of a flexible Stokesian flagellar swimmer realised as a yarn made of two intertwined elastomer fibres, one active and the other one passive. Finally, reshaping of active textiles actuated by bending of Janus fibres is described. We show a great variety of shapes, determined by minimising the overall energy of the fabric, that can be produced by varying bending directions determined by the orientation of Janus fibres. Under certain conditions, alternative equilibrium states, one absolutely stable and the other metastable coexist, and their relative energy may flip its sign as system parameters, such as the extension upon actuation, change. A snap-through reshaping in a specially structured textile reproduces the Venus flytrap effect.

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4 Poster

Vortices in thin-film micromagnetics

Marco Baffetti, *University of Nottingham*

Let $\Omega \subset \mathbb{R}^2$ be a bounded simply connected domain. We consider a family of energy functionals E_ϵ defined on $H^1(\Omega)$, depending on a parameter $\epsilon > 0$, that arise in the context of micromagnetics. As ϵ tends to 0, critical points u_ϵ of E_ϵ satisfying a logarithmic energy bound $E_\epsilon(u_\epsilon) \leq M|\log\epsilon|$ tend to harmonic functions whose boundary traces are in $BV(\partial\Omega)$ and jump by a multiple of π at finitely many points (the *vortices*). For minimizers and critical points whose vortices are assumed to be *separated* we know that there can only be single jumps. We prove that this is in fact true for general critical points satisfying the given energy bound.

Rotational induced normal force in meta-materials

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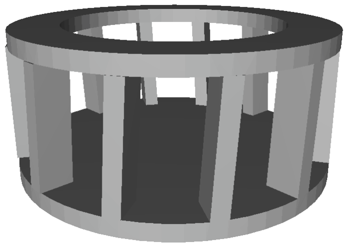
Applying torsion on a liquid or solid often causes stresses in the perpendicular directions called as normal stress. A critical question in the field of meta-material design would be the rational design of a material with desirable normal force induced by torsion. To approach this problem, we design an asymmetric cylindrical unit cell, in which the Maxwell-Betti's reciprocity relation is not valid [1]. We define the isolation and susceptibility, similar to the parameters in wave propagation and electromagnetic systems and calculate these parameters for our system [2]. By performing experiments and theoretical modeling, we study the normal force induced by torsion, and we observe that the structure has a high capability in mechanical force cancellation, and energy absorption. Due to the significant response of the system to the small rotational deflections, this simple unit cell provides a powerful platform for designing meta-materials with controllable normal force induced by torsion or controllable torsion by compression/tension.



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Nematic liquid crystals on curved surfaces - a thin film limit

Ingo Nitschke, *Faculty of Mathematics, TU Dresden*

We consider a thin film limit of a Landau-de Gennes Q-tensor model. In the limiting process we observe a continuous transition where the normal and tangential parts of the Q-tensor decouple and various intrinsic and extrinsic contributions emerge. Main properties of the thin film model, like uniaxiality and parameter phase space, are preserved in the limiting process. For the derived surface Landau-de Gennes model, we consider an L^2-gradient flow. The resulting tensor-valued surface partial differential equation is numerically solved to demonstrate realizations of the tight coupling of elastic and bulk free energy with geometric properties.

Thin film limit of the vector-valued Laplace equation for different boundary conditions

Ingo Nitschke, *Faculty of Mathematics, TU Dresden*

To clarify the impact of boundary conditions in a thin film, we consider the homogeneous vector-valued Laplace equation with Neumann, Navier, and Hodge boundary conditions (BC) as a consequence of the Euler-Lagrange (EL) equation for similar distortion energies, where these BCs are natural in tangential direction. Moreover, we present a thin film limit of the thin film PDE as well as the energies We observe that the limiting process and the EL equation commute and see how curvature quantities contribute to the resulting surface PDEs depending on the choice of BCs.

Hydrodynamic interactions in polar liquid crystals on evolving surfaces

Sebastian Reuther, *Faculty of Mathematics, TU Dresden*

We consider the derivation and numerical solution of the flow of polar liquid crystals whose molecular orientation is subjected to a tangential anchoring on an evolving curved surface. The underlying model is a simplified surface Ericksen-Leslie model, which is derived as a thin-film limit of the corresponding three-dimensional equations with appropriate boundary conditions. A finite element discretization is considered and the effect of hydrodynamics on the interplay of topology, geometric properties and defect dynamics is studied on various surfaces. Additionally we propose a surface formulation for an active polar viscous gel.

Lagrangian mechanics of cilia carpets

Anton Solovev, *Center for Advancing Electronics Dresden, TU Dresden*
(joint work with Benjamin M. Friedrich)

Cilia are thin elastic filaments grown on epithelia surfaces that exhibit active regular bending waves; collections of cilia can synchronize their beat into mesoscale metachronal waves.
We study hydrodynamic synchronization in cilia carpets, using Lagrangian Mechanics of Active Systems as a multi-scale modelling framework. Each cilium is described as a phase oscillator, where the phase represents a generalized degree of freedom that parametrizes a limit-cycle of

ciliar shapes measured in experiments. We compute generalized forces and hydrodynamic interactions between cilia, using low-Reynolds number hydrodynamic simulations (three-dimensional Stokes equation) based on a fast multipole boundary element method. We find mutual synchronization between pairs of flagella.
As the next step, we will develop generalized Kuramoto models of coupled phase oscillators, with coupling functions calibrated by hydrodynamic simulations, to understand synchronization in the presence of active ciliar fluctuations and disorder in cilia orientation.

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A geometric theory of nonlinear morphoelastic shells

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Morphoelastic shells are elastic two-dimensional bodies that can grow and remodel (the evolution of spontaneous curvatures) in time. It is an idealization of the behaviour of thin growing bodies, such as biological membranes, that can deform in-plane (stretch) and/or out-of-plane (bend). Here, we formulate a general geometric theory of nonlinear morphoelastic shells that can model the time evolution of the shell geometry as well as the residual stresses within induced by bulk growth and remodelling. In this geometric framework, growth and remodelling are modeled using an evolving referential configuration for the shell. We consider the evolution of both the first and second fundamental forms in the material manifold by considering them as dynamical variables in the variational problem. Then, we use a Lagrange-d'Alembert field theory to derive the governing equations of motion and the kinetic equation governing the geometric evolution of the shell. To prove the versality of the theory, we discuss a few examples: stress-free evolution of initially flat shells; and find the residual stress evolution in growing shells.