Vector- and Tensor-Valued Surface PDEs

Stefan Neukamm¹, Simon Praetorius¹, and Axel Voigt¹

¹Institute of Scientific Computing, TU Dresden, Germany. {stefan.neukamm, simon.praetorius, axel.voigt}@tu-dresden.de

Abstract

The workshop will delve into the intricate coupling between surface geometry and PDEs, with a particular emphasis on vector- and tensor-valued surface fields. Traditional approaches for scalar-valued equations on curved surfaces are no longer sufficient for tackling the complexities presented by vector- and tensorvalued surface PDEs. Therefore, this event seeks to bridge the gap between different communities and develop innovative numerical methods and computational simulations as well as applications and experiments to address these challenges.

Specific problems from various application areas will be investigated, including fluidic membranes, active matter, viscoelastic properties of a cell cortex, prestrained elastic structures, and nematic liquid crystal elastomers. These topics represent highly active research fields where reliable and predictive simulations play a crucial role in catalyzing further developments.

Program¹

Wednesday, Nov 29

- $\mathbf{08:55}-\mathbf{09:00}$ Opening
- 09:00 09:50 Max Wardetzky: Efficient simulations of random walks on Riemannian manifolds
- 09:50 10:15 Stefan Neukamm Derivation of a homogenized bending theory for prestrained plates
- $10{:}15-10{:}45 \ \rightsquigarrow {\rm Coffee \ break}$
- 10:45 11:35 Sami Al-Izzi: A twist on active membranes
- 11:35 12:00 Eloy de Kinkelder: Numerical simulation of active surface deformations during division of biological cells
- $12:00-13:35 \ \rightsquigarrow \ Lunch \ break$
- 13:35 14:25 Chandrasekhar Venkataraman: Stokes-flow free boundary problems, with applications to the growth of biological tissues
- 14:25 14:50 Yadong Liu: On a compressible fluid-structure interaction problem with slip boundary conditions
- $14{:}50-15{:}20 \ \rightsquigarrow {\rm Coffee \ break}$
- 15:20 15:55 Andrea Poiatti: Phase separation on evolving surfaces
- 15:55 16:20 Petr Pelech: Modeling of bacterial cell division
- 16:20 17:00 Fridtjof Brauns: Geometry, topology and morphogen gradients govern orientational order during Hydra morphogenesis

¹All times are given in Central European Standard Time (UTC+1)

Thursday, Nov 30

- 09:00 09:50 Evan Gawlik: Intrinsic curvature approximation with Regge finite elements
- $09{:}50-10{:}15$ Michael Neunteufel: Analysis of distributional Riemann curvature tensor in any dimension
- $10{:}15-10{:}45 \ \rightsquigarrow \ Coffee \ break$
- 10:45 11:35 Helmut Abels: Sharp interface limit of a Navier–Stokes/Allen–Cahn system with vanishing mobility
- $\label{eq:11:35-12:00} \begin{array}{c} \text{Lucas Benoit-Maréchal: Amplitude expansion of the phase-field crystal model on deformable surfaces} \end{array}$
- $12:00 13:35 \rightsquigarrow$ Lunch break
- 13:35 14:25 Robert Nürnberg: Parametric finite element methods for Navier–Stokes equations on evolving surfaces
- 14:25-14:50 Hanne Hardering: Parametric finite element discretizations of the surface Stokes equations
- $14:50 15:20 \rightsquigarrow \text{Coffee break}$
- 15:20 15:55 Veit Krause: Derivation and simulation of a two-phase fluid deformable surface
- 15:55 16:20 Paul Schwering: An Eulerian finite element method for tangential Navier–Stokes equations on evolving surfaces
- 16:20 17:00 Alan Demlow: Nodal FEM for the surface Stokes equations

Friday, Dec 01

- 09:00 09:50 Shuo Yang: Accelerated energy minimizing flows for large bending deformations of non-linear plates
- 09:50 10:15 Philipp Tscherner: Modeling and simulation of thin sheet folding
- $10:15 10:45 \rightsquigarrow Coffee break$
- 10:45 11:35 André Massing: Symmetric pressure stabilizations and BDF 1–6 time stepping schemes for the transient Stokes problem on surfaces.
- 11:35 12:00 Tristan Goodwill: A fast integral equation solver for surface PDEs
- 12:00 12:25 Alejandra Foggia: A meshfree collocation scheme for scalar and vector surface differential operators on point clouds
- 12:25 12:30 Closing

Sharp Interface Limit of a Navier–Stokes/Allen–Cahn system with vanishing mobility

<u>Helmut Abels¹</u>, Mingwen Fei², and Maximilian Moser³

¹Fakultät für Mathematik, Universität Regensburg.
²Department of Applied Mathematics, Anhui Normal University.
³ISTA Klosterneuburg, Austria.
helmut.abels@mathematik.uni-regensburg.de

Abstract

We consider the sharp interface limit of a Navier–Stokes/Allen–Cahn system, when a parameter $\varepsilon > 0$ that is proportional to the thickness of the diffuse interface tends to zero, in a two dimensional bounded domain. In dependence on the mobility coefficient in the Allen–Cahn equation in dependence on $\varepsilon > 0$ different limit systems or non-convergence can occur. In the case that the mobility is proportional to the square root of $\hat{I}\mu$ solutions convergence to a solutions of a classical sharp interface model on short times for well-prepared and sufficiently smooth initial data. To this end we construct a suitable approximation of the solution of the Navier–Stokes/Allen–Cahn system using an expansion with half-integer powers of ε and suitable solutions of a linearized limit system. Then the difference of approximate and exact solution is estimated with the aid of a suitable spectral estimate of the linearized Allen–Cahn operator.

This is a joint work with Mingwen Fei (Anhui Normal University, China), and Maximilian Moser (ISTA Klosterneuburg, Austria).

- H. Abels. (Non-)convergence of solutions of the convective Allen-Cahn equation. Partial Differ. Equ. Appl., 3(1):Paper No. 1, 11, 2022.
- [2] H. Abels, M. Fei, and M. Moser. Sharp interface limit for a Navier-Stokes/Allen-Cahn system in the case of a vanishing mobility. *Preprint*, arXiv:2304.12096, 2023.
- [3] S. Hensel and Y. Liu. The sharp interface limit of a Navier–Stokes/Allen–Cahn system with constant mobility: Convergence rates by a relative energy approach. SIAM J. Math. Anal., 55(5):4751–4787, 2023.

A twist on active membranes

<u>Sami Al-Izzi¹</u> and Gareth P. Alexander²

¹University of Oslo, Department of Mathematics. ²The University of Warwick, Department of Physics. samiali@math.uio.no

Abstract

I will discuss some of our recent results on active chiral and nematic membranes. The chiral stresses we consider give rise to a novel form of odd elasticity. To outline this phenomenology I will give explicit calculations outlining spontaneous flow transitions and shape instabilities. I will discuss the relevance of these results in developmental biology and their relation to active nematics, in particular how certain limits of active nematic membranes can reduce to a theory of an isotropic membrane with an active stress defined by the deviatoric part of the shape operator.

Short Bio

Sami Al-Izzi completed his PhD in Mathematics of Systems as a cotutelle between the University of Warwick and Sorbonne Université before moving to Sydney for a postdoc at the EMBL-Australia node based at UNSW. He recently moved to the University of Oslo as a postdoc. Sami's research interests are, broadly speaking, in the role of geometry, topology and mechanics in biology/soft matter, with a particular focus of active hydrodynamics in deforming geometries.

Amplitude expansion of the phase-field crystal model on deformable surfaces

Lucas Benoit–Maréchal¹ and Marco Salvalaglio¹

¹Institute of Scientific Computing, Technische Universität Dresden lucas.benoit-marechal@tu-dresden.de

Abstract

We study deformations and defects in thin, flexible sheets with crystalline order using a coarse-grained Phase-Field Crystal (PFC) model. The PFC model describes crystals at diffusive timescales through a continuous periodic field representing the atomic number density. In its amplitude expansion (APFC), a coarse-grained description featuring slowly varying fields retaining lattice deformation, elasticity, and an advanced description of dislocations is achieved.

We introduce surface PFC and APFC models in a convenient height formulation encoding normal deformation. With this framework, we then study general aspects of the buckling of strained sheets, defect nucleation on a prescribed deformed surface, and out-of-plane relaxation near dislocations.

We benchmark and discuss our results by looking at the continuum limit for buckling under elastic deformation, and at evidence from microscopic models for deformation at defects and defect arrangements. We shed light on the fundamental interplay between lattice distortion at dislocations and out-of-plane deformation by looking at the effect of the annihilation of dislocation dipoles. The scale-bridging capabilities of the devised mesoscale framework are also showcased with the simulation of a representative thin sheet hosting many dislocations.

Geometry, topology and morphogen gradients govern orientational order during Hydra morphogenesis

Fridtjof Brauns¹, Zihang Wang¹, and M. Cristina Marchetti¹

¹Kavli Institute for Theoretical Physics, University of California, Santa Barbara. fbrauns@ucsb.edu

Abstract

Orientational order, encoded in anisotropic fields, plays an important role during the development of an organism. A striking example of this is the freshwater polyp Hydra, where topological defects in the muscle fiber orientation have been shown to localize to key features of the body plan. This body plan is organized by morphogen concentration gradients, raising the question how muscle fiber orientation, morphogen gradients and body shape interact. Here, we introduce a minimal model that couples nematic orientational order to the gradient of a morphogen field. We show that on a planar surface, alignment to a radial concentration gradient can induce unbinding of topological defects, as observed during budding and tentacle formation in Hydra, and stabilize aster/vortex-like defects, as observed at a Hydra's mouth. On curved surfaces mimicking the morphologies of Hydra in various stages of development-from spheroid to adult-our model reproduces the experimentally observed reorganization of orientational order. Our results suggest how gradient alignment and curvature effects may work together to control orientational order during development and lay the foundations for future modeling efforts that will include the tissue mechanics that drive shape deformations.

Short Bio

- Since 2021 PostDoc Fellow at KITP Santa Barbara. Work on cell and tissue mechanics during morphogenesis (with Boris Shraiman) and on non-reciprocal pattern formation (with Cristina Marchetti)
- 2015-2021 PhD student with Erwin Frey at LMU Munich. Work on pattern formation in mass-conserving reaction-diffusion systems

Nodal FEM for the surface Stokes equations

<u>Alan Demlow¹</u> and Michael Neilan²

¹Department of Mathematics, Texas A&M University. ²Department of Mathematics, University of Pittsburgh. demlow@tamu.edu

Abstract

The surface Stokes equations have attracted significant recent attention in the numerical analysis literature as their numerical solution presents some challenges not present in the Euclidean case. In particular, their solution yields vector fields which should simultaneously be continuous and tangential to the given surface. This is not problematic on smooth surfaces, but is not possible in a typical finite element context where the underlying actual smooth surface is approximated by a polyhedral counterpart. Thus most finite element methods for surface Stokes problems to date have involved penalization in order to weakly enforce either tangentiality or continuity. In this talk we present FEM for the surface Stokes problems based on the MINI element. Our method is strongly tangential and H1 nonconforming, but possesses sufficient weak continuity properties that penalization is not necessary. This is the first surface Stokes methodology which allows for direct translation of common Euclidean Stokes element such as MINI, Taylor–Hood, and Scott–Vogelius to the standard surface FEM context.

This is joint work with Michael Neilan.

A meshfree collocation scheme for scalar and vector surface differential operators on point clouds

Alejandra Foggia^{1,2,3}, Abhinav Singh^{1,2,3}, and Ivo F. Sbalzarini^{1,2,3,4}

¹Technische Universität Dresden, Faculty of Computer Science, Dresden, Germany.
²Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany.
³Center for Systems Biology Dresden, Dresden, Germany.
⁴Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany.
foggia@mpi-cbg.de

Abstract

Vector-valued partial differential equations (PDEs) on surfaces describe flow processes across science and engineering. These surfaces can have a complex shape, demanding methods that provide accurate solutions beyond approximated and simplified geometries.

We propose a numerical framework that uses a mesh-free collocation method to solve PDEs on curved surfaces. We generalize the Discretization-Corrected Particle Strength Exchange (DC-PSE) [1] method to surface differential operators in a (pseudo) embedding-free way requiring fewer computational resources compared with other embedding and mesh-based methods. Our method can be combined with surface representation methods, such as (meshless) level sets [2], to operate on arbitrary surfaces. Moreover, it is scalable on multi-CPU, enabling simulations of large geometries.

We benchmark the algorithm by computing the Gauss and mean curvature of an ellipsoid and of the Stanford bunny. In addition, we compare the solution of the scalar heat equation on a flat surface with a bump obtained with our method and with several Finite Element methods [3]. We demonstrate the ability of the algorithm to work with vector PDEs by solving diffusion models and in surface-flow problems on closed curved manifolds.

- B. Schrader, S. Reboux and I. F. Sbalzarini (2010). Discretization correction of general integral PSE operators for particle methods. J. Comp. Phys., 229, 4159–4182.
- [2] S. Osher and J. A. Sethian (1988). Fronts Propagating with curvature-dependent speed: Algorithms based on Hamilton-Jacobi formulations. J. Comp. Phys., 79, 12–49.
- [3] E. Bachini, P. Brandner, T. Jankuhn, M. Nestler, S. Praetorius, A. Reusken and A. Voigt. Diffusion of tangential tensor fields: numerical issues and influence of geometric properties. J. Num. Math., 2023.

Intrinsic curvature approximation with Regge finite elements

Evan Gawlik¹

¹Department of Mathematics, University of Hawaii at Manoa. egawlik@hawaii.edu

Abstract

The lengths of the edges of a simplicial triangulation determine a piecewise constant Riemannian metric possessing single-valued tangential-tangential components along codimension-1 simplices. This Riemannian metric is the simplest example of a tensor field belonging to the Regge finite element space, which consists of piecewise polynomial symmetric tensor fields with tangential-tangential continuity. Given such a metric, one can ask how to compute intrinsic curvatures like the scalar curvature, Ricci tensor, and Riemann curvature tensor, none of which are well-defined in the classical sense because of the metric's low regularity. This talk will address some of these questions, focusing mainly on the scalar curvature. We give a definition of scalar curvature for Regge metrics, prove a convergence result in a negative-order Sobolev norm, and discuss extensions to other curvature tensors.

Short Bio

Evan Gawlik is an assistant professor of mathematics at the University of Hawaii. His research interests lie in numerical analysis, with an emphasis on numerical methods for partial differential equations and numerical linear algebra. His work often explores the interplay between numerical analysis and differential geometry.

A fast integral equation solver for surface PDEs

<u>Tristan Goodwill¹</u>

¹Committee on Computational and Applied Mathematics, University of Chicago. tgoodwill@uchicago.edu

Abstract

Elliptic PDEs on a surface embedded in three dimensions occur frequently in computer graphics, including in shape analysis and surface interpolation problems. They also occur in many areas of physics, including molecular dynamics and fluid dynamics. They are particularly useful in magnetostatics and plasma physics problems, where they are used to construct the Hodge decomposition of tangential vector fields.

In this talk, we present a method for converting a broad class of scalar elliptic PDEs on a general smooth surface into second kind Fredholm integral equations. Doing so ensures the equations are well conditioned and makes it possible to construct high-order numerical solvers. To derive the integral equation, we extend the known method for the Laplace–Beltrami problem [1] on a sphere to a broader class of equations on general smooth surfaces. Specifically, we observe that the Green's function of a corresponding PDE in the plane gives a parametrix (an approximate Green's function) for the PDE on a surface. We then use that parametrix to derive an integral equation form of the PDE.

If time allows, we will also talk about how the structure and simplicity of the resulting integral equation can be leveraged to efficiently solve the discretized linear system.

- M. C. A. Kropinski and N. Nigam (2014). Fast integral equation methods for the Laplace-Beltrami equation on the sphere. Adv. Comp. Math., 40 577–596
- [2] E. K. Rodriguez, A. Hoger, and A. D. McCulloch (1994). Stress-dependent finite growth in soft elastic tissues. Journal of Biomechanics, 27(4):455-467.

Parametric finite element discretizations of the surface Stokes equations

<u>Hanne Hardering</u>^{*1} and Simon Praetorius^{*2}

¹Institute of Numerical Mathematics, Technische Universität Dresden. ²Institute of Scientific Computing, Technische Universität Dresden. hanne.hardering@tu-dresden.de

Abstract

We present a higher-order surface finite-element (SFEM) penalty-based discretization of the tangential surface Stokes problem. Several discrete formulations are investigated which are equivalent in the continuous setting. The impact of the choice of discretization of the diffusion term and of the divergence term on numerical accuracy and convergence, as well as on implementation advantages, is discussed. We analyze the inf-sup stability of the discrete scheme in a generic approach by lifting stable finite-element pairs known from the literature. A discretization error analysis in tangential norms then shows optimal order convergence of an isogeometric setting that requires only geometric knowledge of the discrete surface.

This is joint work with Simon Praetorius (TU Dresden).

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Numerical simulation of active surface deformations during division of biological cells

Eloy de Kinkelder¹ and Sebastian Aland¹

¹Institute of Numerical Mathematics and Optimization, TU Bergakademie Freiberg. eloymerlijn.dekinkelder@htw-dresden.de

Abstract

Shape changes of single cells are governed by the actomyosin cortex, a thin layer of active material underneath the cell surface. Besides the imposed rigidity, the cortical surface exerts an active contractile tension, the strength of which being controlled by the concentration of force-generating molecules.

The complex interplay of molecule transport and surface hydrodynamics gives rise to pattern formation and self-organized shape dynamics. Despite the biological importance of these phenomena, the system is far from being understood.

To improve this understanding, we present a numerical model of such an active surface immersed in viscous fluids. The cortex is modelled as a viscoelastic surface material, described by a freely evolving Finite-Element grid. The dynamics are coupled to a surface concentration equation of force-generating molecules (e.g. actomyosin).

We analyze the emerging mechanochemical patterns and shape changes and show that the activity of the surface can lead to cell division or cell migration.

Derivation and Simulation of a two-phase fluid deformable surface model

<u>Veit Krause¹</u>, Elena Bachini², Ingo Nitschke¹, and Axel Voigt¹

¹Institute of Scientific Computing, Technische Universität Dresden. ²Department of Mathematics "Tullio Levi-Civita", University of Padua. veit.krause@tu-dresden.de

Abstract

We consider two-phase fluid deformable surfaces as model systems for biomembranes. Such surfaces are modelled by incompressible surface Navier–Stokes-Cahn–Hilliard-like equations with bending forces. We derive this model using the Lagrange–D'Alembert principle considering various dissipation mechanisms. The highly nonlinear model is solved numerically to explore the tight interplay between surface evolution, surface phase composition, surface curvature and surface hydrodynamics. It is demonstrated that hydrodynamics can enhance bulging and furrow formation, which both can further develop to pinch-offs. The numerical approach builds on a Taylor-Hood element for the surface Navier–Stokes part, a semi-implicit approach for the Cahn–Hilliard part, higher order surface parametrizations, appropriate approximations of the geometric quantities, and mesh redistribution. We demonstrate convergence properties that are known to be optimal for simplified sub-problems.

On a Compressible Fluid-Structure Interaction Problem with Slip Boundary Conditions

Yadong Liu¹, Sourav Mitra², and Šárka Nečasová³

¹Fakultät für Mathematik, Universität Regensburg.
²Department of Mathematics, Indian Institute of Technilogy Indore.
³Institute of Mathematics, Czech Academy of Scineces.
yadong.liu@ur.de

Abstract

In this talk, I will present a recent project on a compressible barotropic fluid system interacting with a linear (visco)-elastic solid equation. In particular, the elastic structure formulates the moving boundary of the fluid, and the Navier-slip type boundary condition is taken into account. Depending on the reference geometry (flat or not), we show the existence of weak solutions to the coupled system provided the adiabatic exponent satisfies $\gamma > \frac{12}{7}$ without damping and $\gamma > \frac{3}{2}$ with structure damping, utilizing the domain extension and regularization approximation.

This talk is based on joint work with Sourav Mitra (IIT, Indore) and Šárka Nečasová (IMCAS, Prague).

Symmetric pressure stabilizations and BDF 1–6 time stepping schemes for the transient Stokes problem on surfaces.

André Massing¹, Alessandro Contri¹, and Balázs Kovács²

¹Department of Mathematical Sciences, Norwegian University of Science and Technology. ³Numerische Mathematik, University of Paderborn andre.massing@ntnu.no

Abstract

We present a new stability and error analysis of fully discrete approximation schemes for the transient Surface Stokes equation. For the spatial discretization, we consider a wide class of Galerkin finite element methods which includes both very recently proposed inf-sup stable spaces and symmetric pressure stabilized (SPS) formulations.

In particular, we discuss how the classical SPS framework from Burman and Fernández [1] can be extended to surface flow problems. Afterwards we present a unified theoretical analysis of backward difference formulae (BDF methods) of order 1 to 6. The main novelty of our approach lies in deriving optimal-order stability and error estimates for both the velocity and the pressure using Dahlquist's G-stability concept together with multiplier techniques introduced by Nevanlinna and Odeh and recently by Akrivis et al. Throughout the presentation, we provide a number of numerical experiments illustrating the properties of the spatial and temporal schemes.

This is joint work with Alessandro Contri (NTNU) and Balázs Kovács (University of Paderborn)

Short Bio

André received his PhD in Computional Mathematics from the University of Oslo in 2012. After working as Postdoc and Assistant Professor at Umeå University in Sweden, he returned to Norway, where he is currently an Associate Professor at the Department of Mathematical Sciences at the Norwegian University of Science and Technology in Trondheim. André's research centers around the analysis, algorithmic realization and applications of novel discretization method for solving partial differential equations (PDEs) with a particular emphasis on complex multiphysics problems. In recents years, he has focused on surface PDEs and mixed-dimensional PDEs arising in e.g. computational cell biology.

References

 E. Burman and M. A. Fernández, Galerkin Finite Element Methods with Symmetric Pressure Stabilization for the Transient Stokes Equations: Stability and Convergence Analysis, SIAM J. Numer. Anal., 47 (2009), pp. 409–439

Derivation of a homogenized bending theory for prestrained plates

<u>Stefan Neukamm¹</u>

¹Institute of Scientific Computing, Technische Universität Dresden. stefan.neukamm@tu-dresden.de

Abstract

The presence of prestrain has a profound effect on the mechanical behavior of thin structures and can lead to curved configurations in equilibrium. In the talk, we consider nonlinear bending plates with a prescribed, microheterogeneous prestrain. Our goal is to analyze the relationship between the microheterogeneity and the shape of the energy minimizers.

To this end, we present an approach that combines analytical and numerical methods. We start with a 3D nonlinear elasticity model for a periodic material occupying a plate-like domain of small thickness. We consider a spatially periodic prestrain modeled by a multiplicative decomposition of the deformation gradient. By simultaneous dimension reduction and homogenization, we rigorously derive (in the Γ -limit of vanishing thickness and period) a homogenized nonlinear bending model for plates with an emergent spontaneous curvature term that can lead to non-flat equilibrium shapes. The effective properties of the plate model (bending stiffness and spontaneous curvature) are characterized by corrector problems. These allow to relate the microstructural configuration of the 3D plate to the shape of the minimizers of the effective 2D model. We study this analytically and numerically and discuss applications to self-forming wood bilayers.

Analysis of distributional Riemann curvature tensor in any dimension

Michael Neunteufel¹, Jay Gopalakrishnan², Joachim Schöberl¹, and Max Wardetzky³

¹Institute of Analysis and Scientific Computing, TU Wien. ²Maseeh Department of Mathematics + Statistics, Portland State University. ³Institute of Numerical and Applied Mathematics, University of Göttingen. michael.neunteufel@tuwien.ac.at

Abstract

The intrinsic curvature of an N-dimensional Riemannian manifold (M, g) with metric tensor g is given by the fourth-order Riemann curvature tensor. Regge calculus was originally developed for solving Einstein field equations in general relativity by discretizing the metric tensor by piece-wise constant metrics and approximating the curvature utilizing angle defects.

Regge finite elements have been recently developed consisting of piece-wise symmetric matrix-valued polynomials with specific continuity conditions over element interfaces. Only the tangential-tangential components are single-valued. These elements are beneficial for discretizing strain and metric fields in several applications, such as continuum mechanics, shells, and (discrete) differential geometry.

Due to the weak continuity of Regge elements, taking derivatives leads to distributions rather than regular functions. In the last four years, a concept of approximating and analyzing curvature quantities like the Gauss curvature and connection 1-form in 2D and scalar curvature in any dimension has been successfully developed.

In this talk, we propose a novel definition of the distributional (densitized) Riemann curvature tensor in any dimension. We prove that in a negative Sobolev norm, we obtain convergence towards the smooth curvature of rate k + 1, if a sequence of Regge metrics interpolating the smooth metric tensor g into Regge finite elements of polynomial order k is provided. In dimension N = 2 the rate holds for all non-negative integers k, whereas for dimension 3 or higher, one requires at least linear Regge elements.

We confirm with numerical examples, implemented in the open-source finite element software NG-Solve (www.ngsolve.org), that the proven theoretical rates are sharp.

Parametric finite element methods for Navier–Stokes equations on evolving surfaces

Robert Nürnberg¹ and Harald Garcke²

¹University of Trento, Department of Mathematics. ²Fakultät für Mathematik, Universität Regensburg. robert.nurnberg@unitn.it

Abstract

We consider the Navier–Stokes equations on an evolving surface, where the movement of the surface is prescribed by the fluid velocity on it. The equations may feature external and intrinsic forcings, the latter arising, for example, from a simple bending energy. Then the obtained system serves as a very simple model for fluidic biomembranes. We propose a parametric finite element approximation based on piecewise linear elements, and study stability and conservation properties.

This is joint work with Harald Garcke.

Short Bio

Robert graduated with a Diplom in Mathematics from Humboldt University Berlin in 2000. He received his PhD in 2003 at Imperial College London, as a student of John W. Barrett, and worked there subsequently on a permanent position first as Lecturer and then as Senior Lecturer. Since 2020 he is an Associate Professor at the University of Trento.

Robert works on the numerical approximation of moving interface problems, using both phasefield methods and parametric front tracking methods.

Modeling of bacterial cell division

Petr Pelech¹, Christoph Allolio², and Luke H. Chao³

¹Charles University, Faculty of Mathematics and Physics. ²Mathematical Institute, Charles University. ³Blavatnik Institute, Harvard Medical School. pelech@karlin.mff.cuni.cz

Abstract

To divide, Gram-negative bacteria must remodel their cell wall at the division site. However, how they overcome the internal turgor pressure to remodel their cell wall to a smaller diameter, remains still unclear. It is debated, whether remodeling alone can drive membrane constriction, or if a constrictive force from the tubulin homolog FtsZ is required. Recent numerical experiments conducted by Nguyen et al. [1] support indirectly the later option, observing the initial constriction phase only when the Z-ring force exceeds a certain level. Nevertheless, it is still an open question whether also the later division stages can be explained by such a mechanical model.

We hypothesized the growth is driven purely by stress, taking the theory of morphoelasticity (Rodriguez et al. [2]) as basis for our model. The internal turgor pressure and the constrictive Z-ring force were the only mechanical inputs.

Both constriction and septation phase were correctly reproduced by our model, which supports the hypothesis that Z-ring force plays an essential and unique role in the bacteria division process.

This is a joint work with Christoph Allolio (Charles University) and Luke Chao (Harvard).

- L. T. Nguyen, C. M. Oikonomou, H. J. Ding, M. Kaplan, Q. Yao, Y. Chang, M. Beeby, and G. J. Jensen (2019). Simulations suggest a constrictive force is required for Gram-negative bacterial cell division. Nat Commun. 10, 1259.
- [2] E. K. Rodriguez, A. Hoger, and A. D. McCulloch (1994). Stress-dependent finite growth in soft elastic tissues. Journal of Biomechanics, 27(4):455-467.

Phase separation on evolving surfaces

<u>Andrea Poiatti¹</u>, Maurizio Grasselli¹, Charles M. Elliott², and Diogo Caetano²

¹Department of Mathematics, Politecnico di Milano. ²Mathematics Institute, University of Warwick. andrea.poiatti@polimi.it

Abstract

In this talk I would like to present some recent results about the mathematical analysis of phase-field models on evolving surfaces, obtained in collaboration with Maurizio Grasselli, Charles M. Elliott and Diogo Caetano. First, in [1] we analyze the Cahn–Hilliard equation on an evolving two-dimensional surface, whose evolution is assumed to be given a priori. We show the instantaneous regularization property of weak solutions. Exploiting this result, we are able to show the validity of the instantaneous strict separation property, i.e., we prove that any weak solution stays instantaneously away from the pure states. Applications of these models can be found in the cell membrane phase separation, leading to the formation of lipid rafts. Nevertheless, the evolution in time of the surface should not be a priori prescribed . Taking inspiration from the recent [3], we derived a system of equations coupling a multicomponent Cahn–Hilliard equation with a fourth order equation for the evolution of the surface, under the assumption of small deformations. The surface evolves in time due to the presence of the different chemical species undergoing phase separation. We have analyzed this system ([2]) and obtained the well-posedness of weak solutions, together with their instantaneous regularization and the validity of the instantaneous strict separation property. In conclusion, we proved the convergence of each trajectory to a single equilibrium.

- Caetano, D., Elliott, C.M., Grasselli, M., Poiatti, A. (2023), Regularisation and separation for evolving surface Cahn-Hilliard equations, SIAM J. Math. Anal. 55(6), 6625-6675.
- [2] Caetano, D., Elliott, C.M., Grasselli, M., Poiatti, A., Mathematical analysis of a multi-component phase field model for spherical biomembranes, in preparation.
- [3] Elliott, C.M., Hatcher, L. (2021), Domain formation via phase separation for spherical biomembranes with small deformations, European J. Appl. Math. 32, 1127-1152.

An Eulerian finite element method for tangential Navier–Stokes equations on evolving surfaces

Paul Schwering^{*1}, Maxim A. Olshanskii^{†2}, and Arnold Reusken¹

¹Institut für Geometrie und Praktische Mathematik, RWTH Aachen University. ²Department of Mathematics, University of Houston. schwering@igpm.rwth-aachen.de

Abstract

The motion of an inextensible viscous fluid layer represented by a material surface can be described by the evolving surface Navier–Stokes equations. We introduce a method for the numerical solution of a simplified problem consisting of tangential surface Navier–Stokes equations (TSNSE) posed on a passively evolving smooth closed surface embedded in \mathbb{R}^3 . For discretization of the TSNSE, we consider a geometrically unfitted finite element method known as TraceFEM. The TraceFEM applies to a fully Eulerian formulation of the problem and does not require a surface triangulation, which makes it convenient for deforming surfaces. In TraceFEM, one uses standard (bulk) finite element spaces to approximate unknown quantities on the surface $\Gamma(t)$ which propagates through a given triangulation of an ambient volume Ω , i.e. $\Gamma(t) \subset \Omega$ for all times t. The discrete formulation does not need a surface parametrization and uses tangential calculus in the embedding space \mathbb{R}^3 . For scalar PDEs on evolving surfaces, variants of TraceFEM are known in the literature. For the TSNSE we choose a hybrid (finite difference in time - finite elements in space) approach since it is more flexible in terms of implementation and the choice of elements. We use a BDF scheme for the time-discretization and a stable Taylor-Hood pair of finite elements in space. To represent the surface, we use a level-set description and a higher-order method to calculate integrals on the surface approximation. Theoretical results show the optimal order of convergence. In this presentation, we explain the method and present numerical experiments that illustrate the optimality of the convergence.

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Modeling and Simulation of Thin Sheet Folding

Philipp Tscherner¹, Sören Bartels¹, Andrea Bonito², and Peter Hornung³

¹Abteilung für Angewandte Mathematik, Albert-Ludwigs-Universität Freiburg. ²Department of Mathematics, Texas A&M University ³Institut für Geometrie, Technische Universität Dresden philipp.tscherner@mathematik.uni-freiburg.de

Abstract

In this project we study foldable objects by means of modeling, numerical simulation and geometrical analysis. For the latter, a relation between the fold angle, the geodesic and the normal curvature of a folding arc is derived, giving rise to interesting geometrical observations of isometric structures involving curved folds. To model objects including kinks, a 2D energy is identified as the Γ -limit of a 3D elastic energy that accounts for discontinuities of the deformation gradient along a prescribed curve. The reduced model is discretized by a discontinuous Galerkin method that allows for a practical description of foldable structures by neglecting gradient jumps of the deformation along the folding curve. The discretized nonlinear model, that is based on a reconstruction of the Hessian and a relaxation of the isometry condition, Γ -convergences to the continuous model under appropriate density assumptions on smooth folded isometries. A priori and a posteriori error estimates are derived for the corresponding linear model that describes configurations with small deflections and does not include the isometry condition. Various numerical experiments are carried out to study the physical behaviour of foldable objects like flytraps.

Stokes-flow free boundary problems, with applications to the growth of biological tissues

Chandrasekhar Venkataraman¹

¹Mathematics, University of Sussex. C.Venkataraman@sussex.ac.uk

Abstract

We formulate, analyse and numerically simulate what are arguably the two simplest Stokes-flow free boundary problems relevant to tissue growth, extending the classical Stokes free boundary problem by incorporating (i) a volumetric source (the nutrient-rich case) and (ii) a volumetric sink, a surface source and surface compression (the nutrient-poor case). A number of phenomena are identified and characterised thereby, most notably a buckling-associated instability in case (ii). Regularisations of case (ii), which may otherwise be ill posed, will also be discussed.

Short Bio

Chandrasekhar Venkataraman is a senior lecturer in mathematics at the University of Sussex. Chandrasekhar obtained his PhD in Mathematics at Sussex in 2011. Following this, Chandrasekhar was an EPSRC funded postdoctoral fellow at Warwick till 2012 and Sussex 2012–2015. Chandrasekhar was appointed to the permanent post of Lecturer in Mathematical Biology at the University of St Andrews in 2015, before returning to Sussex in 2018. Chandrasekhar is broadly interested in mathematical biology with a particular focus on problems involving biological growth and pattern formation.

Efficient Simulations of Random Walks on Riemannian Manifolds

Max Wardetzky¹, Michael Herrmann², Simon Schwarz³, and Anja Sturm³

¹Institut für Numerische und Angewandte Mathematik, Georg-August-Universität Göttingen.
²Institut für Partielle Differentialgleichungen, Technische Universität Braunschweig.
³Institut für Mathematische Stochastik, Georg-August-Universität Göttingen.
wardetzky@math.uni-goettingen.de

Abstract

According to a version of Donsker's theorem, geodesic random walks on Riemannian manifolds converge to the respective Brownian motion. From a computational perspective, however, evaluating geodesics can be costly. We therefore introduce approximate geodesic random walks based on the concept of retractions. We show that these approximate walks converge to the correct Brownian motion in the Skorokhod topology as long as the geodesic equation is approximated up to second order. As a result we obtain an efficient algorithm for sampling Brownian motion on compact Riemannian manifolds. We will also discuss some open questions concerning possible extensions of our method to the anisotropic setting.

This is joint work with Michael Herrmann, Simon Schwarz and Anja Sturm.

Accelerated energy minimizing flows for large bending deformations of nonlinear plates

Shuo Yang¹, Guozhi Dong², and Hailong Guo³

¹Yanqi Lake Beijing Institute of Mathematical Sciences and Applications. ²School of Mathematics and Statistics, Central South University, China. ³School of Mathematics and Statistics, University of Melbourne, Australia. shuoyang@bimsa.cn

Abstract

In recent years, there have been some numerical explorations of large bending deformations in nonlinear plates, including single layer, prestrained, and bilayer plates. The mathematical problems consist of minimizations of bending energy functionals while subject to nonlinear and non-convex metric constraints. In previous works, the computation of such non-convex constrained energy minimization problems has relied on gradient flows. While these approaches are known for their stability, they often exhibit slow convergence, especially when dealing with highly non-convex problems. In this presentation, we introduce new iterative schemes that surpass existing gradient flow algorithms in terms of speed and efficiency. In our accelerated flows, we linearize the metric constraint through incremental updates to a tangent plane, building upon the previous iteration. Rigorous analysis confirms the stability of these accelerated flows, and also proves the proper control over constraint violations. Furthermore, we discuss other related properties, including the convergence of the flow.

We note that people have spatially discretized these problems using approaches such as Kirchhoff Finite Element Method (FEM), interior penalty Discontinuous Galerkin (DG), and local DG. In contrast, our work adopts Morley FEM for spatial discretization, offering a simpler formulation compared to previous methods. We establish a Gamma convergence theory specific to the Morley discretization of these problems, aligning with established analysis in previous works. We further present a series of numerical simulations that illustrate the acceleration effect and various properties of our new approach.

My collaborators on this work: Guozhi Dong (Central South University, China) and Hailong Guo (University of Melbourne).

Short Bio

Shuo Yang got his Ph.D degree from University of Maryland in 2021, under the supervision of Ricardo Nochetto. He joined Yanqi Lake Beijing Institute of Mathematical Sciences and Applications (BIMSA) as a postdoctoral fellow in 2021, and is going to become an assistant research fellow in the same institute starting from September of 2023. BIMSA is a newly founded mathematics institute located in Beijing, China, and is currently administrated by Tsinghua University.