Book of Abstracts

Modelling and Simulation in Biomedical Applications

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Recent advances for numerical simulation in brain research

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Numerical simulation is a widely used tool to investigate the function and dysfunction of the human brain. One area of interest is the use of source analysis using Electro- and Magnetoencephalography (EEG, MEG) to non-invasively localize electrical activity within the brain. In order to solve the EEG and MEG inverse problem, an accurate solution of the forward problem using numerical simulation is needed. A challenging problem in the simulation of these signals is the discretization of the singular source distribution. A different area of research is the reciprocal simulation of brain stimulation. The latter introduces an electrical current to the brain using electrodes on the head surface. In order to understand the current flow and to plan and compute optimal stimulation protocols, numerical simulation is used. Both applications share the problem of constructing an appropriate discrete head geometry due to the complex shape of the computational domain. We will present recent advances for numerical simulations in these areas of bioelectromagnetism. Several different finite element methods have been investigated, including discontinuous Galerkin methods as well as cut-cell methods. These discretizations make use of the Dune framework and employ multigrid techniques to solve the resulting linear systems.

Explicit Vectorization for Algebraic Multigrid Methods

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Abstract

Modern hardware architectures provide a formidable challenge to the design of algorithms with portable performance across different flavors of multicore CPUs, manycore accelerators, and graphics processors. I will present a case study of an algebraic multigrid method for uncertainty quantification [1] to show the applicability of explicit vectorization techniques as a general design tool for massively parallel software.

References

[1] D. Schaden, "Efficient Parallel PDE-Solvers for Uncertainty Quantification," master thesis, Technische Universität München, 2016.

Automated Finite Element Assembling

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In this talk we present implementation aspects of the general purpose Finite Element software NGSolve. In particular we address the steps to transform a variational formulation given by the user in a high-level representation into an algorithm to assemble element matrices. This framework assists with numerical experiments in a wide area of fields that involve partial differential equations.

We also present various examples and an application in nuclear magnetic resonance, which includes generating tetrahedral meshes from voxel data using the meshing software Netgen.

SIMD Directived Parallelization for a Solver of the Bidomain Equations

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Cardiovascular simulations include coupled PDEs (partial differential equations) for electrical potentials, non-linear deformations and systems of ODEs (ordinary differential equations) all of them are contained in the simulation software CARP (Cardiac Arrhythmia Research Package). We focus in this talk on the solvers for the elliptical part of the bidomain equations describing the electric stimulation of the heart for an anisotropic tissue. The existing conjugate gradient and GMRES solver with an algebraic multigrid preconditioner is already parallelized by MPI+OpenMP/CUDA.

We investigate the OpenACC parallelization of this solver on one GPU especially its competitiveness with respect to the highly optimized CUDA implementation on recent GPUs. The OpenACC performance can achive the CUDA performance if the implementation is especially careful written. Further, we show first results of the GPU parallelizaiton with OpenMP 4.5.

Keywords
OpenACC, OpenMP 4.5, Multigrid

Modeling cell biomechanics is flows

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Computational modeling is becoming increasingly important in studies of cells in microvascular and microfluidic flows. In this talk, we will present a particle-based computational models and simulation framework that can be employed in simulations of cells in complex flow domains. Validation of simulation results using quantitative experimental data will also be presented.

Model-based estimation of internal heart power in aortic valve disease patients.

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Introduction: Aortic valve disease (AVD) causes pressure overload of the left ventricle (LV) which may trigger adverse remodeling and, eventually, precipitate progression towards heart failure (HF). AVD can be treated by transvenous aortic valve implant (TAVI) which aims at reducing the transvalvular pressure gradient. However, depending on the specific AVD etiology, TAVI does not always reverse HF symptoms. **Objectives:** We aim to develop personalized computer models of LV electromechanics (EM) to predict acute TAVI-induced changes in LV function and derive clinical biomarkers such as internal heart power (IHP) which are believed to offer prognostic value of longer term outcomes. **Methods:** We developed $N = 15$ *in silico* EM models of LV and aorta of patients suffering from AVD. Models comprised electrophysiological, mechanical and circulatory components which were all personalized using clinical datasets including anatomical 3D whole heart MRI scans, LV volume traces, pressure drop across the valve as well as LV peak pressure. EM simulations of a heartbeat fitted to pretreatment conditions were carried out and validated against complementary clinical data such as strain and torsion measurements that were not used for model fitting. Based on the assumption of a reduced transvalvular pressure gradient < 20 mmHg, a change in characteristic impedance of the aorta was estimated to simulate post-treatment

conditions. IHP was computed under pre- and post-treatment conditions and compared against the image-based clinical estimation of these quantities. **Results and Conclusion:** The developed workflow enabled us to efficiently model LV EM in a larger cohort of AVD patients. All *in silico* models replicated clinical markers within prescribed margins of accuracy in terms of LV hemodynamics and deformation as assessed by pressure-volume loop analysis and circumferential slice strains, respectively. Model predictions of IHP were comparable to the clinically derived analog, however, non-negligible discrepancies were also observed in many cases likely attributable to limitations of clinical IHP calculations based on Laplace's law. Our study suggests that computational models provide a more accurate, reliable and robust method of determining IHP than currently used standard clinical procedures.

Stabilized Finite Element Methods for Computational Design of Blood-Handling Devices

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The development of reliable blood damage (hemolysis) models is a key issue for the virtual design of ventricular assist devices (VADs). Commonly used stress-based hemolysis models assume an instantaneous deformation of red blood cells. Therefore, a strain-based model is considered, which is able to compute the time-dependent (viscoelastic) deformation of the cells.

The flow and hemolysis quantities are computed by stabilized finite element methods. The stabilization theory is critically reviewed and tailored to the individual problem statements. Efficient and accurate variational multi-scale formulations for anisotropic meshes, in combination with discontinuity-capturing, will be presented. Furthermore, we will discuss turbulence modeling with large eddy simulation and the handling of rotating objects with multiple reference frames or moving mesh techniques.

For the hemolysis estimations, we will discuss a logarithm transformation for a viscoelastic tensor equation that is able to improve the convergence of the equation system significantly. The numerical methods will be applied to benchmark devices and state-of-the-art VADs.

Homogenization of the generalized Poisson–Nernst–Planck problem in a two-phase medium

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We investigate a generalized Poisson–Nernst–Planck system of nonlinear partial differential equations describing cross-diffusion of multiple charged particles in various electro-kinetics phenomena in bio-medical and electro-chemistry applications. A two-phase domain is endowed with inhomogeneous, nonlinear conditions at the interface between the solid and the pore parts. These features together bring the most difficulties to the homogenization procedure. Based on the asymptotic methods, periodic unfolding, and compensated compactness, we arrive at the homogenized problem supported by proper correctors and provided rigorously by residual error estimates.

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Algebraic multigrid methods for a space–time finite element discretization of parabolic problems

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In this talk, we will present some numerical studies on algebraic multigrid methods for solving the linear system of algebraic equations arising from a space–time finite element discretization of parabolic problems. The finite element discretization is based on the recent results [O. Steinbach: Space–time finite element methods for parabolic problems, Comput. Methods Appl. Math., 15:551–566, 2015]. We will mainly focus on robustness of the algebraic multigrid methods for solving the discretized model problems, that are relatively robust with respect to the mesh discretization parameter, material constant and a certain regularization parameter.

Fluid-Structure-Interaction methods based on domain decomposition algorithms for problems with nonlinear anisotropic arterial wall models

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Transmural wall stress distributions of in vivo arteries are a major factor driving arteriosclerosis and arteriogenesis. In this talk, we focus on fluid-structure interaction (FSI) using sophisticated nonlinear structural models which have already been developed and adapted to experiments in the past. In particular, we use an anisotropic, polyconvex hyperelastic structural model for FSI simulations in an idealized benchmark geometry and in realistic patient-specific geometries of coronary arteries. The coupled FSI problems are solved using a monolithic approach based on domain decomposition, i.e., overlapping Schwarz and Dirichlet-Neumann methods. Our solver environment combines the FEM software packages LifeV and FEAP, which provide the nonlinear models for the fluid and a nonlinear, polyconvex, anisotropic model for the structure. Furthermore, we discuss improvements in the computing time of our FSI simulations, e.g., due to the use of suitable parallel domain decomposition preconditioners.

Modeling the impact of stenting of aortic coarctations upon left ventricular load

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Hemodynamic models of blood flow in the left ventricle (LV) and aorta are important tools for analyzing the mechanistic links between myocardial deformation and flow patterns in human hearts. Typically, computational fluid dynamics (CFD) models driven by image-based kinematic models are employed aiming to predict the acute response to an intervention. While such models have proven to be suitable for analyzing the hemodynamic status quo of a patient, they are of limited predictive power as they rely upon the tacit assumption that the kinematics of the heartbeat remains unaffected by the intervention. Electro-mechano-fluidic (EMF) models that capture the entire physics of ventricular electromechanics (EM) promise high potential to overcome this limitation. Such models render feasible the prediction of changes in essential parameters such as myocardial wall stresses and work rates, which are known to be key factors driving ventricular remodeling and disease progression and their potential reversal post-treatment.

In a recent study we built a cohort of twenty in silico electro-mechanical LV and aorta models of patients suffering from aortic valve disease (AVD) and/or aortic Coarctations (CoA). All models comprising electrophysiological, mechanical and circulatory components were parameterized for individual patients using comprehensive clinical datasets. These

validated EM models were fed into our recently developed in-house CFD solver.
In this talk we will present our general workflow together with first results on hemodynamics in the LV for some peronalized EM models.

Coarse space-discretization of bidomain equation: effect on conduction velocity and front shape

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The bidomain equation is the most commonly used model to describe in detail the spatial and temporal electric activity of the heart. The solutions are often travelling waves characterised by a very steep front, about 0.1 mm thick (in the longitudinal direction). This yields a considerable computational effort on patient-specific human geometries.

By means of a perturbation argument, it is possible to analyse in detail the effect of a specific discretisation in space on traveling wave solutions of the bistable (or Nagumo) equation, which is a simple but mathematically reasonable approximation of the dynamics at the front of the wave. We show how specific discretisation schemes (FD, FE, Hermite), and the choice of a coarse grid, can affect the solution, leading so to possibly erroneous physiological conclusions. We also analyse the impact of mass lumping, adopted by several authors in relation with operator splitting schemes.

Secondly, we exploit the error estimates to design a robust numerical scheme for the problem of interest. We propose and analyse two different schemes: the first one is a fourth-order (in space) scheme obtained by a weighted average of the finite difference and the finite element method. The second one is a "stabilised" finite element scheme, where we introduce a numerical conductivity to consistently adjust the conduction velocity.

Finally, we test the methodology on realistic ionic models and geometries. The results are in excellent agreement with our analytical results based on the bistable model, thus showing the validity of the approach.

Optimization based estimation of activation sites in the heart

Karl Kunisch Aurel Neic Gernot Plank Philip Trautmann

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This talk is concerned with an inverse problem in cardiac electrophysiology. In particular, the locations of the activation sites in the heart are estimated from the arrival times of the excitation wave on the epicardium of the heart. The electrophysiologic activity of the heart is often modeled using the Bidomain equations, whose numerical solution is very expensive. If one is only interested in the activation times T of the tissue, the Bidomain model can be reduced to the simpler viscous Eikonal equation

$$\begin{cases} -\varepsilon \operatorname{div}(M\nabla T) + M\nabla T \cdot \nabla T = 1 & \text{in } \Omega, \\ T = g_a & \text{on } \Gamma, \\ \varepsilon \nabla T \cdot n = 0 & \text{on } \Gamma_N. \end{cases} \tag{1}$$

The domain Ω models the geometry of the heart. The epicardium of the heart is denoted by Γ_N and the boundaries of the activation region (activation sites) by Γ. The matrix M describes the fiber orientation of the heart tissue and the function g_a the activation times in the activation regions. On the basis of this model we formulate the inverse problem in the following form

$$\min_{\Gamma} J(\Gamma) := \frac{1}{2} \int_{\Gamma_N} (T(\Gamma) - z)^2 \, \mathrm{d}x \quad \text{subject to (1)}, \tag{2}$$

where z is the measured data on the epicardium. Problem (2) constitutes a shape optimization problem. We approach problem (2) using a gradient descent method. Thus we calculate the shape derivative DJ of J with respect to Γ on the continuous level. The numerical calculation of a perturbation field for Γ based on DF involves the numerical solution of (1), the adjoint equation of the linearized version of (1) and a vector-valued elliptic equation. These equations are discretized using linear finite elements and the non-linearity is treated using a quasi Newton method. The talk is concluded with the presentation of numerical experiments on a three-dimensional heart geometry with synthetic data.

TOWARDS HEMODYNAMIC AND FSI ANALYSIS IN HYPERTROPHIC CARDIOMYOPATHY

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Hypertrophic cardiomyopathy is the most prevalent form of inherited heart failure, affecting 1:500 individuals. Progression into more severe symptoms occurs in approximately 2 out of 3 patients, with disease progression commonly associated with obstruction of the aortic valve and significant hemodynamic losses. How patients progress and how to best treat this condition depends on the severity of disease and the key factors influencing increased hemodynamic burden. In this talk, we present our latest work toward understanding the hemodynamics of the ventricle using PCMRI, introducing a new technique for interpreting relative pressure gradients. While this technique is helpful in facilitating our understanding of the ventricular function, understanding the drivers of disease requires knowledge of the influence of the left ventricular muscle, mitral valve, and blood flow. For this, we introduce a novel extension of our previous FSI work in the heart for handling this complex multi-physics system, relying on local enrichment of finite element velocity space. Preliminary test results are presented on classic FSI benchmark problems.

METHODS AND ALGORITHMS FOR SIMULATION OF RADIO FREQUENCY HEPATIC TUMOR ABLATION

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The Radio Frequency (RF) ablation destroys the unwanted tissue by heating, arising when the energy dissipated by the electric current flowing through the RF probe is converted to heat. The processes to be simulated include electricity field, flows in porous media and heat transfer in the related soft tissues. The mathematical model is described by a nonlinear time-dependent system of PDEs. The bio-heat equation is coupled with the Arrhenius equation which asses the level of thermal cell necrosis. The computational domain has complicated geometry and interphases, extracted from high resolution 3D medical images. A finite element discretization in space and Backward Euler scheme in time are used. Then, the algebraic multigrid (AMG) method is applied to solve the arising large-scale unstructured sparse linear systems. The presented numerical experiments are run on supercomputer IBM Blue Gene/P where the parallel version of BoomerAMG is utilized. They show, for instance: (i) the weighted impact of blood circulation trough the portal vane and trough the capillarity network, and (ii) the indicators V_1 and $V_{4.6}$, denoting the volume of efficient ablation where the cells are destroyed with a probability of 66% and 99% respectively. The issues of strong and weak parallel scalability are also addressed.