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Book of Abstracts

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TIME DOMAIN BOUNDARY ELEMENTS AND MESH REFINEMENTS

HEIKO GIMPERLEIN*

ABSTRACT

We discuss recent [1, 2, 3] and on-going progress for time-domain boundary element methods for wave and elastodynamic problems, with a focus on locally refined meshes. Solutions of the time-dependent equations exhibit singularities due to geometry (corners), mixed or nonlinear (contact) boundary conditions. We discuss well-posed formulations for such problems as well as their approximation on locally refined meshes by h- and hp-versions. A priori and a posteriori estimates for the approximation error are presented for both the weakly singular and the hypersingular integral equations. The a posteriori estimates lead to an adaptive mesh refinement procedure. Numerical experiments illustrate the theoretical results.

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SPACE–TIME VIRTUAL ELEMENTS FOR THE HEAT EQUATION

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ABSTRACT

We present a space–time virtual element method for the discretization of the heat equation. The design, analysis, and implementation of the method are independent of the spatial dimension, as the global virtual element space is chosen as nonconforming across *time-like* facets. Moreover, functions in this space are solutions to local heat problems with polynomial data. The information between time slabs is transmitted by means of upwind terms that involve the traces of suitable polynomial projections of the discrete functions. Several numerical experiments validate the theoretical results and show the advantages of the proposed method.

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OPTIMAL COARSENING FOR ADAPTIVE MICROMAGNETISM

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ABSTRACT

We present an adaptive approximation algorithm that allows us to approximate a given vectorfield with pointwise length constraint with quasi-optimal complexity in the H^1-norm.

The approach ensures that the approximations satisfy the same constraint but are still quasi-optimal within the unconstrained class of approximations. As an application, we consider the Landau-Lifshitz-Gilbert equation, which models the magnetisation of ferromagnetic materials on a microscopic level. Since this time dependent equation requires adaptive refinement of the spatial meshes, we use the approximation routine as a coarsening step in the time integrator to avoid overrefinement, e.g. caused by moving singularities.

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DISCRETE CHAIN RULES FOR FINITE-VOLUME DISCRETIZATIONS OF CROSS-DIFFUSION SYSTEMS

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ABSTRACT

Cross-diffusion systems appear in many applications, like population dynamics, cell biology, and gas mixtures. The underlying entropy structure allows for the derivation of (discrete) gradient estimates and makes the analysis of numerical schemes possible. This analysis needs a nonlinear chain rule, and the main difficulty is to adapt this rule to the discrete level and to the system case. In this talk, we present two strategies to define a discrete nonlinear chain rule, leading to structure-preserving finite-volume schemes. We prove the existence of discrete solutions and the convergence of the numerical schemes.

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ADAPTIVE EXPONENTIAL MULTI-OPERATOR SPLITTING FOR MHD

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ABSTRACT

We construct splitting methods for the solution of the equations of magnetohydrodynamics (MHD). The physical and mathematical properties of the involved operators imply that splittings into three or even four operators with positive coefficients are appropriate for a physically correct and efficient solution of the equations of motion. To obtain a solution approximation with reliable accuracy efficiently, adaptive choice of the time-steps is important particularly in the light of the unsmooth dynamics of the system. Thus, we construct new method coefficients in conjunction with associated error estimators by optimizing the leading local error term similarly as in [1]. The new coefficients are given in the collection
`https://www.asc.tuwien.ac.at/auzinger/splitting/`
As a proof of concept, we demonstrate that adaptive splitting faithfully reflects the solution behavior also in the presence of a shock for the viscous Burgers equation, which serves as a simplified model problem displaying several features of the Navier–Stokes equation for incompressible flow, see [2].

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WKB-BASED METHODS FOR THE 1D STATIONARY SCHRÖDINGER EQUATION IN THE HIGHLY OSCILLATORY REGIME

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ABSTRACT

We are concerned with the numerical solution of differential equations of the type $\varepsilon^2\varphi''(x) + a(x)\varphi(x) = 0$ when $a(x) > 0$. Since, for a small parameter $\varepsilon > 0$, the solution exhibits rapid oscillations with a wave length proportional to ε, standard schemes for ODEs become inefficient as they would have to resolve every oscillation. We present two different numerical approaches based on well known WKB-techniques from quantum mechanics: First, an explicit one-step ODE-solver, which relies on an analytical pre-processing of the given ODE and a special treatment of highly oscillatory integrals, which rely on the Picard-approximation of the solution. Global error bounds are presented. Second, the (global in x) WKB approximation series, whereby differentiations and integrations involved in the computation of the coefficient functions of the asymptotic series are carried out using spectral methods. We conclude with several numerical examples.

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ADAPTIVE (SPACE-TIME) FEM FOR DISTRIBUTED OPTIMAL CONTROL PROBLEMS

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ABSTRACT

We present an abstract framework for the discretization of a distributed optimal control problem. In particular, we are interested in bounding the norm between the computed solution and the target function with respect to the relaxation parameter, the regularity of the target and the approximation property of our finite element space. The framework presented, will lead to a so called energy-regularization and will, in particular, show how the regularity of the control and the state are related. This concept is applied to several examples, including the energy regularization for the Poisson equation and for the wave equation. The theoretical findings will be supported by numerical examples. Furthermore, an adaptive refinement strategy is proposed and possible extensions are discussed.

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FINITE ELEMENT METHODS FOR REDUCED LANDAU-DE GENNES MINIMIZATION PROBLEMS OF NEMATIC LIQUID CRYSTALS AND FERRONEMATIC SYSTEMS

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ABSTRACT

In this talk, we first discuss the finite element approximation of non-linear elliptic partial differential equations that model the equilibrium configurations of a two-dimensional nematic liquid crystal device. In the second part, we focus on the analysis of a free energy functional, that models a dilute suspension of magnetic nanoparticles in a two-dimensional nematic well, referred as ferronematics. We discuss the asymptotic analysis of global energy minimizers in the limit of vanishing elastic constant, where the re-scaled elastic constant is inversely proportional to the domain area. We establish the existence and local uniqueness of the discrete solutions of the associated Euler-Lagrange PDE, error estimates in the energy and L^2 norms with parameter dependency. The theoretical results are complemented by the numerical experiments on the discrete solution profiles, and the numerical convergence rates that corroborates the theoretical estimates.

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GPU-ACCELERATED MATRIX-FREE SOLVERS FOR THE EFFICIENT SOLUTION OF CARDIAC ELECTROPHYSIOLOGY IN LIFE^X

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ABSTRACT

Cardiac elecrophysiology can be modeled by the monodomain equation, describing the space–time evolution of the transmembrane potential, coupled with proper ionic models, representing how chemical species move across ionic channels. The most challenging aspect is the requirement of high temporal and spatial resolution dictated by the solution to such problem, as it resembles a propagating wavefront with very steep gradients. The computational cost of solving the discretized problem is such that direct methods quickly become too expensive. We exploit modern hardware architectures to develop a GPU-accelerated matrix–free solver that can be readily employed for mixed CPU-based and GPU–based, massively parallel, large-scale electrophysiology simulations. We rely on matrix-free solvers and on the sum-factorization, two computational techniques that have proven to be effective ways to reduce the computational complexity. In this framework, we propose and implement two different time discretization schemes for the monodomain equation: the 2nd-order Backward Differentiation Formula (BDF2), resulting in a semi-implicit time scheme, and the 2nd-order Runge-Kutta scheme (RK2), giving an explicit scheme. While the former requires the solution of a linear system at each time-step, the latter can perform a DoF-by-DoF update, as the space discretization is based on Spectral Element Method with Numerical Integration (SEM-NI). Moreover, the RK2 scheme is theoretically much faster, but constrained by a severe stability condition on Δt. We perform a thorough comparison among the different solvers under p-refinement, *i.e.* by increasing the polynomial degree of the basis functions, in terms of computational cost and accuracy.

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ANALYSIS AND NUMERICAL APPROXIMATION OF HEAT TRANSFER VIA INTERFACES AND RADIATION

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ABSTRACT

We consider heat transfer in a three-dimensional multi-part component where different parts might not be perfect in contact. We assume that this leads to temperature jumps across such interfaces and therefore we consider Robin jump conditions on them. Additionally, heat radiation in form of nonlinear Stefan-Boltzmann boundary conditions is taken into account on outer boundaries. A corresponding transient model that includes these conditions is presented and existence and uniqueness of a solution is examined. Furthermore, the convergence behavior for solutions obtained using finite element approximations in space and the implicit Euler method in time is examined. To fix the locking phenomena occurring if meshes are non-conforming across interfaces and the thermal resistivity parameter is small, a Nitsche-type mortaring method is used [1]. Order optimal convergence rates independent of the thermal resistivity can then be shown.

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DISTRIBUTIONAL CURVATURES ON DISCRETE SURFACES WITH APPLICATION TO SHELLS

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ABSTRACT

To compute the Gaussian or mean curvature of a surface embedded in $\mathbb{R}^3$ a C^1-surface is required. For a piece-wise affine triangulation this assumption is no longer fulfilled. The approximation of curvature quantities is still a field of intensive research in discrete differential geometry (DDG). The Hellan–Herrmann–Johnson (HHJ) method avoids C^1-conforming finite elements for the biharmonic plate problem by means of a mixed method discretizing the bending moments by tensor valued elements, where only the normal-normal component is globally continuous [1]. Regge finite elements, which are matrix-valued and solely tangential-tangential continuous, turned out to be the appropriate space for discretizing strains and metrics [5]. In this talk we combine DDG with HHJ and Regge finite elements to introduce well-defined distributional curvature quantities. We apply this framework to nonlinear shells for the bending energy [3] and show how the problem of membrane locking can be mitigated [4]. We demonstrate the performance of the method by means of benchmark examples implemented in the finite element software NGSolve (www.ngsolve.org).

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SLOWLY DECAYING KOLMOGOROV n-WIDTH: MODEL ORDER REDUCTION BY MEANS OF TRANSPORT MAPS

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ABSTRACT

I present a Model Order Reduction (MOR) procedure based on a preprocessing of the snapshots in the offline phase. The goal is to apply it to a Fluid–Structure Interaction (FSI) problem of interest, that exhibits a slow decay of the Kolmogorov n-width [3]: this is reflected, at the numerical level, by a slow decay in the magnitude of the eigenvalues returned by a Proper Orthogonal Decomposition on the solution manifold. By means of a preprocessing procedure, I will show how we are able to control the decay of the Kolmogorov n-width of the obtained solution manifold. The preprocessing employed is based on the composition of the snapshots with a map belonging to a family of smooth and invertible mappings from the physical domain into itself [1]. In order to assess the capabilities and the performance of the proposed MOR strategy, I draw a comparison between the results of the novel offline stage and the standard one, as well as a comparison between the novel online phase and the standard one[2].

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DISCRETIZATION OF SCALAR PARTIAL DIFFERENTIAL EQUATIONS WITH SIGN-CHANGING COEFFICIENTS BASED ON A WEAKLY COERCIVE REFORMULATION

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ABSTRACT

We propose a new computational method for the solution of transmission problems with sign-changing coefficients for smooth interfaces in two and three dimensions. The method is based on a weakly coercive reformulation of the problem, which can be discretized with classical finite element spaces and for which each Galerkin discretization converges unconditionally. The new method leads to a nonstandard sparsity pattern of the system matrix and we explain its implementation in NGSolve. We present computational experiments and discuss the necessity of special quadrature rules.

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AN IMPLEMENTATION OF A HILBERT-TRANSFORMED TDBEM FOR THE WAVE EQUATION IN 3D

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ABSTRACT

Motivated by a series of recent works by O. Steinbach and M. Zank, in this talk we address the challenges of an implementation of a Hilbert-transform of the time-domain boundary element method (TDBEM) for the wave equation in 3D. In order to keep an overview of the challenges, we only consider a Dirichlet problem with the retarded single layer operator. We apply a tensor product ansatz, in particular piecewise constant ansatz resp. test functions in space and time. We observe symmetric Toeplitz blocks until a certain time, which we can benefit from, but the whole space-time system is not a Toeplitz matrix. Therefore we have a densely populated space-time system, which needs to be solved. Finally, we close the talk with numerical examples.

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BOURGAIN TECHNIQUES FOR ERROR ESTIMATES AT LOW REGULARITY

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ABSTRACT

Standard numerical integrators such as splitting methods or exponential integrators suffer from order reduction when applied to semilinear dispersive problems with non-smooth initial data. In this talk, we focus on the cubic nonlinear Schrödinger equation with periodic boundary conditions. For such problems, we present filtered integrators that exhibit superior convergence rates at low regularity. Furthermore, due to the nonexistence of suitable embedding results, the error analysis at very low regularity cannot be carried out in the usual framework of Sobolev spaces. Instead, completely new techniques are required. They are based on Bourgain's seminal work and will be sketched in the talk. Numerical examples illustrating the analytic results will be given.

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A MODIFIED SPLITTING METHOD FOR SEMILINEAR DAMPED WAVE EQUATIONS

DUY PHAN*, ALEXANDER OSTERMANN

ABSTRACT

We employ the Strang splitting method to solve a class of semilinear damped wave equations

$$\partial_{tt}u - \alpha\Delta(u) - \beta\Delta(\partial_t u) + \gamma\partial_t u + \delta u = g(u) + h(\partial_t u), \quad \text{in } \Omega \times (0,T).$$
$$u(t,x) = 0 \qquad \text{on } \partial\Omega \times (0,T),$$
$$u(0,x) = p(x), \qquad \partial_t u(0,x) = q(x).$$

Here Ω is a connected, bounded domain. The diffusion coefficient α is positive, whereas all other coefficients β, γ, δ are non-negative. The original equation is split into two parts: the linear part and the nonlinear part. Employing the exact exponential integrators introduced in [1], the linear flow can be computed in a fast and reliable way. The nonlinear flow can be evaluated accurately by solving a corresponding second-order ODE or approximated by standard Runge-Kutta methods. This approach covers the traditional Störmer-Verlet scheme (leapfrog method). Some numerical simulations demonstrate the efficiency of the modified splitting method compared with Störmer-Verlet approach.

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A FINITE-VOLUME SCHEME FOR NONLOCAL CROSS-DIFFUSION SYSTEMS

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ABSTRACT

Cross-diffusion systems arise in the modeling of the dynamics of several species. If we take into account that each species can have an interaction radius, the system becomes nonlocal, thus making its analysis more challenging.

In [1] we used the entropy method to prove existence of solutions to such a nonlocal cross-diffusion system. While this is a step torwards the understanding of nonlocal cross-diffusion systems, there are still a lot of open questions, one of them being for example: Do different (initially separated) species stay separated over time? A suitable numerical scheme can give answers to these questions or at least point us towards the right direction.

In this talk I will present an implicit Euler finite-volume scheme for nonlocal cross-diffusion systems. We will sketch how to "translate" the entropy calculations for the continuous equations, that were done in [1], to the finite-volume scheme in order to prove existence of solutions to the scheme. Numerical experiments will illustrate some properties of the scheme and round off the presentation. This talk is based on our preprint [2].

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GEOMETRY-BASED APPROXIMATION OF WAVES PROPAGATING THROUGH COMPLEX DOMAINS

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ABSTRACT

We consider wave propagation problems over 2-dimensional domains with piecewise-linear boundaries, possibly including scatterers. Under the assumption that the initial conditions and forcing terms are radially symmetric and compactly supported (which is common in applications), we propose an approximation of the propagating wave as the sum of some special nonlinear space-time functions: each term in this sum identifies a particular ray, modeling the result of a single reflection or diffraction effect. We describe an algorithm for identifying such rays automatically, based on the domain geometry.

To showcase our proposed method, we present several numerical examples, such as waves scattering off wedges and waves propagating through a room in presence of obstacles. We will also present some simple examples of inverse problems, where our method can be applied to drastically speed up computations.

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AN OPTIMAL AFEM FOR ELASTOPLASTICITY WITH THE APPLICATION OF THE AXIOMS OF ADAPTIVITY

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ABSTRACT

In this talk a proof of optimal convergence of an AFEM for elastoplasticity with combined linear kinematic and isotropic hardening is discussed. The proof applies the axioms of adaptivity. The verification of the axioms in this setting draws from an already existing result on optimal convergence for AFEM for elastoplasticity. These two approaches to proving optimal convergence are then compared to highlight differences and similarities between their methodologies.

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AN ADAPTIVE LEAST SQUARES BOUNDARY ELEMENT METHOD FOR ELLIPTIC BOUNDARY VALUE PROBLEMS

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ABSTRACT

We formulate and analyze a least squares boundary element method for the weakly singular boundary integral equation which is related to the solution of a Dirichlet boundary value problem for a second order partial differential equation, with the Laplacian as model problem. In particular we may assume less regular boundary data $g \notin H^{1/2}(\Gamma)$ but $g \in L^2(\Gamma)$. For this we consider the single layer boundary integral operator $V : H^{-1}(\Gamma) \to L^2(\Gamma)$, i.e., we will solve the boundary integral equation $Vw = f$ by minimizing $\frac{1}{2}\,\|Vw - f\|^2_{L^2(\Gamma)}$. This results in a mixed variational formulation where we use piecewise constant approximations to discretize both the primal unknown $w \in H^{-1}(\Gamma)$ and the adjoint $p := f - Vw \in L^2(\Gamma)$. Using nested boundary element spaces $S^0_H(\Gamma) \subseteq S^0_h(\Gamma)$ we can prove stability and related error estimates for both the primal and adjoint approximations, w_H and p_h, respectively. When considering the approximate adjoint p_h on a finer mesh than the primal w_H, we can use $\|p_h\|_{L^2(\Gamma)}$ as a posteriori error indicator for the error $\|w - w_H\|_{H^{-1}(\Gamma)}$ to drive an adaptive mesh refinement. Note that this defines an adaptive boundary element method also for regular boundary data $g \in H^{1/2}(\Gamma)$. Numerical examples confirm the theoretical results.

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THE α-MOSOLOV PROBLEM - A VARIATIONAL APPROACH

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ABSTRACT

A *hp*-finite element discretization for the α-Mosolov problem, a scalar variant of the Bingham problem [1] but with the α-Laplacian operator, is being analyzed. Its weak formulation is either a variational inequality of second kind or equivalently a non-smooth but convex minimization problem. For any $\alpha \in (1, \infty)$, we prove in [2] convergence, including guaranteed convergence rates in the mesh size h and polynomial degree p of the FE-solution of the corresponding discrete variational inequality. Moreover, we derive a family of reliable a posteriori error estimators which are applicable to any "approximation" of the exact solution and not only to the FE-solution and can therefore be coupled with an iterative solver. We prove that any quasi-minimizer of this family of a posteriori error estimators satisfies an efficiency estimate. All our results contain the known results for the Mosolov problem by setting $\alpha = 2$. Numerical results underline our theoretical findings.

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ADAPTIVE FEM FOR LINEAR ELLIPTIC PDES: OPTIMAL COMPLEXITY

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ABSTRACT

We consider a general nonsymmetric second-order linear elliptic PDE in the framework of the Lax–Milgram lemma. We formulate and analyze an adaptive finite element algorithm with arbitrary polynomial degree p that steers the adaptive mesh-refinement and the inexact iterative solution of the arising linear systems. More precisely, the iterative solver employs, as an outer loop, the so-called Zarantonello iteration to symmetrize the system and, as an inner loop, a uniformly contractive algebraic solver, e.g., an optimally preconditioned conjugate gradient method [1] or an optimal geometric multigrid algorithm[2, 3]. We prove that the proposed inexact adaptive iteratively symmetrized finite element method (AISFEM) leads to full linear convergence and, for sufficiently small adaptivity parameters, to optimal convergence rates with respect to the overall computational cost, i.e., the total computational time [4].

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AUTOMATIC SEGMENTATION TOOL FOR ABDOMINAL AORTIC ANEURYSM

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ABSTRACT

In this work, we want to develop an automatic segmentation tool for abdominal aortic aneurysm (AAA). Abdominal aortic aneurysm is a vascular pathology with a high mortality rate and consists of a local enlargement of the abdominal aorta called aneurysm. The aneurysm is formed by two components, the lumen, which is the passageway through which blood flows, and the thrombus, a blood clot surrounding the lumen. In many cases, the aneurysm grows too much and the only way to proceed is surgery. Doctors require quantitative information about the aneurysm both for diagnosis and pre-surgical planning. This type of information can be obtained by analyzing, manually, the scans taken from medical imaging, i.e. X-rays, Magnetic Resonance Imaging (MRI), or Computed Tomography (CT). The automatic segmentation tool aims to accelerate and automatize the manual procedure, in order to give to doctors useful information concerning the aneurysm. In our case, we want to extract, from the medical images, the lumen and the thrombus and, to do that, we have to choose the criterion of extraction. We first segment the lumen, relying on its geometry, then we face the thrombus's segmentation, formulating and solving a minimization problem through morphological operators. At the end of the segmentation, we are also able to compute quantitative indicators which, together with the reconstruction of the aneurysm, can help doctors in their decisions.

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MODELING AND ENERGY STABLE NUMERICAL SCHEMES OF NETWORK DEVELOPMENT IN BIOLOGY GELS

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ABSTRACT

We consider the modeling and simulation of the network development in biological gels. A thermodynamically consistent model with homogenous Neumann or periodic boundary condition is derived based on the Rayleighian method. Two fully discrete numerical schemes are proposed to solve the problem. Energy stability is achieved at the discrete level for both schemes. Positivity-preserving property can be shown for the Flory—Huggins potential at continuous and discrete levels. Numerical results are also shown and are in agreement with theory.

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HIGH-ORDER CELL METHODS FOR THE TIME-DEPENDENT MAXWELL'S EQUATIONS

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ABSTRACT

We are concerned with the efficient numerical approximation of solutions of the time-domain Maxwell system. Methods like the classical finite-difference time-domain method or finite integration techniques rely on the approximation of the electric and the magnetic field on two interlaced (Cartesian) grids respectively.

Our method expands this idea to general triangular meshes by defining a dual grid using the barycentric subdivision of the primal mesh, resulting in a decomposition of each mesh into quadrilaterals. Contrary to previous approaches we use a Lagrangian polynomial basis with respect to tensor product integration points on the unit square which are subsequently re-mapped to the quadrilaterals of the reference element. This approach also provides a generalization of the method to three space dimensions and enables us to use lumped mass matrices which significantly increases the computational efficiency of our method.

Numerical experiments underline the facts that the resulting algorithm provides converging, spurious-free solutions and is efficient, compared to competing methods.

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TWO-LEVEL ERROR ESTIMATION FOR THE INTEGRAL FRACTIONAL LAPLACIAN

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ABSTRACT

We consider an adaptive finite element method for the integral fractional Laplacian of the classical SOLVE-ESTIMATE-MARK-REFINE form. As a-posteriori error indicator, we take a two-level error estimator. Based on certain saturation assumptions, we show reliability and efficiency of the error estimator on meshes generated by newest vertex bisection, which implies linear convergence of the Galerkin error generated by the adaptive algorithm. Moreover, in two space dimensions, we obtain convergence of the algorithm with optimal algebraic rates.

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UNIFORM STABILITY AND FEM FOR PARABOLIC EQUATIONS

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ABSTRACT

For the discretization of time-dependent partial differential equations, the standard approaches are explicit or implicit time-stepping schemes together with finite element methods in space. An alternative approach is the usage of space-time methods, where the space-time domain is discretized and the resulting global linear system is solved at once. In this talk, the model problem is the heat equation. First, a space-time variational formulation in fractional-order Sobolev spaces for the heat equation is discussed, where a modified Hilbert transformation [1, 2] is used such that ansatz and test spaces are equal. A conforming discretization of this space-time variational formulation in fractional-order Sobolev spaces leads to a space-time Galerkin finite element method, which is unconditionally stable, i.e. an inf-sup condition holds in an appropriate space-time norm. However, this space-time norm differs from the norm used for the continuous variational setting. In this talk, a new space-time finite element method is introduced, and its uniform stability is investigated. In the last part of the talk, numerical examples are shown and discussed.

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