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FINITE ELEMENT METHODS FOR ICE SHEET MODELLING

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An ice sheet model is a type of computational fluid dynamics model describing the very viscous, non-Newtonian flow of the ice on Greenland and Antarctica. Traditionally, finite differences has been the discretization method of choice, but finite element models are now becoming more common. The FEM models used for ice sheet modelling typically employ FEM techniques developed for general computational fluid dynamics problems. However, these methods are not optimal for ice sheet simulations which offers peculiar challenges such as moving meshes and varying viscosity. In this talk we present methods for computing ice velocity by solving the p-Stokes equations on a thin, moving ice domain.

PRECONDITIONERS FOR HIGH ORDER FEM MASS MATRIX ON TRIANGLES

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It is well-known that the stiffness matrix that arises in high order finite element discretisation of elliptic PDEs is generally ill-conditioned as the polynomial order p is increased. Although the mass matrix for low order (h-version) finite element approximation is well-conditioned, the mass matrix for the p-version is, like the stiffness matrix, generally ill-conditioned. For transient and singularly perturbed problems, it is necessary to invert the mass matrix, or a perturbation thereof, in order to carry out time stepping.

iWe present an algorithm for preconditioning the two dimensional mass matrix which results in a preconditioned system whose condition number is independent of the polynomial order and the mesh size. Although the preconditioner is applicable to any choice of basis for the high order polynomials, we show that the preconditioner can be implemented efficiently in the case where a Bernstein polynomial basis is chosen. Numerical examples are presented illustrating the performance of the algorithm for a range of challenging applications.

A REGULARIZED ENTROPY-BASED MOMENT METHOD FOR KINETIC EQUATIONS

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We present a new entropy-based moment method for the velocity discretization of kinetic equations. This method is based on a regularization of the optimization problem defining the original entropy-based moment method, and this gives the new method the advantage that the moment vectors of the solution do not have to take on realizable values. We show that this equation still retains many of the properties of the original equations, including hyperbolicity, an entropy-dissipation law, and rotational invariance. The cost of the regularization is mismatch between the moment vector of the solution and that of the ansatz returned by the regularized optimization problem. However, we show how to control this error using the parameter defining the regularization. This suggests that with proper choice of the regularization parameter, the new method can be used to generate accurate solutions of the original entropy-based moment method, and we confirm this with numerical simulations.

GMSFEM FOR SOLVING REDUCED DARCY FLOW MODEL IN FRACTURED POROUS MEDIA

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In This talk, I will present a reduced model for Darcy flow in fractured porous media. We solve this reduced model using Generalized Multiscale Finite Element Method (GMsFEM). Our approach is based on modeling the fracture flow in one dimension and the matrix flow in two dimensions. And then the GMsFEM is used to construct, efficiently, a lower dimension space that approximates the coupled Darcy flows in the matrix and the fracture. The advantage of using GMsFEM is to represent the fracture effects on a coarse grid via multiscale basis functions constructed using local spectral problem. Solving local problem leads to consider small scale information in each coarse grid. On another hand, the multiscale basis functions generated offline following GMsFEM framework can be reused for any input parameter to solve the problem in the online stage. Our goal is to combine GMsFEM with a reduced model for Darcy flow in fractured porous media. In this work, we consider a general case for the permeability in both fracture and matrix domain. Here, we would like to note that other research considered special case when the fracture permeability is much larger than the matrix permeability. Our experiment, at current stage, shows that the finite element solution for the matrix pressure in the case when the fracture permeability being much larger than the matrix permeability is almost continuous, while in the opposite case we will have discontinuity along the fracture.

NON-LOCAL SMOOTH INTERFACES IN CONTINUUM SOLVATION

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Continuum models to handle solvent and electrolyte effects in an effective way have a long tradition in quantum-chemistry simulations and are nowadays also being introduced in computational condensed-matter and materials simulations. A key ingredient of continuum models is the choice of the solute cavity, i.e. the definition of the sharp or smooth boundary between the regions of space occupied by the quantum-mechanical (QM) system and the continuum embedding environment. The cavity, which should really reflect the region of space accessible to the degrees of freedom of the environmental components (the solvent), is usually defined by an exclusion approach in terms of the degrees of freedom of the system (the solute), typically the atomic position of the QM system or its electronic density.

While standard approaches to define the cavity lead to comparably high accuracies, some shortcomings are present in most local definitions and limit the transferability of the models to more complex simulations. In particular, local definitions of the interface are often uneffective in characterizing the solvent-excluded regions of space, i.e. regions of space where the solvent molecules would not be able to enter, but the continuum medium can penetrate. Moreover, standard definitions of continuum interfaces require a separate parametrization to handle solvation of charged species, due to the fact that charged solutes more strongly bind the solvent molecules.

In a smooth-interface continuum solvation framework it is possible to capture these additional effects by exploiting non-local definitions of the interface, while keeping the methods computationally inexpensive and without affecting the calculation of derivatives, e.g. as required for running a self-consistent field optimization of the electronic density of a geometry optimization. Here, the solvent-aware and field-aware approaches to continuum interfaces will be presented, the type of parameters involved in these models will be analyzed and the effects of these methods on continuum solvation calculations in condesed-matter simulations will be discussed.

VARIATIONAL TIME DISCRETIZATION OF HIGHER ORDER AND HIGHER REGULARITY WITH APPLICATION TO WAVES AND INCOMPRESSIBLE FLOW

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We present families of variational space-time finite element discretisations which we combine with collocation conditions in order to get solutions of higher-order regularity in time of the fully discrete approximations. By condensation, linear systems show up that have less degrees of freedom than the corresponding pure variational formulations but lead to the same order of convergence, cf. [3].

Firstly, we apply this approach to the hyperbolic wave equation, written as a first-order in time system

$$\partial_t u - v = 0\,, \quad \partial_t v - \nabla \cdot (c\nabla u) = f$$

and equipped with appropriate initial and boundary conditions. This system is studied as a prototype model for elastic waves with applications in, e.g., non-destructive material inspection. We derive the linear system that leads to a globally C^1-regular in time solution. Optimal order error estimates for the fully discrete scheme are given and illustrated by challenging numerical experiments, cf. [1, 2].

Next, we extend our investigations to the incompressible nonstationary Navier–Stokes equations

$$\partial_t \vec{v} + (\vec{v} \cdot \nabla)\vec{v} - \nu\Delta\vec{v} + \nabla p = \vec{f}\,, \quad \nabla \cdot \vec{v} = 0\,.$$

We solve the resulting nonlinear system by Newton's method and analyze the convergence properties of the C^1-regular in time discrete solution numerically.

The subproblems of wave propagation and fluid flow are studied as building blocks for fluid-structure interaction which will be our work for the future.

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HIGH-ORDER DISCONTINUOUS GALERKIN METHODS FOR ELASTO-ACOUSTIC WAVE PROPAGATION PROBLEMS ON POLYGONAL AND POLYHEDRAL GRIDS

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We present the spatial discretization of an evolution problem arising from the coupling of elastic and acoustic wave propagation phenomena by employing high-order discontinuous Galerkin methods on polygonal and polyhedral meshes. The coupled nature of the problem is ascribed to suitable transmission conditions imposed at the interface between the solid (elastic) and fluid (acoustic) domains. We state and prove a well-posedness result for the strong formulation of the problem, present a stability analysis for the semi-discrete formulation, and finally prove a priori hp–version error estimates for the resulting formulation in a suitable (mesh-dependent) energy norm. We also discuss the time integration scheme employed to obtain the fully discrete system. The convergence results are validated by numerical experiments carried out in both two- and three-dimensions.

UNIFIED FORMULATION FOR POLYTOPIC DISCONTINUOUS GALERKIN APPROXIMATION OF FLOWS IN FRACTURED POROUS MEDIA

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We propose a formulation based on discontinuous Galerkin (DG) methods on polygonal and polyhedral grids for the simulation of flows in fractured porous media. Our method is very flexible from the geometrical point of view, being able to handle meshes made of arbitrarily shaped elements, with edges/faces that may be in arbitrary number (potentially unlimited) and whose measure may be arbitrarily small. Our approach is then very well suited to tame the geometrical complexity featured by most of applications in the computational geoscience field. More precisely, we adopt a model for single-phase flows where fractures are treated as a $(d-1)$-dimensional interfaces between d-dimensional subdomains, $d = 2, 3$. In the model, the flow in the porous medium (bulk) is assumed to be governed by Darcy's law and a suitable reduced version of the law is formulated on the surfaces modelling the fractures. The two problems are then coupled through physically consistent conditions. We focus on the numerical approximation of the coupled bulk-fractures problem, presenting and analysing, in the unified setting of [D. N. Arnold et al., Unified analysis of discontinuous Galerkin methods for elliptic problems, 2001/02], all the possible combinations of primal-primal, mixed-primal, primal-mixed and mixed-mixed formulations for the bulk and fracture problems, respectively. Finally, the validity of the theoretical analysis is assessed through numerical experiments.

NUMERICAL ANALYSIS FOR DIRICHLET CONTROL PROBLEMS

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An overview of discretization error estimates for Dirichlet control problems with L^2-regularization is presented. State and control are discretized by piecewise linear and continuous functions. Singularities of the solution at corners of the domain are taken into account by using graded finite element meshes. These singularities are different for unconstrained and control constrained problems.

EXPONENTIAL DECAY OF THE RESONANCE ERROR IN NUMERICAL HOMOGENIZATION VIA PARABOLIC AND ELLIPTIC CELL PROBLEMS

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The present work concerns the numerical homogenization of multiscale elliptic PDEs of the form $-\nabla \cdot (a^\varepsilon(x)\nabla u^\varepsilon(x)) = f(x)$, where a^ε characterizes a microscopically nonhomogeneous medium, which has variations with a wavelength $\varepsilon \ll |\Omega|$. A direct numerical approximation of such a PDE is prohibitevely expensive as it requires resolutions down to the finest scales in the problem. An alternative idea is to look for a homogenized PDE of the form $-\nabla \cdot (a^0(x)\nabla u^0(x)) = f(x)$ describing the average response of the system, where the homogenized coefficient a^0 has only slow variations. Once a^0 is determined, u^0 can be approximated at a cost independent of the small scale parameter ε. Explicit formulas for the homogenized coefficient a^0 are available only for limited theoretical settings, such as purely periodic or stationary ergodic media. When the exact period of the coefficient is unknown or when the coefficient has more complex non-periodic variations, the available formulas for the a^0 either break down or are simply inaccurate, and more general multiscale numerical methods are needed to approximate u^0.

Several multiscale approaches, such as the heterogeneous multiscale methods (HMM), have been developed in the past. These approaches rely on upscaling certain effective quantities, e.g., the homogenized coefficient a^0, by solving elliptic cell-problems over microscopic boxes of size $\delta^d > \varepsilon^d$, where d is the dimension of the problem. This will then imply an artifical boundary condition on the boundary of the microscopic domain, which will lead to an $O(\varepsilon/\delta)$ resonance error, dominating all other discretization errors coming from a multiscale coupling. Different strategies have been developed to improve the decay rate of the resonance error to higher orders, see [1, 2, 3]; each coming with some computational challenges. In the present work, we propose two new methods based on parabolic and elliptic cell-problems, which result in an exponential decay of the boundary error, and improve the overall decay rate to arbitrarily high orders in ε/δ without increasing the computational cost in comparison to solving standard elliptic cell-problems.

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A *PRIORI* ERROR ESTIMATES OF FULLY DISCRETE FINITE ELEMENT GALERKIN METHOD FOR KELVIN-VOIGT VISCOELASTIC FLUID FLOW MODEL

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In this talk, a finite element Galerkin method is applied to the Kelvin-Voigt viscoelastic fluid model, when its forcing function is in $L^\infty(\mathbf{L^2})$. Some new *a priori* bounds for the velocity as well as for the pressure are derived which are independent of inverse powers of retardation time κ. Optimal error estimates for the velocity in $L^\infty(\mathbf{L^2})$ as well as in $L^\infty(\mathbf{H}_0^1)$-norms and for the pressure in $L^\infty(L^2)$-norm of the semidiscrete method are discussed which hold uniformly with respect to κ as $\kappa \to 0$ with the initial condition only in $\mathbf{H}^2 \cap \mathbf{H}_0^1$. For the complete discretization of the semidiscrete system a first order accurate backward Euler method is applied and the fully discrete optimal error estimates are established. Finally, the talk will be concluded by presenting some numerical results. The results discussed in this talk are sharper than those derived earlier for finite element analysis of the Kelvin-Voigt viscoelastic fluid model in the sense that the error estimates hold true uniformly even as $\kappa \to 0$.

HP-ADAPTIVE FEM FOR VIS IN OPTIMAL CONTROL PROBLEMS

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A distributed elliptic control problem with control constraints is typically formulated as a three field problem and consists of two variational equations for the state and the co-state variables as well as of a variational inequality for the control variable. In view of a flexible adaptive scheme, the three variables are discretized independently by (non-conforming) *hp*-finite elements. While that discrete formulation is well suited for computations, it is less favorable for numerical analysis. We therefore rewrite the weak three field formulation as an equivalent variational inequality with an operator of the type $B = I + \alpha^{-1}A^{-2}$ formulated in the control variable only. Analogously, we condense out the state and the co-state variables from the discrete three field formulation. This implicates to deal with an approximation of the operator B, as A^{-2} cannot be realized numerically, depending on the independent discretization spaces for the eliminated state and co-state variables.

We provide sufficient conditions for the unique existence of a discrete solution triple. Also a priori error estimates and guaranteed convergence rates are derived, which are stated in terms of the mesh size as well as of the polynomial degree. Moreover, reliable and efficient a posteriori error estimates are presented. The efficiency estimate rests on an analytic solution of an optimization problem to find the best conforming approximation of the non-conforming discrete solution.

Several numerical experiments demonstrate the applicability of the discretization with *hp*-finite elements, the efficiency of the a posteriori error estimates and the improvements with respect to the order of convergence resulting from the application of *hp*-adaptivity. In particular, the *hp*-adaptive schemes show superior convergence rates.

LOW-ORDER DIVERGENCE-FREE FINITE ELEMENT METHODS IN FLUID MECHANICS

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It is a well-known fact that the finite element approximation of equations in fluid mechanics (e.g., the Navier-Stokes equations) is simpler, and more accurate, if the finite element method delivers an exactly divergence-free velocity. In fact, in such a case the convective term remains antisymmetric in the discrete setting, without the need to rewrite it, and the stability analysis can be greatly simplified. Now, when the finite element spaces used are the conforming $\mathbf{P}_1$ for velocity and $\mathbf{P}_0$ for pressure, then, in addition to add appropriate terms to stabilise the pressure, some extra work needs to be done in order to compensate for the lack of incompressibility of the discrete velocity.

In this talk I will present two recent applications of a technique developed previously in [2] to overcome the limitations described in the previous paragraph. The first example presented is the application of this idea to the steady-state Boussinesq equation [1]. Then, the transient Navier-Stokes equations will be analysed, where some error estimates independent of the Reynolds number will be shown.

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OPTIMAL CONTROL PROBLEMS AND ALGEBRAIC FLUX CORRECTION SCHEMES

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Solutions of convection-diffusion-reaction equations may possess layers, i.e., narrow regions where the solution has a large gradient (in particular for convection dominated equations). Standard finite element methods lead to discrete solutions which are polluted by spurious oscillations. The main motivation for the construction of the so-called algebraic flux correction (AFC) schemes is the satisfaction of the DMP to avoid spurious oscillations in the discrete solutions. We apply an AFC scheme to an optimal control problem governed by a convection-diffusion-reaction equation. Due to the fact that the AFC schemes are nonlinear and usually non-differentiable the approaches "optimize-then-discretize" and "discretize-then-optimize" do not commute. We use the "optimize-then-discretize" approach, i.e., we discretize the state equation and besides the adjoint equation with the AFC method.

OPTIMAL ORDER ERROR ANALYSIS FOR GALERKIN–COLLOCATION APPROXIMATION OF WAVE PROBLEMS AND RELATED SCHEMES

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The elucidation of many physical problems in science and engineering is subject to the accurate numerical modelling of complex wave propagation phenomena. In multi-physics, time derivatives of unknowns can be involed as coefficient functions in some of the subproblems. Over the last decades high-order numerical approximation schemes for partial differential equations have become well-established tools.

Here we propose the combined higher-order variational and collocation approximation in time of wave equations. Continuous and discontinuous finite element approaches are used for the discretization in space. The conceptual basis is the establishment of a direct connection between the Galerkin method for the time discretization and the classical collocation methods, with the perspective of achieving the accuracy of the former with reduced computationals costs provided by the latter in terms of less complex linear algebraic systems. Higher order regularity in time of the discrete solution is ensured. Moreover, a related class of schemes that is based on a computationally cheap post-processing in time is proposed. The key ingredient is the construction of a special lifting operator that improves the discrete solution's regularity and approximation quality in time. A posteriori error control and adaptive mesh refinement mechanisms become feasible.

A unified framework for the derivation of optimal order a priori error estimates in time and space and in various norms is presented. For stabilty reasons, optimal-order error estimates for the time derivative are derived first and, then, used to bound the approximation error of the solution itself. For homogeneous right-hand side terms the conservation of energy is proved for the proposed classes of schemes which is a key feature in the numerical approximation of wave phenomena.

The results are a joint work with S. Becher, G. Matthies, F. Radu and F. Schieweck.

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SHAPE OPTIMIZATION OF ACOUSTIC DEVICES USING CUTFEM AND LEVEL-SET GEOMETRY DESCRIPTIONS

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CutFEM is a recent framework for computations using non-body-conforming meshes [Burman, Claus, Hansbo, Larson, Massing, *Int. J. Numer. Meth. Engng.* 104, 472–501, 2015]. The framework is particularly useful in the context of shape optimization to evade the need for remeshing or deforming meshes. A less well-known added benefit with fixed meshes is that the exact expression for the shape derivative in the discrete case then is typically given by a surface integral over the design boundary. In contrast, when deforming meshes are used, the exact discrete shape derivative is more cumbersome to compute; it is given by a volume integral that explicitly involves the mesh deformation also in the interior of the domain.

In our approach to shape optimization in the CutFEM framework, the boundary is defined as the zero contour of a level-set function. The level-set function is, in turn, defined as the finite-element solution of a Poisson problem in which the nodal values of the right-hand side forcing function constitute the design variables that are actually updated by the gradient-based optimization algorithm. This conditioning of the design variables with the inverse Laplace operator enforces smooth design updates and can also be used for shape regularization by adding a Tikhonov term to the objective function.

In a recent application of this scheme, we consider the problem of designing, in full 3D, the internal geometry (the *phase plug*) of a *compression driver* aimed as the sound source for a mid-to-high-frequency acoustic horn in a public-address audio system. We rely on the FeniCS computing platform for the implementation. A particular feature of this application is that visco-thermal acoustic boundary-layer losses at solid walls are taken into account in the computations. These losses are modeled by a Wenztell boundary condition, that is, a generalized impedance (Robin) boundary condition involving a tangential diffusion operator. This condition is enforced at the boundary that cuts through the fixed background mesh in the CutFEM discretization. The presence of the tangential diffusion also affects the sensitivity analysis; since the geometry is only piecewise smooth, the jumps in the surface normal make additional contribution to the surface-based gradient expressions.

For the optimization, we chose a driver with a 2"-diameter membrane and with a phase plug consisting of 32 radial slits in circumferential symmetry, whose shape was designed using our approach. The optimization objective was to match the frequency response, in a least-squares sense, to a given idealized frequency response evaluated at 27 frequencies, 0.625–10 kHz. The target frequency response was accurately captured by the optimized design, and we concluded that the visco-thermal boundary layer losses are significant in the higher end of the spectrum and thus that the modeling of these are necessary to obtain realistic results.

OPTIMAL CONVERGENCE RATES IN L^2 FOR A FIRST ORDER SYSTEM LEAST SQUARES FINITE ELEMENT METHOD

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We consider a Poisson-like second order model problem written as a system of first order equations. For the discretization an $\boldsymbol{H}(\Omega, \mathrm{div}) \times H^1(\Omega)$-conforming least squares formulation is employed. A least squares formulation has the major advantage that regardless of the original formulation the linear system resulting from a least squares type discretization is always positive semi-definite, making it easier to solve. Even though our model problem in its standard $H^1(\Omega)$ formulation is coercive our methods and lines of proof can most certainly be applied to other problems as well, see [2, 3] for an application to the Helmholtz equation. A major drawback of a least squares formulation is that the energy norm is somewhat intractable. Deducing error estimates in other norms, e.g., the $L^2(\Omega)$ norm of the scalar variable, is more difficult. Numerical examples in our previous work [2] suggested convergence rates previous results did not cover. Closing this gap in the literature will be the main focus of the talk. To that end we showcase a duality argument in order to derive L^2 error estimates of the scalar variable, which was the best available estimate in the literature. We then perform a more detailed analysis of the corresponding error terms. This analysis then leads to optimal convergence rates of the method. The above procedure can then be applied to more complicated boundary conditions, for which an analogous result is a nontrivial task. As a tool, which is of independent interest, we develop $\boldsymbol{H}(\Omega, \mathrm{div})$-conforming approximation operators satisfying certain orthogonality relations. For the analysis, a crucial tool are recently developed projection based commuting diagram operators, see [4].

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EQUILIBRATED STRESS APPROXIMATION AND ERROR ESTIMATION WITH APPLICATION TO SOLID MECHANICS

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A stress equilibration procedure for linear elasticity is presented with emphasis on the behavior for nearly incompressible materials. It is based on the displacement-pressure approximation computed with a stable finite element pair and constructs an H(div)-conforming, weakly symmetric stress reconstruction. The construction leads then to reconstructed stresses by Raviart- Thomas elements of degree k which are weakly symmetric. The computation is performed locally on a set of vertex patches. The resulting error estimator constitute a guaranteed upper bound for the error with a constant that depends only on the shape regularity of the triangulation. The extension to the Signorini contact problem is straightforward.

TIME INTEGRATION ERRORS AND ENERGY CONSERVATION PROPERTIES OF THE STORMER VERLET METHOD APPLIED TO MPM

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The great practical success of the Material Point Method (MPM) in solving many challenging problems nevertheless raises some open questions regarding the fundamental properties of the method. as grid crossing and null-space errors and for example nonlinear stability. The question of the energy conservation of the method has been addressed by Bardenhagen and Love and Sulsky but has not been considered further. In this work both the time integration errors and the energy conservation of MPM is extended by including the impact of particle movement and grid-crossing and a different time integration approach. It is shown that the properties of the spatial methods used play an important role in time accuracy and in conservation. In particular it is shown that a lack of smoothness in the spatial basis functions results in a loss of time accuracy. Furthermore it is shown that it is helpful for the basis functions to possess a commutative property. The error in energy conservation is evaluated and as a result, a more accurate method based upon the Stormer-Verlet method is applied. This method is symplectic and very widely used in many applications such as molecular dynamics and planetary orbits and even dates back to Newton. An analysis of this method as applied to MPM is undertaken and the method is shown to have globally second order accuracy in energy conservation and locally third order accuracy of energy conservation in time. This is in contrast to the globally first order accuracy both in the solution and in energy conservation of the the Symplectic Euler Methods that are used in many MPM calculations This theoretical accuracy is demonstrated numerically on standard MPM test examples

GOAL-ORIENTED ADAPTIVITY FOR ELLIPTIC PDES WITH PARAMETRIC OR UNCERTAIN INPUTS

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In this talk, we present a goal-oriented adaptive algorithm for approximating linear quantities of interest derived from solutions to elliptic partial differential equations (PDEs) with parametric or uncertain inputs. Specifically, we consider a class of elliptic PDEs where the underlying differential operator has affine dependence on a countably infinite number of uncertain parameters and employ the stochastic Galerkin finite element method to approximate the solutions to the corresponding primal and dual problems.

Our algorithm follows the standard adaptive loop: $\mathsf{SOLVE} \Longrightarrow \mathsf{ESTIMATE} \Longrightarrow \mathsf{MARK} \Longrightarrow \mathsf{REFINE}$. Here, the error in the goal functional (e.g., the expectation of the quantity of interest) is *estimated* by the product of computable estimates of the energy errors in Galerkin approximations of the primal and dual solutions. Drawing information from the spatial and parametric contributions to these error estimates, the *marking* is performed by extending the strategy proposed in [4]. Finally, following the methodology developed in [3, 2], a balanced adaptive *refinement* of spatial and parametric components of the approximation space is performed by combining the associated error reduction indicators computed for the primal and dual solutions (see [1]).

We will discuss the results of numerical experiments that demonstrate the effectiveness of our goal-oriented adaptive strategy for a representative model problem with parametric coefficients and for various quantities of interest (including the approximation of pointwise values).

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BEMPP-CL: FAST GPU AND CPU ASSEMBLY OF INTEGRAL OPERATORS WITH OPENCL

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The Bempp boundary element library is a UCL lead project that has been developed since 2011. It consists of a fast C++ core and a user friendly Python interface. It supports the Galerkin discretisation of Laplace, Helmholtz and Maxwell boundary integral operators, either as dense matrices or via ACA based H-Matrix compression.

However, over the last 10 years a revolution has taken place in advanced computing architectures. Massively multicore Xeon CPUs with up to 56 cores are expected to be released in 2019. Each of these cores supports AVX-512 registers that allow the parallel execution of eight double precision or sixteen single precision instructions. At the same time GPU architectures have become mainstream with the fastest Nvidia Volta V100 GPUs having over 5000 compute cores with a peak performance of almost 16 TFlops per second in single precision.

While Bempp performs well on classical multi-core architectures with a few parallel cores, performance issues arise in massive multicore environments. Moreover, it is not able to take advantage of modern vectorized instructions or GPU computing environments.

These considerations have lead to the decision to completely redevelop the library with modern compute architectures in mind. The new library should support advanced vector instruction sets on CPUs and vendor-independent GPU computing. Moreover, the new library should consist only of Python code that would not require any pre-compilation of C or C++ modules. The outcome of these efforts is the Bempp-cl library, which is expected to be released in May 2019. So far it supports the dense Galerkin assembly of Laplace, Helmholtz and Maxwell operators. The performance profiles are significantly improved compared to Bempp, making it possible to assemble dense matrices in the dimension of tens of thousands within seconds on a modern CPU or GPU node. This is especially useful for highly oscillatory problems, which are challenging for standard H-Matrix compression algorithms. Indeed, we will demonstrate high-frequency examples, where the dense assembly in Bempp-cl is significantly more performant than the H-Matrix assembly in previous Bempp versions.

In this talk we present an overview of Bempp-cl, discuss the optimised implementation of assembly routines on modern vector CPU and GPU devices, and present a number of application benchmarks.

A POSTERIORI ERROR ANALYSIS FOR THE MIXED LAPLACE EIGENVALUE PROBLEM

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We review some a posteriori estimators for the Laplace eigenvalue problem in mixed form and show how to extend them to the corresponding eigenvalue problem.

The standard residual error estimator is known to work well and it has been proved to provide an optimally convergent adaptive scheme when used in combination with the usual Dörfler marking strategy [D. Boffi, D. Gallistl, F. Gardini, L. Gastaldi, Math. Comp., 86(307) (2017) 2213-2237].

On the other hand, non residual error estimators are more challenging to be analyzed. Using the Prager-Synge hypercircle approach with local flux reconstructions, a fully computable upper bound for the flux error in the L2-norm is derived when the problem is discretized using Raviart–Thomas finite elements of arbitrary polynomial degree. Efficiency of the local error estimators is proved and numerical experiments with optimal convergence rates are provided [F. Bertrand, D. Boffi, R. Stenberg, arXiv:1812.11203]. The extension of the result to other mixed finite elements, such as BDM spaces, is not straightforward.

MAXWELL-LLG COUPLING VIA CONVOLUTION QUADRATURE

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We consider the Landau-Lifshitz-Gilbert-equation (LLG) on a bounded domain Ω with Lipschitz-boundary Γ coupled with the linear Maxwell equations on the whole space. As the material parameters outside of Ω are assumed to be constant, we are able to reformulate the problem to a MLLG system in Ω coupled to a boundary equation on Γ. We define a suitable weak solution (which still has a reasonable trace for the boundary equation) and propose a time-stepping algorithm which decouples the Maxwell part and the LLG part of the system and which only needs linear solvers even for the nonlinear LLG part. The approximation of the boundary integrals is done with convolution quadrature. Under weak assumptions on the initial data and the input parameters we show convergence of the algorithm towards weak solutions, which especially guarantees the existence of solutions to the MLLG system.

Keywords: convolution quadrature · maxwell · maxwell-LLG · linear scheme · ferromagnetism · boundary elements · transparent boundary conditions · convergence

Mathematics Subject Classifications (2010): 35Q61, 65M12, 65M38, 65M60

THE RATIONAL SPDE APPROACH FOR GAUSSIAN RANDOM FIELDS WITH GENERAL SMOOTHNESS

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A popular approach for modeling and inference in spatial statistics is to represent Gaussian random fields as solutions to stochastic partial differential equations (SPDEs) of the form $L^\beta u = W$, where W is Gaussian white noise, L is a second-order differential operator, and $\beta > 0$ is a parameter that determines the smoothness of u. However, this approach has been limited to the case $2\beta \in \mathbb{N}$, which excludes several important covariance models and makes it necessary to keep β fixed during inference.

We introduce a new method, the rational SPDE approach, which is applicable for any $\beta > 0$ and therefore remedies the mentioned limitation. The presented scheme combines a finite element discretization in space with a rational approximation of the function $x^{-\beta}$ to approximate u. For the resulting approximation, an explicit rate of strong convergence to u is derived and we show that the method has the same computational benefits as in the restricted case $2\beta \in \mathbb{N}$ when used for statistical inference and prediction. Numerical experiments are performed to illustrate the accuracy of the method, and an application to climate reanalysis data is presented.

A HYBRID HIGH-ORDER METHOD FOR KIRCHHOFF–LOVE PLATE BENDING PROBLEMS

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We present a novel Hybrid High-Order (HHO) discretization of fourth-order elliptic problems arising from the mechanical modeling of the bending behavior of Kirchhoff–Love plates, including the biharmonic equation as a particular case. The proposed HHO method supports arbitrary approximation orders on general polygonal meshes, and reproduces the key mechanical equilibrium relations locally inside each element. When polynomials of degree $k \geq 1$ are used as unknowns, we prove convergence in h^{k+1} (with h denoting, as usual, the meshsize) in an energy-like norm. A key ingredient in the proof are novel approximation results for the energy projector on local polynomial spaces. Under biharmonic regularity assumptions, a sharp estimate in h^{k+3} is also derived for the L^2-norm of the error on the deflection. The theoretical results are supported by numerical experiments.

EFFICIENT DISCRETIZATIONS OF NON-LINEAR AND ANISOTROPIC PDES ON CARTESIAN GRIDS

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I will describe Voronoi's first reduction, a tool coming from the field of additive lattice geometry, which turns out to be particularly efficient for the discretization of anisotropic PDEs on cartesian grids.

This approach is versatile, and yields monotone and second order consistent finite difference schemes for various PDEs, ranging from anisotropic elliptic PDEs to the Monge-Ampère equation, and more. In turn, these applications raise new questions on Voronoi's reduction, related to its continuity or its extension to inhomogeneous forms. Numerical results illustrate the method's robustness and accuracy.

CLASSICAL DENSITY FUNCTIONAL THEORY APPROACH TO MOLECULAR SOLVATION

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I will present a molecular version of classical DFT (MDFT) at the basic Hyper-Netted-Chain (HNC) level, i.e. second-order Taylor expansion around a fixed homogeneous density, and beyond. The solvent around a molecular solute is represented by a continuous molecular density field depending on positions and orientations (3 + 3 variables discretised on a spatial and angular grid).[1, 2, 3] Technically, the orientations can be handled efficiently using generalized spherical harmonics expansions and the angular version of FFT's.[3] The approach is illustrated by a few solvation problems : prediction of solvation free energies and microscopic solvation profiles for organic molecules datasets, identification of water molecules around proteins, electron transfer rates close to surfaces. The necessity of introducing so-called bridge excess functionals beyond the HNC approximation will be discussed.

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THE VIRTUAL ELEMENT METHOD FOR GEOPHYSICAL SIMULATIONS

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The flexibility of the Virtual Element Method (VEM) in handling polytopal meshes can be of great help when devising methods for the simulation of physical phenomena in domains that are characterized by huge geometrical complexities. Indeed, discretizing such domains with good quality triangular or tetrahedral meshes can be very hard and require a high number of degrees of freedom.

In this talk we review some strategies based on polytopal meshes to deal with flow and transport simulations in fractured media [3, 1, 4, 2, 5] and for elastic and elasto-plastic problems. Particular focus is given to the computation of the local projectors involved in the VEM discrete formulation: we describe a matrix-based strategy to compute local matrices that can be easily implemented exploiting vectorialization to optimize multiplications.

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P-MULTILEVEL SOLUTION STRATEGIES FOR HHO DISCRETIZATIONS

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Nowadays most of the production runs in the field of fluid mechanics are accomplished by means of second order accurate numerical schemes. The promise of high-order methods to deliver high-fidelity computations for a comparable computational effort hasn t been delivered yet. The lack of high-order mesh generation techniques and the lack of ad-hoc solution strategies are certainly to be blamed. In the case of implicit time marching strategy employing Krylov solvers, a very common combination in the context of CFD, the number of degrees of freedom and the number of Jacobian non-zeros entries strongly impacts the efficiency of the solution strategy, the other relevant parameter being the number of Krylov iterations. Recently introduced Hybrid High Order (HHO) discretizations of the incompressible Navier-Stokes equations [L. Botti, D. A. Di Pietro, J. Droniou, A Hybrid High-Order method for the incompressible Navier Stokes equations based on Temam's device, Journal of Computational Physics, 376, pp. 786–216, 2019] have demonstrated the potential to deal with convection dominated flow regimes and provide local mass conservation properties. Thanks to static condensation, the globally coupled velocity unknowns are coefficients of polynomials expansions in d-1 variables defined over mesh faces, where d is the problem dimension. Similarly, all but piecewise constants pressure degrees of freedom defined over mesh elements can be condensed-out. When high-order discretization are considered, dramatic savings in terms of Jacobian non-zeros entries are expected with respect to discontinuous Galerkin discretizations. Still, the ability to efficiently solve the linearized linear systems arising from such discretizations hasn t been demonstrated. In this work I will consider p-multivel solution strategies as an effective mean of accomplishing such task.

TWO SCALES ADAPTATION AND SEARCH SPACE RECYCLING FOR ADAPTIVE MULTIPRECONDITIONED FETI

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In a previous work, we developed a new domain decomposition method: Adaptive Multipreconditioned FETI (AMPFETI). AMPFETI is the combination of the dual domain decomposition method FETI and the adaptive multipreconditioned conjugate gradient. AMPFETI is robust enough to solve ill conditioned finite element systems arising from large scale non linear industrial problems. At each iteration, AMPFETI generates as many search directions as there are subdomains in the decomposition. Depending on the result of the adaptive test, these search directions are then kept separatly or gathered. In the case of large and ill-conditioned systems, the memory needed to store all kept search directions may become excessive. This motivated a new version of AMPFETI in which the multipreconditioning is defined at a coarser level: subdomains are grouped in aggregates and each aggregate provide a search direction. It allows a better control off the memory consumption. In this contribution we present a new variant of AMPFETI in which aggregates evolve during the krylov iterations. We also couple AMPFETI with classic deflation techniques and show some new results on real industrial testcases.

BASIC IDEAS ON VIRTUAL ELEMENT METHODS AND SOME RECENT DEVELOPMENTS

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The talk will be (roughly) split in two parts. The first, meant for people not familiar with Virtual Elements, will briefly recall the basic ideas: Virtual Elements Spaces are made of piecewise smooth functions (or vector valued functions) on decompositions made of very general polygons or polyhedra. They are defined as solutions of suitable (systems of) PDE equations inside each element, but "the name of the game" is that one does not solve these problems, but uses the degrees of freedom to compute suitable projections from the local VEM space to spaces of polynomials. Everything is made in such a way that the Patch-Test will always be satisfied. In the beginning VEMs were introduced for solving simple problems, as Laplace equation, but then they were extended to more complicated ones, like linear and non-linear elasticity, Stokes and Navier-Stokes equations, Plate bending problems, Magnetostatic problems, etc. Some of the more recent among such developments will be briefly hinted in the second part of the talk, to give an idea of the typical demeanor used to deal with these methods.

DUALITY BASED SPACE-TIME ADAPTIVITY FOR CONVECTION-DOMINATED PROBLEMS

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The DWR philosophy offers great potential in the field of efficient error control for problems characterizing diverse complex phenomena like flow, transport, waves and multi-physics systems. Challenges are for example the appropriate resolution of sharp layers and moving fronts as well as the design of scalable and economical data structures for the underlying numerical approximations; cf. [4]. Using duality arguments the DWR method provides an a posteriori error estimator based on a target functional of physical interest that serves as an indicator for adaptive refinement in space and time.

In this contribution we present a space-time adaptive algorithm based on the Dual Weighted Residual method as well as the underlying software design for the implementation process. Flexible data structures for the open source `deal.II` library are presented that are indispensable to handle the complex software architecture for solving the primal and dual problem in the course of the DWR philosophy. In particular, these structures offer huge potential for the application to large scale problems of practical interest. As a prototype we consider a time-dependent convection-diffusion-reaction equation

$$\partial_t u - \nabla \cdot (\varepsilon \nabla u) + \mathbf{b} \cdot \nabla u + \alpha u = f \tag{1}$$

with a small diffusion coefficient $0 < \varepsilon \ll 1$. These convection-dominated problems are characterized by interior or boundary layers and still remain challenging issues; cf. [3]. To avoid unphysical oscillations within the numerical solutions the adaptive refinement is combined with the streamline upwind Petrov-Galerkin method (SUPG), a residual based stabilization technique. In numerical experiments the applicability of the presented algorithm is studied. Its efficiency is demonstrated for benchmark problems of convection-dominated transport; cf. [1, 2, 4].

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ANALYSIS AND NUMERICS FOR A VISCOELASTIC PHASE SEPARATION MODEL

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The viscoelastic phase separation plays an important role in polymer physics, especially in the separation of solvent and polymer. Due to the mutual difference in size and scale of the ingredients one expects a dynamical asymmetry in this process. In our model the dynamic asymmetry will be induced by viscoelastic effects.
A typical phase separation model consists of a coupled Cahn-Hilliard-Navier-Stokes system for the evolution of volume fraction and velocity and is mainly driven by a mixing potential.
In our case we consider an additional viscoelastic tensor equation associated to the shear stress. Here we choose the diffusive Peterlin equation as rheological model, see [1]. Further, we include a scalar viscoelastic equation which acts as an extra pressure on the divergence between polymer and solvent velocity. This equation will be responsible for introducing the dynamic asymmetry. It turns out that this additional equation is strongly coupled to the diffusion in the Cahn-Hilliard equation and together they form a cross-diffusion subsystem. The model is consistent with the second law of thermodynamics and exhibit an interesting energetic structure.
The nonlinear dependence of typical dimensionless numbers, like Reynolds and Weissenberg number, on the volume fraction allows one to observe a variety of interesting effects.
The aim of this talk is to present some results on the existence of dissipative weak solutions for a viscoelastic phase separation model and their numerical approximation.

We will shortly discuss the existence results and the applied methods of the proof. The main part of the talk will focus on the Lagrange-Galerkin finite element method for the numerical approximation [2]. Therefore, we consider a $P1$ finite element approximation for every variable in space and the first-order characteristic scheme for the material derivative. We will present several simulations and numerically confirm that the scheme is mass conservative and energy dissipative.

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MODELLING FRICTION IN A PARTICLE TO PARTICLE SPH CONTACT ALGORITHM.

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Previous work developed a particle-to-particle contact algorithm for frictionless sliding between two bodies discretised by SPH particles. A particle to particle formulation removes the requirement to construct surfaces or approximate a surface normal. This algorithm has been successfully applied to the analysis of a range of engineering problems and extended to treat contact between finite element and SPH domains. This paper extends this particle-to-particle contact algorithm to include a friction model to broaden the applicability of the contact algorithm. A simple friction model has implemented that generates a lateral contact force between individual particle pairs, with the friction force vector being orthogonal to the local contact force vector. 2D and 3D sensitivity studies show that the friction model works effectively with the overall contact algorithm and agrees with analytical predictions.

FINITE ELEMENT SIMULATIONS AND TRACTION FORCE MICROSCOPY INVERSE PROBLEMS

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Traction force microscopy measures the deformation of the substrate when a cell migrates. The inverse problem—the recovery of the force applied by the cell—can be solved directly for a linear elastic substrate, but presents more difficulties in complex media.

We present a Bayesian approach to solve the inverse problem in traction force motility by means of a finite element approximation of the forward problem and a parallel Markov Chain Monte Carlo method. We use a linear elasticity model as a benchmark for the method, but our approach is readily applicable to more complex substrates, such as anisotropic media and three-dimensional cell migration.

In order to validate the results, we use an experimental dataset that includes not only the substrate deformation but also the focal adhesions. We solve the inverse problem using only the substrate deformation information, and we verify the result by comparing the recovered force with the location of the focal adhesions.

As an example of the application of this results, we use a simple coupled-bulk-surface model to predict the direction of migration of the cell when the force is known.

HP-VERSION SPACE-TIME DISCONTINUOUS GALERKIN METHODS FOR PARABOLIC PROBLEMS ON GENERAL PRISMATIC MESHES.

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We present the *hp*-version space-time interior penalty discontinuous Galerkin (dG) finite element method for parabolic equations on general spatial meshes, giving rise to prismatic space-time elements. A key feature of the proposed method is the use of space-time elemental polynomial bases of total degree defined in the physical coordinate system. This approach leads to a fully discrete hp-dG scheme using fewer degrees of freedom for each time step compared to standard dG time-stepping schemes whereby spatial elemental bases are tensorized with temporal basis functions. A second key feature of the new space-time dG method is the incorporation of very general spatial meshes consisting of polygonal/polyhedral elements with arbitrary number of straight/curved faces.

CONVERGENCE AND OPTIMALITY IN ADAPTIVE HP-FEMS

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In the last few years, the numerical analysis of adaptive FEM discretizations of hp-type for second-order boundary-value problems has made significant progress. In particular, an abstract setting has been designed [1], in which such methods can be framed.

For problems with given forcing term, a general adaptive algorithm (termed hp-AFEM) is based on alternating a solution stage, which provides a new approximate solution with guaranteed error reduction, and an adaptation stage, which yields a new hp-near best partition at the expense of a mild increase of the error. Under reasonable assumptions, this algorithm is proven to be convergent with geometric rate, and instance optimal [1, 2].

Such approach has been recently extended the hp-adaptive approximation of eigenvalue problems, by introducing an iterative procedure for computing a selected eigenvalue and its eigenspace [3]. Convergence and optimality properties can be established under mild conditions on the initial mesh and the operator coefficients. The error reduction is based on a Doerfler-type marking, which uses a computable p-robust equilibrated-flux estimator. For such estimator, a saturation result implies a contraction property for the eigenfunction error in the energy norm.

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HOW TO SOLVE TRANSMISSION PROBLEMS WITH SIGN-CHANGING COEFFICIENTS: PART II. WHEN HYPER-SINGULAR BEHAVIORS APPEAR.

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In electromagnetic theory, the effective response of specifically designed materials can be modeled by strictly negative coefficients: these are the so-called negative materials. Transmission problems with discontinuous, sign-changing coefficients then occur in the presence of negative materials surrounded by classical materials. For general geometries, establishing Fredholmness of these transmission problems is well-understood thanks to the T-coercivity approach [3].
Let σ be a parameter that is strictly positive in some part of the computational domain (characterizing a classical material), and strictly negative elsewhere (characterizing the negative material). We focus on the scalar source problem in two dimensions: find u such that $\mathrm{div}(\sigma\nabla u)+\omega^2 u = f$ plus boundary condition, where f is some data and ω is the pulsation. Denoting by σ^+ the strictly positive value, and by σ^- the strictly negative value, one can prove that there exists a critical interval, such that the scalar source problem is well-posed in the Fredholm sense if, and only, if, the ratio σ^-/σ^+ lies outside the critical interval. The bounds of this critical interval depends on the shape of the interface separating the two materials.
When the ratio σ^-/σ^+ lies inside the critical interval, the problem is ill-posed due to hyper-singular solutions appearing at the corners of the interface. One can recover a well-posed formulation by taking into account those singularities in an extended framework.
We present two approaches to approximate the solution in the extended framework using finite element method. The first approach consists in rescaling the mesh according to the singularities' oscillations, and using Perfectly Matched Layers at the corners [2]. The second approach consists in explicitly computing the singularities, and subtract them from the solution to use standard meshes (Singular Complement Method, [1]).

The case where the ratio σ^-/σ^+ lies outside the critical interval is addressed in the talk given by P. Ciarlet "How to solve problems with sign-changing coefficients: part I. Classical theory".

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CALCULATION OF THE SOLVENT AND ION ATMOSPHERE OF MACROMOLECULES USING 3D-RISM

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The ionic atmosphere around highly charged molecules, like DNA and other macromolecules, involves a complex interplay of co-ions, counter-ions and water. Rigorously modeling such an environment requires accounting for the discrete molecular nature of the solvent. The reference interaction site model (RISM) uses explicit molecular solvent models to provide a complete equilibrium sampling of bulk solvent and solvent around a solute of arbitrary shape and size.[1] Results are similar to those obtained from explicit solvent molecular dynamics (MD) but at a fraction of the cost. In this talk, I will first introduce RISM theory with special attention for thermodynamic qualities, such as preferential interaction parameters and solvation free energies and entropies. Examples will include the distribution of water and ions around a 24 base pair strand of DNA,[2] and of G-quadruplexes,[3] making comparisons to both experiment and to results from molecular dynamics simulations.

Recent developments allow 3D-RISM calculations to be performed with periodic boundary conditions, opening the way to the description of solvent properties in macromolecular crystals, where the solvent may occupy 50% or less of the volume of the unit cell. Numerical methods akin to the particle-mesh Ewald scheme allow an efficient evaluation of both the potential and the resulting forces on the solute atoms. This opens the way to new models for the "bulk-solvent" contribution to X-ray scattering.

These codes can be obtained as a part of the AmberTools distribution[4] (`http://ambermd.org`).

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A PRESSURE-ROBUST HYBRID HIGH-ORDER METHOD FOR THE STEADY INCOMPRESSIBLE NAVIER-STOKES PROBLEM

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In this work we introduce and analyze a novel pressure-robust hybrid high-order method for the steady incompressible Navier-Stokes equations. The proposed method supports arbitrary approximation orders, and is (relatively) inexpensive thanks to the possibility of statically condensing a subset of the unknowns at each nonlinear iteration. For regular solutions and under a standard data smallness assumption, we prove a pressure-independent energy error estimate on the velocity of order $(k+1)$. More precisely, when polynomials of degree $k \geq 0$ at mesh elements and faces are used, this quantity is proved to converge as h^{k+1} (with h denoting the meshsize). In order to achieve pressure-independence, a divergence preserving velocity reconstruction operator is constructed to discretize the body forces (as done in [1]), and the nonlinear term in rotational form (as similarly done in [2] and [3]). Numerical results are presented to support the theoretical analysis.

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AN EFFICIENT MATRIX-FREE FINITE ELEMENT SOLVER FOR THE CAHN–HILLIARD EQUATION

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Lithium ion batteries are key technologies for mobile power devices, as for example in smartphones, laptops or electric vehicles. For the better understanding of the electrode materials we investigate the temporal evolution of the concentration profile of lithium ions in a single electrode particle during the (dis-)charge process. Due to changes in the host material, for example $LiFePO_4$, a separation into lithium-rich and lithium-poor phases is possible. This behaviour can be described with a phase-field model, see [3, 2].

We focus on the efficient numerical solution of the resulting time-dependent fourth-order PDE, also known as the Cahn–Hilliard equation. The main challenges arise from the high nonlinear character and the spatial as well as the temporal properties of this equation, which includes the handling of the almost sharp moving phase boundary and processes on different time scales. In addition, different to the classical formulation of the Cahn–Hilliard equation, a nonlinear boundary condition of exponential-type models the (dis-)charge of the electrode particles.

For the numerical solution of the arising system we employ a higher order standard finite element method ($p \geq 3$) together with an adaptive second order time integrator. Since we want to incorporate the strong anisotropic lattice structure of the electrode material $LiFePO_4$, the simulation of three-dimensional geometries is inevitable. For this, however, we have to manage a huge amount of degrees of freedom. Especially therefore we have developed a fully parallelisable, highly efficient finite element solver, which totally avoids the necessity of storing matrices. The implementation is based on the matrix-free framework within the open-source finite element library deal.II [1].

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AN HDG METHOD FOR THE STOKES-DARCY PROBLEM

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We propose a hybridized discontinuous Galerkin (HDG) method to solve the Stokes-Darcy problem monolithically. We approximate the fluid velocity and pressure in the entire domain, the velocity trace in the Stokes region only and Stokes and Darcy pressure traces in their respective domains. We prove that the method satisfies point-wise mass conservation, pressure-robustness and divergence-conformity properties while having a high order accuracy. We present numerical examples to demonstrate the theoretical results.

ANISOTROPIC HIGH-ORDER ADAPTIVE BOUNDARY ELEMENT METHODS FOR 3D WAVE PROPAGATION

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The main advantage of the Boundary Element Methods (BEMs) is that only the domain boundaries are discretized. They are also well suited to problems in large-scale or infinite domains since they exactly account for radiation conditions at infinity. This dimensional advantage is offset by the fully-populated system matrix, with solution times rapidly increasing with the problem size.

Mesh adaptation is a technique to reduce the computational cost of a numerical method by optimizing the positioning of a given number of degrees of freedom on the geometry of the obstacle. For wave scattering problems, adaptation is particularly important for obstacles that contain geometric or solution singularities. The best strategy to achieve these goals is via so-called "anisotropic" mesh adaptation for which an extensive literature exists for volume-based methods. However, there is relatively little research attention being paid to mesh adaptation in a boundary element context. With the development of fast BEMs, the capabilities of BEMs are greatly improved such that efficient adaptive mesh strategies are needed to optimize further the computational cost. So far BEM adaptivity methods have been confined to isotropic techniques (by using Dörfler marking) and formulated specifically for a system of equations.

The first originality of our work is the extension of metric-based anisotropic mesh adaptation (AMA) [3] to the BEM [2]. The metric-based AMA generates a sequence of non-nested meshes with a specified complexity. The different meshes are defined according to a metric field derived from the evaluation of the linear interpolation error of the (unknown) exact solution on the current mesh. The advantages of this approach are that it is ideally suited to solutions with anisotropic features, it is independent of the underlying PDE and discretization technique, and it is inexpensive. The second originality is the combination of two acceleration techniques, namely metric-based AMA and Fast Multipole accelerated BEM [1]. If no fast BEM is used, the capabilities of anisotropic mesh techniques cannot be fully demonstrated for realistic large scale scattering scenarios.

In this talk, we will show the performance of the strategy to recover optimal convergence rates for simple and complex real-world scattering problems. We will also show the importance of the proposition of an efficient preconditioner if highly anisotropic meshes are used.

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SHAPE OPTIMIZATION FOR THE AUGMENTED LAGRANGIAN FORMULATION OF CONTACT PROBLEMS

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Structural optimization has become an integral part of industrial conception, with applications in more and more challenging mechanical contexts. Those contexts often lead to complex mathematical formulations involving non-linearities and/or non-differentiabilities, which causes many difficulties when considering the associated shape optimization problem.

In this talk, we get interested in finding the optimal design of an elastic body in frictional (Tresca) contact with a rigid foundation, taking into account a possible gap between the two. The proposed optimization algorithm is based on shape derivatives and a level-set representation of the shape, as introduced in [1], while the contact problem is written under its well known augmented Lagrangian formulation, see [2]. However, due to the projection operators involved in this formulation, the solution is not shape differentiable in general.

First, working with directional derivatives, we derive sufficient conditions for shape differentiability, and get an expression for the shape derivative of any generic functional. Then, some numerical results, obtained using the finite element method to solve the augmented Lagrangian formulation of the contact problem and finite differences for the advection of the level-set, are presented.

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FREQUENCY-EXPLICIT CONVERGENCE ANALYSIS FOR FINITE ELEMENT DISCRETIZATIONS OF WAVE PROPAGATION PROBLEMS IN HETEROGENEOUS MEDIA

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We consider the Helmholtz equation in a heterogeneous domain $\Omega \subset \mathbb{R}^d$ with $d \in \{2,3\}$. The domain is characterized by its bulk modulus and density $\kappa, \rho : \Omega \to \mathbb{R}^+$, and the boundary $\partial\Omega$ is split into two subdomains Γ_{A} and Γ_{D}. Then, given $f : \Omega \to \mathbb{C}$, we seek a function $u : \Omega \to \mathbb{C}$ such that

$$\left\{\begin{array}{rcll} -\dfrac{\omega^2}{\kappa}u - \boldsymbol{\nabla}\cdot\left(\dfrac{1}{\rho}\boldsymbol{\nabla}u\right) &=& f & \text{in } \Omega \\ u &=& 0 & \text{on } \Gamma_{\mathrm{D}} \\ \dfrac{1}{\rho}\boldsymbol{\nabla}u\cdot\boldsymbol{n} - \dfrac{1}{\sqrt{\kappa\rho}}u &=& 0 & \text{on } \Gamma_{\mathrm{A}}, \end{array}\right. \tag{1}$$

where $\omega > 0$ is the (given) angular frequency.

We assume that the heterogeneous coefficients κ and ρ are piecewise smooth. Specifically, we assume that there exists a partition $\mathscr{P} = \{\Omega_\ell\}$ of Ω such that each Ω_ℓ has a smooth boundary of class $\mathscr{C}^{m+1,1}$ and that $\kappa, \rho \in \mathscr{C}^{m,1}(\overline{\Omega_\ell})$ for all $\Omega_\ell \in \mathscr{P}$ where $m \geq 0$ is a given integer.[1]

We consider finite element discretizations to problem (1) of degree $p \leq m+1$ that are built on shape-regular meshes $\mathscr{T}_h$ compatible with the partition $\mathscr{P}$. We perform a stability and convergence analysis under the assumption that the problem is solvable for all frequencies. Then, for every $\omega > 0$, there exists a real number $\beta_{\mathrm{s}}(\omega)$ such that

$$\|u\|_{0,\Omega} \leq \frac{\beta_{\mathrm{s}}(\omega)}{\omega^2}\|f\|_{0,\Omega}. \tag{2}$$

The behaviour of $\beta_{\mathrm{s}}(\omega)$ is known for several configurations of interest, and in particular, it depends linearly on ω for non-trapping domains.

Our key result is the following: under the assumption that $\omega h + \beta_{\mathrm{s}}(\omega)(\omega h)^p \leq C$, the finite element solution is quasi-optimal, and we have

$$k\|u-u_h\|_{0,\Omega} + |u-u_h|_{1,\Omega} \leq C\left(h + \frac{\beta_{\mathrm{s}}(\omega)}{\omega}(\omega h)^p\right)\|f\|_{0,\Omega}.$$

Recalling that $N_\lambda = (\omega h)^{-1}$ is a measure of the number of elements per wavelength, our analysis shows that the finite element scheme provides a quasi-optimal solution under the assumption that

$$N_\lambda \geq C\max\left(1, \beta_{\mathrm{s}}(\omega)^{1/p}\right). \tag{3}$$

Following estimate (3), our key conclusion is that high order finite element methods are stable on coarser meshes than low order ones, especially in the high-frequency regime.

This crucial observation is corroborated by numerical experiments, which show that the main estimates we derive are sharp, and that higher order methods generally need much less degrees of freedom to achieve a desired accuracy in the high frequency regime.

THRESHOLD DYNAMICS METHOD FOR TOPOLOGY OPTIMIZATION FOR FLUIDS

Huangxin Chen, Haitao Leng,
Dong Wang and Xiao-Ping Wang

In this talk we will introduce an efficient threshold dynamics method for topology optimization for fluids modeled with the Stokes equation. We aim to minimize an objective energy function that consists of the dissipation power in the fluid and the perimeter approximated by nonlocal energy subject to a fluid volume constraint and an incompressibility condition. In order to solve the problem in the whole domain, a one-domain approach for fluids over porous media will be introduced. Then we show that the minimization problem can be solved with an iterative scheme in which the Stokes problem is approached with a Brinkman problem. The indicator functions of the fluid-solid regions are then updated according to simple convolutions followed by a thresholding step. The total energy decaying property of the iterative algorithm can be obtained. Some numerical results will be shown to verify the efficiency of the proposed algorithm.

GENERALIZED MULTISCALE APPROXIMATION OF MIXED FINITE ELEMENTS WITH VELOCITY ELIMINATION FOR SUBSURFACE FLOW

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A frame work of the mixed generalized multiscale finite element method (GMsFEM) for solving Darcy's law in heterogeneous media is studied in this talk. Our approach approximates pressure in multiscale function space that is between fine-grid space and coarse-grid space and solves velocity directly in the fine-grid space. To construct multiscale basis functions for each coarse-grid element, three types of snapshot space are raised. The first one is taken as the fine-grid space for pressure and the other two cases need to solve a local problem on each coarse-grid element. We describe a spectral decomposition in the snapshot space motivated by the analysis to further reduce the dimension of the space that is used to approximate the pressure. Since the velocity is directly solved in the fine-grid space, in the linear system for the mixed finite elements, the velocity matrix can be approximated by a diagonal matrix without losing any accuracy. Thus it can be inverted easily. This reduces computational cost greatly and makes our scheme simple and easy for application. Moreover, the proposed method preserves the local mass conservation property that is important for subsurface problems. Numerical examples are presented to illustrate the good properties of the proposed approach. If offline spaces are appropriately selected, one can achieve good accuracy with only a few basis functions per coarse element according to the numerical results.

MULTIRATE METHODS FOR COUPLED FREE FLOW WITH POROUS MEDIA FLOW PROBLEMS

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We present a decoupled multiple time step finite element scheme for the Stokes/Darcy model. The scheme utilizes small time steps for the fast moving free flow and a relatively larger time step for the slow moving porous media flow. The spatial discretization combines standard inf-sup continuous elements for the Stokes problem and the primal Discontinuous Galerkin method for the porous media flow. We present stability and convergence analysis results for the decoupling scheme. In addition, we compare the fully coupled scheme to the multiple time step decoupling scheme in-terms of CPU time and accuracy. We demonstrate long term stability of the scheme and robustness under realistic parameter regimes.

FINITE ELEMENT APPROXIMATIONS FOR AN OPTIMAL CONTROL PROBLEM RELATED TO BRUSSELATOR SYSTEM

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An optimal control problem related to the Brusselator system is considered. The Brusselator system consists of two coupled nonlinear reaction diffusion PDEs with different diffusion constants. A discontinuous (in time) Galerkin approach, combined with standard finite elements in space is considered for the discretization of the control to state mapping. Using properties of the discrete additive dynamics of the system, and a bootstrap argument, we establish stability bounds in the natural energy norm, with bounds depending polynomially upon the inverse of the diffusion constants. Special care is exercised to avoid any restriction between the temporal and spacial discretization parameters. In addition, a-priori error estimates are presented in the energy norm under a smallness assumption of on the size of the temporal discretization parameter. The error analysis also includes higher order schemes. Finally, we analyze a fully-discrete scheme for a related Robin boundary control problem. The Robin controls satisfy point-wise constraints. The state equation is discretized based on the lowest order discontinuous (in time) Galerkin scheme, while the controls are piecewise constants in space-time. Using the stability estimates under minimal regularity assumptions, we show convergence (in appropriate sense) of the associated discretized optimal control problem to the continuous one.

CLUSTER-BASED MULTISCALE MODEL REDUCTION

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We present a clustering algorithm to study the elliptic PDEs with random coefficients in the multi-query setting. Our method consists of offline and online stages. In the offline stage, we construct a small number of reduced basis functions within each coarse grid block, which can then be used to approximate the multiscale finite element basis functions. In addition, we coarsen the corresponding random space through a clustering algorithm. In the online stage, we can obtain the multiscale finite element basis very efficiently on a coarse grid by using the pre-computed multiscale basis. The new method can be applied to multiscale SPDE starting with a relatively coarse grid, without requiring the coarsest grid to resolve the smallest-scale of the solution. The new method offers considerable savings in solving multiscale SPDEs. Numerical results are presented to demonstrate the accuracy and efficiency of the proposed method for several multiscale stochastic problems without scale separation. This research is partially supported by Hong Kong RGC General Research Fund (Project 14302018) and CUHK Direct Grant for Research 2018-19.

MULTI-CONTINUA UPSCALING FOR FLOWS IN POROUS AND FRACTURE MEDIA

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In this talk, we present multi-continua upscaling methods for multiscale problems. The main idea of these approaches is to use local constraints and solve problems in oversampled regions for constructing macroscopic equations. These techniques are intended for problems without scale separation and high contrast, which often occur in applications. In our method, the local solutions are used as a forward map from local averages (constraints) of the solution in oversampling region. This local fine-grid solution is further used to formulate the coarse-grid problem. Our approach is discussed on several examples and applied to flow problems in porous and fracture media. The numerical results show that we can achieve good accuracy using our new concepts for these complex problems. We will also present the convergence theory for this method. Finally, we present an extension of this method to nonlinear problems. This research is partially supported by Hong Kong RGC General Research Fund (Project 14304217) and CUHK Direct Grant for Research 2017-18.

ANALYSIS OF THE PARALLEL SCHWARZ METHOD FOR GROWING CHAINS OF FIXED-SIZED SUBDOMAINS

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A new class of Schwarz methods was recently presented in the literature for the solution of solvation models, where the electrostatic energy contribution to the solvation energy can be computed by solving a system of elliptic partial differential equations [1, 2]. Numerical simulations have shown an unusual convergence behavior of Schwarz methods for the solution of this problem, where each atom corresponds to a subdomain: the convergence of the Schwarz methods is independent of the number of atoms [1], even though there is no coarse grid correction. Despite the successful implementation of Schwarz methods for this solvation model, a rigorous analysis for this unusual convergence behavior is required.

In this talk, we analyze the behavior of the Schwarz method for the solution of chains of subdomains and show that its convergence does not depend on the number of subdomains in many cases [3, 4]. Moreover, we will present new recent results that study the behavior of the Schwarz method in the cases its convergence depends on the number of subdomains [5].

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HOW TO SOLVE PROBLEMS WITH SIGN-CHANGING COEFFICIENTS: PART I. CLASSICAL THEORY

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In electromagnetic theory, the effective response of specifically designed materials can be modeled by strictly negative coefficients: these are the so-called negative materials. Transmission problems with discontinuous, sign-changing coefficients then occur in the presence of negative materials surrounded by classical materials. For general geometries, establishing Fredholmness of these transmission problems is well-understood thanks to the T-coercivity approach [2].
Let σ be a parameter that is strictly positive in some part of the computational domain (characterizing a classical material), and strictly negative elsewhere (characterizing the negative material). We focus on the scalar source problem: find u such that $\mathrm{div}(\sigma\nabla u) + \omega^2 u = f$ plus boundary condition, where f is some data and ω is the pulsation. Denoting by σ^+ the strictly positive value, and by σ^- the strictly negative value, one can prove that there exists a critical interval, such that the scalar source problem is well-posed in the Fredholm sense if, and only, if, the ratio σ^-/σ^+ lies outside the critical interval. The bounds of this critical interval depends on the shape of the interface separating the two materials [2, 1].
When the ratio σ^-/σ^+ lies outside the critical interval, one can apply the T-coercivity approach at the discrete level to solve the problems numerically. We propose a treatment which allows to design meshing rules for an arbitrary polygonal interface and then recover standard error estimates. This treatment relies on the use of simple geometrical transforms to define the meshes.

The case where the ratio σ^-/σ^+ lies inside the critical interval is addressed in the talk given by C. Carvalho "How to solve problems with sign-changing coefficients: part II. When hyper-singular behaviors appear".

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A TIME DOMAIN COMBINED FIELD INTEGRAL EQUATION FREE FROM CONSTANT-IN-TIME AND RESONANT INSTABILITIES

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Time domain boundary integral equations are used for the modelling of transient scattering by reflecting or penetrable bodies [F. Sayas, Retarded Potentials and Time Domain Boundary Integral Equations: A Road Map, Springer, 2016]. Their advantages include that solutions to these integral equations automatically fulfil radiation conditions, and that only the boundary of the scatter needs to be modelled.

Time domain as opposed to frequency domain solvers have the additional advantages that solutions include information over a broad range of frequencies and that the equations can be coupled to non-linear lumped element circuits or boundary conditions.

Unfortunately, straightforward implementations of the single and double layer based time domain integral equations for the Maxwell equations suffer from a number of problems: (i) the condition number of the system to be solved grows as the mesh parameter tends to zero, (ii) the condition number also grows as the time step tends to infinity, (iii) the system support constant and/or linear in time regime solutions stemming from the scatter's topology, and (iv) the system supports regime solutions related to internal resonances supported by the interior of the scatterer [Y. Beghein at al., A DC-Stable, Well-Balanced, Calderon Preconditioned Time Domain Electric Field Integral Equation, IEEE Trans. AP, vol. 63, no. 12, 2015].

In this contribution, an integral equation is introduced alongside a discrretisation scheme that eliminates these problems. The solver methodology relies on both Calderon or operator preconditioning techniques to control the condition number and a combined field approach to eliminate spurious resonances. To render the system immune from constant and linear in time regime solutions, a non-tensorial space-time discretisation is required subject to a well-chosen Helmholtz decomposition for the discrete currents. The details of the operator preconditioning for the single layer and double layer terms of this combined field equation differ in a technical but critical manner to achieve this.

The discretisation is carefully introduced and its properties are discussed. It will be demonstrated both by investigating late-time solutions and by considering polynomial eigenvalue distributions that the method is free from constant-in-time regime solutions and that, as a result, the method is more robust in the presence of quadrature error and when applied to scattering off multiply connected obstacles.

ON THE INCOMPATIBILITY OF TRADITIONAL LAGRANGIAN MECHANICS AND THE MATERIAL POINT METHOD

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The material point method [D. Sulsky, Z. Chen, H. Schreyer, A particle method for history-dependent materials, *Computer Methods in Applied Mechanics and Engineering* 118 (1994) 179-196] is marketed as the technique to solve problems involving large deformations, particularly in areas where conventional mesh-based methods struggle. However, there are issues with combining the method with traditional total and updated Lagrangian statements of equilibrium. These issues are associated with the basis functions, and particularity their derivatives, of material point methods normally being defined based on an unformed, and sometimes regular, background mesh. It is possible to map the basis function spatial derivatives using the deformation at a material point but this introduces additional algorithm complexity and computational expense. This paper will first present the issues associated with conventional Lagrangian statements of equilibrium and then proposes a new statement which is ideal for material point methods as it satisfies equilibrium on the undeformed background mesh at the start of a load step. The resulting weak form statement of equilibrium for the proposed *previously converged* formulation is

$$\int_{\varphi_{t_n}(\Omega)} (\tilde{P}_{ij}(\nabla_{\tilde{X}}\eta)_{ij} - b_i\eta_i)\mathrm{d}v - \int_{\varphi_{t_n}(\partial\Omega)} (t_i\eta_i)\mathrm{d}s = 0, \tag{1}$$

where φ_{t_n} is the motion of the material body, with domain Ω, evaluated at the previously converged (or for the first load step, the initial) state, $\tilde{X}_i$. The body is subject to tractions, t_i, on the boundary of the domain (with surface, s), $\partial\Omega$, and body forces, b_i, acting over its volume, v. The weak form is derived assuming a field of admissible virtual displacements, η_i. $\tilde{P}_{ij}$ is the Cauchy stress pulled back to the previously converged state $\tilde{P}_{ij} = \Delta J\ \sigma_{im}(\Delta F^{-1})_{jm}$, where ΔF_{ij} is the increment in the deformation gradient over the current loadstep, $\Delta J = \det(\Delta F_{ij})$ is the incremental volume ratio and σ_{ij} is the Cauchy stress. The above weak statement is combined with a linear relationship between elastic logarithmic strains and Kirchhoff stresses and the multiplicative decomposition of the deformation gradient into elastic and plastic components. The resulting equations are discretised by a set of material points that represent the solid body.

The numerical analysis framework is demonstrated using a number of large deformation elasto-plastic problems with both the standard and the generalised interpolation [S.G. Bardenhagen, E.M. Kober, The generalized interpolation material point method, *Computer Modeling in Engineering and Sciences* 5 (2004) 477-495] material point methods, with a specific focus on the convergence towards analytical solutions. Although the formulation is implemented within a implicit material point method, the proposed framework can be applied to all existing material point methods and adopted for both implicit and explicit analysis.

A COUPLED BULK-SURFACE MODEL FOR CELL POLARISATION

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Cell polarisation is the result of intricate networks of biochemical reactions. Recent work on balancing biological complexity with mathematical tractability resulted in the proposal and formulation of a famous minimal model for cell polarisation by [2], known as the wave pinning model. In this talk, we present a three-dimensional generalisation of this mathematical framework through the maturing theory of coupled bulk-surface semilinear partial differential equations in which protein compartmentalisation becomes natural [1]. We show how a local perturbation over the surface can trigger propagating reactions, eventually stopped in a stable profile by the interplay with the bulk component. We present the bulk-surface finite element method which is used to generate numerical simulations over simple and complex geometries, showing pattern formation due to propagation and pinning dynamics. From the mathematical point of view, of the interesting features of the model regards its long time behavior. This will be shown with some explicative and novel simulations over different three-dimensional geometries. The generality of our mathematical and computational framework allows to study more complex biochemical reactions and biomechanical properties associated with cell polarisation in multi-dimensions.

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A PAINLESS AUTOMATIC GOAL-ORIENTED HP-ADAPTIVE STRATEGY FOR NON-ELLIPTIC PROBLEMS

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Despite the existence of several *hp*-adaptive algorithms in the literature (e.g. [1]), very few are used in industrial context due to their high implementational complexity, computational cost, or both. This occurs mainly as a result of two limitations associated with the use of *hp*-adaptive methods: (1) the data structures needed to support *hp*-refined meshes are often complex, and (2) the design of a robust automatic *hp*-adaptive strategy is challenging.

To overcome limitation (1), we adopt the multi-level approach of D'Angela et al. [2]. This method handles hanging nodes via a multilevel technique with massive use of Dirichlet nodes.

Our main contribution in this work is intended to overcome limitation (2) by introducing a novel automatic *hp*-adaptive strategy. Derived from an energy-based *unrefinement* approach developed in [4] for elliptic problems, in here we extend it to the case of goal-oriented adaptivity for non elliptic problems by using a Riez representation of the quantity of interest as presented in [3]. Given an arbitrary grid, the algorithm detects those unknowns that contribute least to an upper bound of an error representation of the quantity of interest, and remove them. Once a sufficient level of unrefinement is achieved, a global h, p, or any other type of refinements can be performed.

We tested and analyzed our algorithm on one-dimensional (1D) and two-dimensional (2D) benchmark cases. We shall illustrate the main advantages and limitations of the proposed goal-oriented *hp*-adapted method.

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A C^1 VIRTUAL ELEMENT METHOD ON POLYHEDRAL MESHES

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In this talk we are interested in H^2-conforming solution of three dimensional linear elliptic problems. If we consider a standard Finite Element framework, the construction of such high regular solution requires high approximation degrees and the discrete functional space becomes really involved.

To avoid these issues and preserve the H^2-conformity, we consider the Virtual Element Method. One of the advantages of such method is a more flexibility in the definition of the discrete spaces. This fact was already exploited to develop C^1 conforming elements in 2d keeping the accuracy order and the number of degrees of freedom at a reasonable level [1, 2]

In this talk we will extend such theory to the three dimensional space. More specifically, we will focus on the lowest order case to better understand the idea behind a Virtual Element discretization. We will show that the number of degrees of freedom is limited with respect to Finite Element indeed they are only 4 per mesh vertex representing function and gradient values. Finally, we will provide some numerical examples on classical fourth order elliptic problems, but also on standard second order elliptic problem where we look for a more regular solution.

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REFINEMENT STRATEGIES FOR POLYGONAL MESHES AND SOME APPLICATIONS TO FLOW SIMULATIONS IN DISCRETE FRACTURE NETWORKS.

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The generation of a triangular conforming mesh for flow simulations in the discrete fracture networks (DNFs) is a challenging problem due to the stochastic nature of the fracture networks obtained sampling probabilistic distributions for dimension, position, size, orientation of the fractures. Moreover, also the distribution of the transmissivities strongly impacts on the solution and on a suitable mesh for its representation. In order to circumvent the creation of a huge number of elements close to intersections, usually required for the conformity, a viable approach can be based on polygonal meshes suitable for DFNs simulations. A possible mesh for Vem discretizations is the "almost minimal" subfractures mesh that can be obtained by a subdivision process of the fractures. This mesh is not usually suited for producing an accurate solution, nevertheless, is a good starting point for a posteriori driven mesh refinement [1, 2, 3, 4]. During the mesh refinement is mandatory to control the aspect ratio of the produced elements and the growing of the number of edges of the elements, as in general the mesh can contain polygons with an highly variable number of edges. In the talk several refinement strategies for convex polygons will be discussed as well as their interplay with the computed Vem solution and the cost of the linear solver.

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THE MRE INVERSE PROBLEM FOR THE ELASTIC SHEAR MODULUS

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Magnetic resonance elastography (MRE) is a powerful technique for noninvasive determination of the biomechanical properties of tissue, with important applications in disease diagnosis. A typical experimental scenario is to induce waves in the tissue by time-harmonic external mechanical osciillation and then measure the tissue's displacement at fixed spatial positions 8 times during a complete time-period, extracting the dominant frequency signal from the discrete Fourier transform in time. Accurate reconstruction of the tissue's elastic moduli from MRE data is a challenging inverse problem, and I will describe a new approach based on combining approximations at different frequencies into a single overdetermined system.

RESIDUAL BASED A-POSTERIORI ESTIMATES BASED ON POST-PROCESSING

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The post-processing of finite element solutions to elliptic problems with the aim to achieve a higher order of approximation has been the focus of numerous studies over the past decades A first contribution was made by Bramble and Schatz (1977) who present an averaging technique that significantly improves the order of convergence of a Galerkin approximation. A second approach was pioneered by Zienkiewicz and Zhu (1992) who used a superconvergent reconstruction of the gradient of approximation to construct an a-posteriori error estimator. Based on this idea a number of further approaches have been suggested quite recently involving for example the reconstruction of function values based on local least squares problems.

In this work we derive a dual weighted residual estimator for elliptic problems based on a general post-processed function u^* to the finite element solution u_h. Our approach requires a simple modification u^{**} of the given reconstruction u^* which converges with the same rate to the exact solution u as u^*. The resulting estimator R^{**} is computable and reliable, i.e., we can show that $J(u - u^{**}) \leq R^{**}$ for general error functionals J. Furthermore, we can show local efficiency of the estimator in the case that the error is measured in the energy norm.

We investigate the numerical properties of the estimator using the *Smoothness Increasing Accuracy Enhancing* (SIAC) filter and a least squares types postporcessing approach. We demonstrate that our modification u^{**} improves on the original reconstruction u^* both in the energy and in the L^2 norm. Also we show some experiments on locally adaptive grids which demonstrate that basing the marking strategy on the post-processed solution u^{**} can greatly improve the efficiency of the adaptive scheme.

HYBRID HIGH–ORDER METHODS FOR INDEFINITE PROBLEMS ON UNFITTED MESHES

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Hybrid High–Order (HHO) methods have been recently introduced in [1]. The unknowns are attached to the cells and faces of the mesh. The cell unknowns can be eliminated locally leading to a global problem coupling the face unknowns only. HHO methods lead to a local conservation principle, are robust in many situations, and are computationally effective. As shown in [2], HHO methods are closely related to Hybrid Discontinuous Galerkin (HDG) methods and to nonconforming Virtual Element Methods (ncVEM).

More recently, HHO methods have been adapted to solve an elliptic interface problem on unfitted meshes [3]. The interface can cut the background mesh in a quite general fashion. Robustness with respect to cuts is achieved by a local cell–agglomeration procedure [3] taking full advantage of the fact that HHO methods support polyhedral meshes.

In the present work, we want to extend those results to indefinite problems, for which the stability analysis is more delicate than for the standard coercive elliptic problem. We consider the Stokes problem. We investigate error estimates and we present numerical simulations.

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FREE AND MOVING BOUNDARY PROBLEMS AND TRANSFINITE INTERPOLATIONS

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In imaging and numerical analysis a *transfinite interpolation* is a special case of an extension of a function defined on a closed subset E of the Euclidean n-dimensional space $\mathbf{R}^n$ to some larger subset of $\mathbf{R}^n$. We first generalize the construction and relax the assumptions of Dyken and Floater [*Transfinite mean value interpolation* (TMI), Computer Aided Geometric Design 26 (2009), 117–134] of an extension to an open domain Ω with compact Lipschitzian boundary and positive reach of a continuous function defined at its boundary $\partial\Omega$. Secondly, we introduce the new family of *k-Transfinite Barycentric Interpolation* (TBI) for compact H^d-rectifiable subsets E of $\mathbf{R}^n$ of arbitrary dimension $0 \leq d < n$. Modulo the specific requirements of the application at hand, it is both computationally simpler and mathematically more general than the TMI for which E is limited to the boundary of an open domain. Thirdly, dynamical versions of the TMI and the TBI are introduced to iteratively construct the rate of change of the position of the points of $\mathbf{R}^n \backslash E$ from the rate of change of the points of E as if E was a moving/deforming body in a fluid medium. This paper is motivated by pressing numerical and theoretical applications in the numerical analysis of free/moving boundary problems, *Arbitrary Lagrangian-Eulerian* (ALE) methods, and iterative schemes in shape/topological optimization and control.

ON NUMERICAL APPROXIMATIONS OF THE SPECTRAL FRACTIONAL LAPLACIAN VIA THE METHOD OF SEMIGROUPS

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As it is well-known, there are several (non-equivalent) ways of defining fractional operators in bounded domains. In this talk we will focus on the so-called spectral fractional Laplacian. Following the heat semi-group formula we consider a family of operators which are boundary conditions dependent and discuss a suitable approach for their numerical discretizations. We will also discuss the numerical treatment of the associated homogeneous boundary value problems. In the end we will talk about possible extensions that can be treated with our approach such as non-homogeneous boundary conditions and discretizations of fractional operators in the whole space.

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ADAPTIVE MULTILEVEL SOLVERS FOR THE DISCONTINUOUS PETROV-GALERKIN METHOD WITH AN EMPHASIS ON HIGH-FREQUENCY WAVE PROPAGATION PROBLEMS

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The work focuses on the development of fast and efficient solution schemes for the simulation of challenging problems in wave propagation phenomena. In particular, emphasis is given in high frequency acoustic and electromagnetic problems which are characterized by localized solutions in problems like ultrasonic testing, laser scanning and modeling of optical laser amplifiers. In wave simulations, the computational cost of any numerical method, is directly related to the frequency. In the high-frequency regime very fine meshes have to be used in order to satisfy the Nyquist criterion and overcome the pollution effect. This often leads to prohibitively expensive problems. Numerical methods based on standard Galerkin discretizations, lack of pre-asymptotic discrete stability and therefore adaptive mesh refinement strategies are usually inefficient. Additionally, the indefinite nature of the wave operator makes state of the art preconditioning techniques, such as multigrid, unreliable.

A promising alternative approach is followed within the framework of the discontinuous Petrov-Galerkin (DPG) method. The DPG method offers numerous advantages for our problems of interest: mesh and frequency independent discrete stability even in the pre-asymptotic region, and a built-in local error indicator that can be used to drive adaptive refinements. Combining these two properties together, reliable adaptive refinement strategies are possible which can be initiated from very coarse meshes. The DPG method can be viewed as a minimum residual method, and therefore it always delivers symmetric (Hermitian) positive definite stiffness matrix. This is a desirable advantage when it comes to the design of iterative solution algorithms. Conjugate Gradient based solvers can be employed which can be accelerated by domain decomposition (one- or multi- level) preconditioners for symmetric positive definite systems.

Driven by the aforementioned properties of the DPG method, an adaptive multigrid preconditioning technology is developed that is applicable for a wide range of boundary value problems. Unlike standard multigrid techniques, our preconditioner involves trace spaces defined on the mesh skeleton, and it is suitable for adaptive hp-meshes. Integration of the iterative solver within the DPG adaptive procedure turns out to be crucial in the simulation of high frequency wave problems. A collection of numerical experiments for the solution of linear acoustics and Maxwell equations demonstrate the efficiency of this technology, where under certain circumstances uniform convergence with respect to the mesh size, the polynomial order and the frequency can be achieved. The construction is complemented with theoretical estimates for the condition number in the one-level setting.

COUPLING OF FINITE ELEMENT METHOD AND SMOOTHED PARTICLE HYDRODYNAMICS FOR MODELLING HIGH-VELOCITY IMPACT DAMAGE IN COMPOSITE MATERIALS

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The impact response of Carbon Fibre Reinforced Polymer materials is important for aerospace applications. Impact threats include birds, runway debris and hail ice. This paper presents research on development of a combined Finite Element Method (FEM) and meshless Smoothed Particle Hydrodynamics (SPH) Method approach to the analysis of composite failure under impact loading. The purpose is to make use of the inherently non-local nature of SPH and treatment of damage based on particle to particle interactions for dealing with composite failure, and at same time to use the efficiency of FEM in areas away from the failure zone. Modelling multiple fractures leading to fragmentation in materials subjected to high-strain rates using continuum mechanics is a challenging problem. Meshless methods such as SPH are well suited to the application of damage and fracture mechanics.

This research is funded by the European project EXTREME (grant agreement no 636549), developing tools for modelling of high velocity impact on aerospace composite structures.

HYBRID HIGH-ORDER METHODS FOR DIFFUSION PROBLEMS ON POLYTOPES AND CURVED ELEMENTS

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Originally introduced in [1, 2], Hybrid High-Order (HHO) methods provide a framework for the discretisation of models based on PDEs with features that set it apart from traditional ones; see [4] for a comprehensive introduction. The construction hinges on discrete unknowns that are broken polynomials on the mesh and on its skeleton, from which two key ingredients are devised:

(i) Local reconstructions obtained by solving small, trivially parallel problems inside each element, and conceived so that their composition with the natural interpolator yields a (problem-dependent) projector on local polynomial spaces;

(ii) Stabilisation terms that penalise residuals designed at the element level so as to ensure stability while preserving the approximation properties of the reconstruction.

These ingredients are combined to formulate local contributions, which are then assembled as in standard Finite Element methods. From this construction, several appealing features ensue: the support of polytopal meshes and arbitrary approximation orders in any space dimension; an enhanced compliance with the physics; a reduced computational cost thanks to the compact stencil along with the possibility to locally eliminate a large portion of the unknowns.

In this presentation, focusing on a diffusive model problem, we introduce the basic construction underlying HHO methods on meshes with straight faces and, following [3], point out an extension to curved elements. The key idea, in the latter case, consists in increasing the polynomial degree of the face unknowns according to the so-called effective (geometric) mapping order. A panel of numerical examples including comparisons with Discontinuous Galerkin methods accompanies the exposition.

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SPACE-TIME DISCONTINUOUS GALERKIN METHOD FOR THE NUMERICAL SOLUTION OF THE RICHARDS EQUATION

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We deal with the numerical solution of the Richards equation describing time-dependent variably-saturated flow though porous media. It can be written in the form

$$\frac{\partial \vartheta(\Psi - z)}{\partial t} - \nabla \cdot (\boldsymbol{K}(\Psi - z))\nabla\Psi) = 0,$$

where Ψ is the hydraulic head [L], z is the geodetic head [L] (distance from the reference level), $\boldsymbol{K}$ is the unsaturated hydraulic conductivity tensor of the second order [L.T^{-1}] and ϑ [-] represents the volumetric water content and the term of a possible storativity of the porous material. The nonlinear function ϑ and $\boldsymbol{K}$ are given by constitutive relations and they can degenerate, i.e., vanish or blow up.

We discretize this problem by an adaptive higher-order space-time discontinuous Galerkin method which employs piecewise polynomial discontinuous approximation with respect to the space and time coordinates. The discretization leads to a system of nonlinear algebraic equations which are solved by a Newton-like method in the combination with the Anderson acceleration. Convergence problems related to the transition between unsaturated and saturated flow are eliminated by a regularization of the constitutive formulas. A special attention is paid to the realization of the seepage boundary condition (or outflow boundary condition) which is treated by a variable penalty in the context of the discontinuous Galerkin method.

We develop an adaptive technique which optimizes accuracy and efficiency by balancing the errors that arise from the space and time discretizations and from the resulting nonlinear algebraic system. Additionally, we adopt a *hp*-anisotropic mesh adaptation technique capable of generating unstructured triangular elements with optimal sizes, shapes, and polynomial approximation degrees. Several numerical experiments are presented to demonstrate the accuracy, efficiency, and robustness of the numerical method.

THE JONES EIGENVALUE PROBLEM IN FLUID-STRUCTURE INTERACTION

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The Jones eigenvalue problem first described by D.S. Jones in [2] concerns unusual modes in bounded elastic bodies: time-harmonic displacements whose tractions and normal components are both identically zero on the boundary. This problem is usually associated with a lack of unique solvability for certain models of fluid-structure interaction. The boundary conditions in this problem appear, at first glance, to rule out any non-trivial modes unless the domain possesses significant geometric symmetries. Indeed, Jones modes were shown to not be possible in most C^∞ domains in [1]. However, while the existence of Jones modes sensitively depends on the domain geometry, such modes do exist in a broad class of domains. This talk presents both theoretical and computational investigations of this eigenvalue problem in Lipschitz domains.

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A-POSTERIORI ERROR ESTIMATOR FOR HP-VERSION DISCONTINUOUS GALERKIN METHODS ON POLYGONAL AND POLYHEDRAL MESHES

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We will present a new framework for deriving the a-posteriori error estimation for the interior penalty discontinuous Galerkin methods on meshes consisting of polygonal/polyhedral (polytopic) elements. The new a-posteriori error estimators are robust with respect to polygonal elements with edge/face degenerations in *hp* setting. Additionally, the new a posteriori error estimator can be bounded from above by the classical a-posteriori error estimator not only on the polytopic meshes but also on simplicial and tensor-product meshes. The new error estimator does not impose any restrictions on the positon of hanging nodes. We will present numerical examples to demonstrate the performance of the proposed estimator on polytopic meshes.

HIGH-ORDER MULTISCALE DISCONTINUOUS GALERKIN METHODS FOR THE ONE-DIMENSIONAL STATIONARY SCHRÖDINGER EQUATION

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We develop high-order multiscale discontinuous Galerkin (DG) methods for one-dimensional stationary Schrödinger equations with oscillating solutions. We propose two types of multiscale finite element spaces and prove that the resulting DG methods converge optimally with respect to the mesh size h in L^2 norm when h is small enough. In the lowest order case, we prove that the second order multiscale DG method has the optimal convergence even when the mesh size is larger than the wave length. Numerically we observe that all these multiscale DG methods have at least second-order convergence on coarse meshes and optimal high-order convergence on fine meshes.

DISCONTINUOUS GALERKIN METHODS FOR THE BIHARMONIC PROBLEM ON POLYGONAL AND POLYHEDRAL MESHES

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We introduce an *hp*-version symmetric interior penalty discontinuous Galerkin finite element method (DGFEM) for the numerical approximation of the biharmonic equation on general computational meshes consisting of polygonal/polyhedral (polytopic) elements. In particular, the stability and *hp*-version a-priori error bound are derived based on the specific choice of the interior penalty parameters which allows for edges/faces degeneration. Furthermore, by deriving a new inverse inequality for a special class of polynomial functions (harmonic polynomials), the proposed DGFEM is proven to be stable to incorporate very general polygonal/polyhedral elements with an arbitrary number of faces for polynomial basis with degree $p = 2, 3$. The key feature of the proposed method is that it employs elemental polynomial bases of total degree $\mathcal{P}_p$, defined in the physical coordinate system, without requiring the mapping from a given reference or canonical frame. Additionally, I will briefly talk about the multigrid algorithm for the propsed DGFEM. A series of numerical experiments are presented to demonstrate the performance of the proposed DGFEM on general polygonal/polyhedral meshes.

A GENERAL NUMERICAL ANALYSIS FRAMEWORK FOR LINEAR AND NON-LINEAR FOURTH-ORDER PROBLEMS

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Fourth-order problems, both linear and non-linear, appear in various domains of mechanics. They model for example thin plates deformations (small or large), as well as 2D turbulent flows through the vorticity formulation of Navier-Stokes equations. Many numerical methods, most of them Finite Elements, have been developed over the years to approximate the solutions of these models. Each method comes with its own convergence analysis carried out using *ad-hoc* arguments.

In this talk, we will present the Hessian Discretisation Method (HDM), a generic analysis framework that encompasses many classical and some less classical numerical methods for fourth-order problems: conforming Finite Elements, non-conforming Finite Elements, methods based on gradient recovery operators, and even Finite Volume-based schemes. The principle of the HDM is to describe a numerical method using a set of four discrete objects, together called a Hessian Discretisation (HD): the space of unknowns, and three operators reconstructing respectively a function, a gradient and a Hessian. Each choice of HD corresponds to a specific numerical scheme. The beauty of the HDM framework is to identify four model-independent properties on an HD that ensure that the corresponding scheme converges for a variety of models, linear as well as non-linear. The HDM is an extension to fourth-order equations of the Gradient Discretisation Method [1], developed for linear and non-linear second-order elliptic and parabolic problems.

We will detail the unified error estimates and convergence analysis that can be obtained using the HDM. For linear models, optimal error estimates can be established [2]. For non-linear models, compactness techniques show the convergence of the HDM without assuming any regularity property on the continuous solution; in some cases (when the continuous solution is non-singular and smooth enough, and when a 'companion' operator can be found for the considered numerical scheme), error estimates can be established [3].

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A HYBRID-HIGH ORDER METHOD FOR THE BRINKMAN MODEL, UNIFORMLY ROBUST IN THE STOKES AND DARCY LIMITS

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The Hybrid High-Order method (HHO) is a recently developed numerical method for diffusion problems [4]. Several key features sets it appart from classical schemes for such models: applicability to generic polygonal and polyhedral meshes, arbitrary order, and easy parallelisability due to its local stencil. The unknowns of the HHO method are (broken) polynomials of degree $k \geq 0$ in mesh elements and on mesh faces. Its construction hinges on local high-order polynomial reconstructions, as well as local stabilisation terms carefully design to preserve the optimal approximation properties of the high-order reconstructions. The typical order of convergence of the HHO method is $(k+1)$ in energy norm. A detailed presentation of the HHO method can be found in the manuscript [2].

In this talk, we will present an HHO method for the Brinkman model, which is an intermediate model between a free flow (Stokes model) and a porous medium flow (Darcy model). These two models are recovered in the limits of vanishing viscosity or permeability. The HHO scheme for the Brinkman model is designed selecting appropriate reconstructions and stabilisations for each component (Stokes and Darcy terms) [1]. The third Strang lemma [3] enables an error estimate for the scheme that highlights a novel physical parameter, the friction coefficient, which measures the (local) proximity of the Brinkman model to each of its limits. Thanks to this coefficient, we can establish an optimal error estimate that is fully robust in both the Stokes and Darcy limit – preserving the optimal convergence order $(k+1)$ in both limits. To our knowledge, no previous numerical analysis of the Brinkman model achieved such robust estimates. The efficiency and practical robustness of the scheme will also be illustrated through numerical results.

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APPROXIMATING MAXWELL EIGENPROBLEM BY A FAMILY OF LAGRANGE ELEMENTS OF ANY ORDER

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In this talk, we propose and study a family of new Lagrange finite element methods for two-dimensional indefinite time-harmonic Maxwell equations and Maxwell eigenproblem. This family of Lagrange elements of polynomials P_ℓ of any order $\ell \geq 1$ can approximate singular solution of H^r regularity with $r < 1$ as well as smooth solution of H^{1+s} regularity with $s \geq 0$, or they are suitable for nonsmooth domains(e.g., nonconvex domains with reentrant corners). We develop a theory for the well-posedness of the proposed finite element method; particularly, the inf-sup condition in the Bubuška sense is established for the indefinite time-harmonic Maxwell equations. Optimal error bounds are obtained for singular solution as well as smooth solution. When applied to the Maxwell eigenproblem, it is shown that this family of Lagrange elements of polynomials P_ℓ of any order $\ell \geq 1$ are all spectral-correct and spurious-free. The spectral theory we have developed for the proposed finite element method includes the key property—the so-called discrete compactness. Consequently, this family of Lagrange elements are particularly very useful for the Maxwell eigenproblem. We must note that the Maxwell eigenproblem is quite different from other eigenvalue problems, because it may have infinitely many singular solutions of H^r regularity for $r < 1$ and may have infinitely many smooth solutions of H^{1+s} regularity for $s \geq 0$; also because there exist some finite element methods of the Maxwell eigenproblem which wrongly approximate the continuous eigenmodes and produce spurious discrete eigenmodes. A quite number of numerical results for the Maxwell eigenproblem on nonsmooth domains are presented for justifying the proposed methods of a family of Lagrange elements and for confirming the theoretical results obtained.

INVERSE PROBLEMS AND HYBRID OPTIMIZATION ALGORITHMS

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Inverse problems are classified as problems with unknown: a) shapes and sizes of the domains, b) boundary and/or initial conditions, c) singularities in /on the domain, d) physical properties of the media, and e) governing system of equations. These types of problems can be solved when additional information, such as over-specified boundary conditions, are provided and enforced. For example, unknown boundary conditions on arbitrary 3D solid objects can be accurately determined non-iteratively for linear models and iteratively for non-linear models where it requires regularization. Similarly, spatial distribution of material properties in arbitrarily shaped, multiply-connected 3D solid objects can be non-destructively determined by minimizing the sum of normalized least-squares differences between measured and calculated boundary values of the field variables. This means also accounting for measurements containing varying levels of noise. These methods can also be used to detect locations, sizes and shapes of unknown domains. The least squares differences between calculated and measured/enforced values was minimized using a cluster of optimization algorithms assembled in a hybrid optimization tool where a set of heuristic rules was used to perform automatic switching among the individual optimizers in order to avoid local minima, escape from the local minima, converge on the global minimum, and reduce the overall computing time. Examples of solved inverse problems governed by systems of ordinary and partial differential equations will be presented with applications in heat transfer, elasticity, aerodynamics, epidemiology, electro-chemistry, and electro-magneto-hydro-dynamics with solidification.

This work was partially supported by the NASA University Leadership Initiative (ULI) program under federal award number NNX17AJ96A, titled Adaptive Aerostructures for Revolutionary Civil Supersonic Transportation".

APPROXIMATION OF TIME DOMAIN BOUNDARY INTEGRAL EQUATIONS

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Time domain boundary integral equations (TDBIEs) are used to model time dependent wave scattering from surfaces in an infinite, homogeneous medium. We concentrate on the acoustic scattering case. The solution can be reconstructed anywhere in space and time in terms of a potential which is computed only on the surface. The approximation of the time dependent surface potential by numerical methods is expensive and sensitive to stability issues, but it can be cheaper than solving the wave equation in a very large space domain. We describe a practical implementation of a full space-time Galerkin TDBIE method derived and analysed by Ha Duong, and its connection with a simpler method, derived by Davies and Duncan, using "backward-in-time" collocation coupled with Galerkin in space.

UNSTRUCTURED CVD-MPFA REDUCED-DIMENSIONAL DFM FINITE-VOLUME METHODS FOR TWO-PHASE FLOW, COUPLED WITH HIGHER RESOLUTION HYBRID UPWIND AND SPECTRAL-VOLUME METHODS

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Objectives/Scope: Novel discrete fracture model (DFM) approximations are presented and coupled with the control-volume distributed multi-point flux approximation (CVD-MPFA) formulation. The reduced-dimensional discrete discontinuous pressure models for intersecting fractures are extended to two-phase flow, including gravity and discontinuous capillary pressure. Higher resolution hybrid upwind methods provide improved flow resolution on unstructured grids. A novel spectral-volume based method with sub-cell resolution is also presented. Performance comparisons are presented for tracer and two-phase flow and fracture problems involving discontinuous capillary pressure and gravity on unstructured meshes. The results demonstrate the importance of the new higher resolution methods coupled with DFM to resolve flow problems including oil trapping in fractures. In addition comparisons between the standard lower order method, the higher resolution hybrid upwind scheme and spectral-volume method shows that the higher resolution methods yields significantly improved flow resolution, which is further enhanced by the spectral-volume method.

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SOME THOUGHTS ON ADAPTIVE STOCHASTIC GALERKIN FEM

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The numerical treatment of random PDEs as examined in Uncertainty Quantification is challenged by the high dimensionality of the problem. The data of the model is commonly characterised by a countable infinite sequence of random variables. However, it is well-known that for many model problems the solution manifold exhibits favourable properties, in particular sparsity and low-rank approximability. In order to practically construct surrogate models, these properties have to be exploited adequately. A successful approach for this task is the stochastic Galerkin FEM steered by an a posteriori error estmation, which has been shown to achieve optimal rates when an affine parameter dependence is assumed.

In this talk we consider two recent extensions with adaptive stochastic Galerkin methods. First, more general coefficients (e.g. lognormal) represented in hierarchical tensor formats are examined. Although the complexity increases substantially, the tensor compression still allows for an efficient computation of an adaptive algorithm. Second, a statistical learning framework (Variational Monte Carlo) for random PDEs is presented. It enables the treatment of very general problems and computes the Galerkin solution with high probability.

NONLOCAL (AND LOCAL) NONLINEAR DIFFUSION EQUATIONS. BACKGROUND, ANALYSIS, AND NUMERICAL APPROXIMATION

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We will consider finite-difference schemes for nonlocal (and local) nonlinear diffusion equations posed in $\mathbb{R}^N \times (0,T)$. Properties needed to perform numerical analysis are going to be discussed. The numerical approximations will converge to the solutions of the equations studied under minimal assumptions including assumptions that lead to very irregular solutions. In other words, the schemes we introduce are robust in the sense that they converge under very unfavourable conditions. Numerical simulations will also be presented.

MULTIGOAL-ORIENTED ERROR CONTROL FOR OPTIMAL CONTROL PROBLEMS

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In this presentation, we consider an optimal control problem subject to a nonlinear PDE constraint such as the p-Laplace equation. We are interested in a posteriori error estimates for multiple quantities of interest. We combine all quantities to one and apply the dual-weighted residual (DWR) method to this combined functional. These a posteriori error estimates are then used for mesh adaptivity. In addition, the estimator allows for balancing the discretization error and the nonlinear iteration error. Several numerical examples demonstrate the excellent performance of our approach.

This work has been supported by the Austrian Science Fund (FWF) under the grant P 29181Goal-Oriented Error Control for Phase-Field Fracture Coupled to Multiphysics Problems in collaboration with the DFG-SPP 1962 Non-smooth and Complementarity-Based Distributed Parameter Systems: Simulation and Hierarchical Optimization.

OPTIMAL ERROR ESTIMATES FOR THE SEMI-DISCRETE OPTIMAL CONTROL PROBLEM OF THE WAVE EQUATION WITH TIME-DEPENDING BOUNDED VARIATION CONTROLS

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We will consider a control problem (P) for the wave equation with a standard tracking-type cost functional and a semi-norm in the space of functions with bounded variations (BV) in time. The considered controls in BV act as a forcing function on the wave equation with homogeneous Dirichlet boundary. This control problem is interesting for practical applications because the semi-norm enhances optimal controls which are piecewise constant.

In this talk we focus on a finite element approximation of (P). In this semi-discretized version, only the state equation is discretized and the controls will not be changed. Under specific assumptions we can present optimal convergence rates for the controls, states, and cost functionals.

COMPUTATION OF SCATTERING RESONANCES IN ABSORPTIVE AND DISPERSIVE MEDIA

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Scattering resonances that refer to a meta-stable behavior in time are for open resonators a natural replacement of eigenvalues for closed systems. The most common finite element methods to approximate scattering resonances uses a perfectly matched layer, infinite elements, or a Dirichlet-to-Neumann map. However, these methods encounter severe spectral instability, which in general results in a large number of spurious (unphysical) eigenvalues in addition to approximations of true scattering resonances. Those spurious solutions are a major problem in scattering resonance computations.

In this talk, we consider Helmholtz type of scattering resonance problems in several dimensions with piecewise constant coefficients as well as graded material properties. For electromagnetic problems we assume that the resonators consist of frequency dependent and lossy materials, such as metals at optical frequencies.

Volume integral based methods are in principle applicable and we encounter, in contrary to the differential operator based methods, no spurious solutions in scattering resonance computations. However, this approach is computationally very demanding, in particularly in higher dimensions. Therefore, we compute first approximations of scattering resonances of a differential operator and use a volume integral equation as residual for removing spurious solutions. This is a joint work with Juan Carlos Araujo-Cabarcas.

EXPONENTIAL CONVERGENCE IN H^1 OF HP-FEM FOR GEVREY REGULARITY WITH ISOTROPIC SINGULARITIES

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For functions $u \in H^1(\Omega)$ in a bounded polytope $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$ which are Gevrey regular in $\overline{\Omega}\backslash\mathcal{S}$ with point singularities concentrated at a set $\mathcal{S} \subset \overline{\Omega}$ consisting of a finite number of points in $\overline{\Omega}$, we prove exponential rates of convergence of hp-version continuous Galerkin finite element methods on families of regular, simplicial meshes in Ω. The simplicial meshes are geometrically refined towards $\mathcal{S}$ but are otherwise unstructured.

IMPROVED EFFICIENCY OF MULTI-INDEX FEM

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We propose a multi-index algorithm for the Monte Carlo (MC) discretization of a linear, elliptic PDE with affine-parametric input. We prove an error vs. work analysis which allows a multi-level finite-element approximation in the physical domain, and apply the multi-index analysis with isotropic, unstructured mesh refinement in the physical domain for the solution of the forward problem, for the approximation of the random field, and for the Monte-Carlo quadrature error. Our approach allows Lipschitz domains and mesh hierarchies more general than tensor grids. The improvement in complexity over multi-level MC FEM is obtained from combining spacial discretization, dimension truncation and MC sampling in a multi-index fashion. Our analysis improves cost estimates compared to multi-level algorithms for similar problems and mathematically underpins the superior practical performance of multi-index algorithms for partial differential equations with random coefficients.

ON THE STABILITY OF THE SPACE-TIME DISCONTINUOUS GALERKIN METHOD FOR NONLINEAR PARABOLIC PROBLEMS IN TIME DEPENDENT DOMAINS

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The paper is devoted to the analysis of the space-time discontinuous Galerkin method (STDGM) applied to the numerical solution of nonstationary nonlinear convection-diffusion initial-boundary value problem in a time-dependent domain. The problem is reformulated using the arbitrary Lagrangian-Eulerian (ALE) method, which replaces the classical partial time derivative by the so-called ALE derivative and an additional convective term. The problem is discretized with the use of the ALE-space time discontinuous Galerkin method (ALE-STDGM). In the formulation of the numerical scheme we use the nonsymmetric, symmetric and incomplete versions of the space discretization of diffusion terms and interior and boundary penalty. The nonlinear convection terms are discretized with the aid of a numerical flux. The goal is to prove the unconditional stability of the method. An important step is the generalization of a discrete characteristic function associated with the approximate solution and the derivation of its properties. It is important that the ALE technique can use different meshes on different time levels and different ALE mappings are prescribed for time slabs separately.

ENFORCING DISCRETE MAXIMUM PRINCIPLES IN DG SCHEMES FOR SCALAR CONSERVATION LAWS

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Many mathematical CFD models involve transport of conserved quantities that must lie in a certain range to be physically meaningful. The solution u of a scalar conservation law is said to satisfy a maximum principle (MP) if global bounds $u_{\min}$ and $u_{\max}$ exist such that $u_{\min} \leq u(t, \mathbf{x}) \leq u_{\max}$. To enforce such inequality constraints for DG solutions at least for element averages, the numerical fluxes must be defined and constrained in an appropriate manner. We introduce a general framework for calculating fluxes that produce non-oscillatory DG approximations and preserve the MP for element averages even if the exact solution of the PDE violates them due to modeling errors or perturbed data. The proposed methodology is based on a combination of flux and slope limiting: The flux limiter constrains changes of element averages so as to prevent violations of global bounds. The subsequent slope limiting step adjusts the higher order solution parts to impose local bounds on pointwise values of the high-order DG solution. Since manipulations of the target flux may introduce a consistency error, it is essential to guarantee that physically admissible fluxes remain unchanged. The novel fractional step flux limiting approach is iterative while in each iteration, the MP property is guaranteed and the consistency error is reduced. Practical applicability is demonstrated by numerical studies for the advection equation (hyperbolic, linear) and the Cahn–Hilliard equation (parabolic, nonlinear). The flux limiter (similar to slope limiter) is a local/parallelizable postprocessing procedure that can be applied to various types of DG discretizations of a wide range of scalar conservation laws.

AN ADAPTIVE NEWTON ALGORITHM FOR OPTIMAL CONTROL PROBLEMS WITH APPLICATION TO OPTIMAL ELECTRODE DESIGN

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We present an adaptive Newton algorithm to solve nonlinear constrained optimisation problems, where the constraint is a system of partial differential equations discretised by the finite element method. The adaptive strategy relies on goal-oriented *a posteriori* error estimates for both the discretisation and the iteration error and builds on the work of Rannacher & Vihharev in the context of nonlinear PDEs (J Numer Math 21(1), 23 62, 2013). The estimation of the iteration error allows us to derive effective stopping criteria for the Newton iterations based on a balancing of iteration and discretisation errors.

The performance of the algorithm is shown for several numerical examples. In particular, we consider the optimisation of electrodes that are used by our medical collaborators to visualise the structure of neuronal networks.

A UNIFIED NITSCHE APPROACH FOR FLUID-STRUCTURE INTERACTIONS AND CONTACT

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We develop Nitsche-based formulations for fluid-structure interaction (FSI) problems with contact. Our approach to model contact is based on the works of Chouly and Hild (SIAM J Numer Anal 51(2):1295–1307, 2013) for contact problems in solid mechanics. Using a suitable extension of the fluid equations below the contact surface, we are able to formulate the FSI interface and the contact conditions simultaneously in equation form on a joint interface-contact surface $\Gamma(t)$. Due to the continuous switch between interface and boundary conditions, the so-called "chattering" phenomenon known in the engineering literature, is prevented.

To deal with the topology changes in the fluid domain at the time of impact, we use a fully Eulerian approach for the FSI problem. We show a stability result and present numerical examples to investigate the performance of the method.

A CONFORMING C^1 FINITE ELEMENT METHOD FOR PDES OF MONGE-AMPÈRE TYPE

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PDEs of Monge-Ampère type arise in the context of optimal transport (OT) problems and related problems in optics. To numerically solve such a fully nonlinear partial differential equation (PDE) usually two processes are involved, a linearisation, e.g. a Newton method, and a discretisation procedure. The question is, how to intertwine these processes? Using a finite element discretisation with C^1 elements renders this question redundant, as the order of performing linearisation and discretisation is commutable [2].

In this talk we present such a C^1 conforming finite element method applicable to equations like

$$\det(D^2u) - \frac{f}{g(\nabla u)} = 0 \qquad \text{in } \Omega, \tag{1}$$

where Ω is a bounded convex domain and $f, g > 0$ are functions such that $\int f = \int g$.

Hereto, we test the PDE (1) in an L^2 sense, linearise and discretise it and finally evaluate it on the C^1-continuous S-spline basis. These trial elements originally were developed in a computer graphics context [1] and are constructed as macro elements, i.e. they are defined piecewise on the reference cell. Thus, their degree can be chosen lower than that of the standard quintic Argyris elements.

Reformulating OT problems yields (1) complemented by nonlinear, so-called transport boundary conditions. We discuss how to enforce these boundary conditions in the context of the C^1 method. The resulting algorithm provides geometric flexibility and high order of approximation for smooth solutions.
In order to solve practically relevant OT problems, we identify the critical parts of the input data and introduce stabilisation techniques within a nested iteration process. We conclude by applying the algorithm to practically relevant mirror and lens design problems.

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VIRTUAL ELEMENT METHOD FOR ELLIPTIC AND PARABOLIC BULK-SURFACE PDES IN TWO DIMENSIONS

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We present a novel method for the numerical approximation of elliptic and parabolic bulk-surface PDEs in two dimensions. To the best of the authors' knowledge, the proposed method is the first application of the Virtual Element Method [1] to bulk-surface PDEs. The method is based on the discretisation of the bulk into polygonal elements with arbitrarily many edges, rather than just triangles. The bulk-surface finite element method on triangular meshes [2] is a special case of the proposed method. The advantage is twofold. First, we show that the ability of the new method of handling general polygons can be exploited to reduce the computational complexity of matrix assembly. Second, we introduce an optimised matrix implementation that can be also exploited in the pre-existing special case of bulk-surface finite elements on triangular meshes [2]. Numerical examples illustrate our findings and experimentally show the optimal convergence rate in space and time.

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A LEAST-SQUARES FINITE ELEMENT METHOD FOR THE OBSTACLE PROBLEM

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In this talk we present recent results on a least-squares finite element method for a first-order reformulation of the obstacle problem. A priori error estimates including the case of non-conforming convex sets are given and optimal convergence rates are shown for the lowest-order case. We provide a posteriori bounds that can be used as error indicators in an adaptive algorithm. Numerical studies are presented.

MULTI-MATERIAL TOPOLOGY OPTIMIZATION BASED ON TOPOLOGICAL DERIVATIVES

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We present a topology optimization method for multiple materials which is based on the concept of topological derivatives. Here, the design, which consists of more than two materials, is represented in an implicit way by a vector-valued level set function. We show a sufficient optimality condition and an iterative algorithm which is based on this condition. Finally, we show numerical results for an academic example, where the the optimal design consists of an arbitrary, but fixed number of materials, as well as for a real world problem, the optimization of an electric motor consisting of three different materials.

CONFORMING AND NONCONFORMING VIRTUAL ELEMENT METHODS FOR EIGENVALUE PROBLEMS

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We analyse the conforming and nonconforming Virtual Element Method (VEM) [1, 2, 3, 4] for the approximation of second order elliptic eigenvalue problems. As a model problem we consider the Laplace eigenvalue problem. We present two possible formulations of the discrete problem, derived respectively by a nonstabilized and stabilized approximation of the L^2-inner product, and we study the convergence properties of the corresponding discrete eigenvalue problem. The proposed schemes provide a correct approximation of the spectrum, in particular we prove optimal-order error estimates for the eigenfunctions and the usual double order of convergence of the eigenvalues. Moreover, we show a large set of numerical tests supporting the theoretical results, including a comparison between the conforming and the nonconforming schemes and present some possible applications of the theory.

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A LAGRANGE MULTIPLIER FORMULATION OF THE FINITE ELEMENT IMMERSED BOUNDARY METHOD

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The approach of the fluid-structure interaction problem with the fictitious method is originated from the finite element version of the Immersed Boundary Method (FE-IBM) developed by Peskin in the finite difference framework. Actually, the introduction of a Lagrange multiplier allows to consider the FE-IBM as a Fictitious Domain formulation for FSI. At each time step a steady problem in mixed form has to be solved. Existence and uniqueness results for suchsolution have been proved. We are going to present some results on the analysis of the scheme including error estimates both in time and space and the stability of a time splitting approach. At the end, we shall show how our technique can handle the case of compressible solids as well.

C^0 INTERIOR PENALTY METHODS FOR AN OPTIMAL CONTROL PROBLEM ON NONCONVEX POLYGONAL DOMAINS

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In this talk we design and analyze C^0 interior penalty methods for an elliptic distributed optimal control problem on nonconvex polygonal domains with pointwise state constraints. We reformulate the elliptic distributed optimal control problem with pointwise state constraints as a fourth order variational inequality. For convex domains Ω this approach has been analyzed in [2]. In this talk we generalize this approach to nonconvex domains Ω with solutions in the space $\mathring{E}(\Omega;\Delta) = \{y \in H_0^1(\Omega) \ : \ \Delta y \in L_2(\Omega)\}$, where Δy is understood in the sense of distributions. The fourth order obstacle problem is discretized with the C^0 interior penalty method enriched by suitable approximations of singular functions at re-entrant corners. We present convergence results for uniform and graded meshes. Numerical results demonstrate the proven convergence rates for two exemplary nonconvex domains.

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IMPROVEMENTS TO THE TREECODE-ACCELERATED BOUNDARY INTEGRAL (TABI) POISSON-BOLTZMANN SOLVER

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The Poisson-Boltzmann (PB) model is an effective implicit solvent approach for simulating solvated biomolecular systems. By treating the solvent with a mean field approximation and capturing the mobile ions with the Boltzmann distribution, the PB model largely reduces the degree of freedom and computational cost. However, solving the PB equation suffers from many numerical difficulties arising from interface jump conditions, complex geometry, charge singularities, and boundary conditions at infinity. In addressing these difficulties, we recently developed a treecode-accelerated boundary integral (TABI) solver for solving Poisson-Boltzmann (PB) equation. The solver has combined advantages in accuracy, efficiency, memory, and parallelization as it applies a well-posed boundary integral formulation to circumvent many numerical difficulties associated with the PB equation and uses an O(N*log(N)) treecode to accelerate the GMRES iterative solver. In this talk, we report our recent improvements to the TABI solver including parallelization, precondition, and surface triangulation. In addition, we provide some biological applications such as the calculation of binding energy and pKa values.

HYPOCOERCIVITY COMPATIBLE HP-FEM FOR KINETIC EQUATIONS

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We present a family of *hp*-version Galerkin finite element methods for Kolmogorov and Fokker-Planck equations. These serve as a sufficiently rich, for our purposes, class of model problems for kinetic-type equations, characterised by diffusion in *some, but not all,* spatial directions only. Nonetheless, solutions to such equations can decay properties to some long time equilibrium, depending on closure by suitable boundary/decay-at-infinity conditions. Our aim is to transfer this fundamental property to general numerical methods methods for very general families of triangulations. The method construction uses ideas by the general theory of *hypocoercivity* developed by Villani (see, e.g., Villani's "Hypocoercivity" Memoir AMS 2009) along with judicious choice of numerical flux functions. These developments turn out to be sufficient to imply that the proposed finite element methods admit a priori error bounds with constants *independent of the final time*, despite such equation's degenerate diffusion nature. Thus, the new methods provably allow for robust error analysis for final times tending to infinity.

HP-VERSION DISCONTINUOUS GALERKIN METHODS ON ESSENTIALLY ARBITRARILY-SHAPED ELEMENTS AND THEIR IMPLEMENTATION

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We extend the applicability of the popular interior-penalty discontinuous Galerkin (dG) method discretizing advection-diffusion-reaction problems to meshes comprising of extremely general, essentially arbitrarily-shaped element shapes. In particular, our analysis allows for *curved* element shapes, arising, *without* the use of (iso-)parametric elemental maps. The feasibility of the method relies on the definition of a suitable choice of the discontinuity-penalization parameter, which turns out to be essentially independent on the particular element shape. A priori error bounds for the resulting method are given under very mild structural assumptions restricting the magnitude of the local curvature of element boundaries. Numerical experiments are also presented, indicating the practicality of the proposed approach. This work generalizes our earlier work detailed in the monograph [1] from polygonal/polyhedral meshes to essentially arbitrary element shapes involving curved faces without imposing any additional mesh conditions.

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LARGE-SCALE STOCHASTIC PDE-CONSTRAINED OPTIMIZATION

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We consider optimization problems governed by PDEs with infinite dimensional random parameter fields. Such problems arise in numerous applications: optimal design and control of systems with stochastic forcing or uncertain material properties or geometry; inverse problems with stochastic forward problems; or Bayesian optimal experimental design problems with the goal of minimizing the uncertainty or maximizing the information gain in the inferred parameters.

Monte Carlo evaluation of the objective as per the popular Sample Average Approximation (SAA) algorithm results in an optimization problem that is constrained by N PDE systems, where N is the number of samples. This results in an optimization problem that is prohibitive to solve, especially when the PDEs are "complex" (e.g., large-scale, nonlinear, coupled) and discretization of the infinite-dimensional parameter field results in a high-dimensional parameter space.

We discuss high-order derivative-based approximations of the parameter-to-objective maps that exploit the structure of these maps, in particular their smoothness, geometry, and low effective dimensionality. Their use as a basis for variance reduction, in combination with randomized linear algebra algorithms, is demonstrated to accelerate Monte Carlo sampling by up to three orders of magnitude and permit efficient solution of large scale stochastic PDE-constrained optimization problems with up to with $O(10^6)$ uncertain parameters and $O(10^6)$ optimization variables. Applications to optimal control of turbulent flow and optimal design of acoustic metamaterials are presented.

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A DISCONTINUOUS GALERKIN METHOD FOR SOLVING ELLIPTIC EIGENVALUE PROBLEMS ON POLYGONAL MESHES WITH HP-ADAPTIVITY

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We present a discontinuous Galerkin method for solving elliptic eigenvalue problems on polygonal meshes [1] based on the discontinuous Galerkin composite finite element method (DGCFEM) [2]. In this talk, the key idea of generally shaped element domains in DGCFEM is used to construct polygonal elements and applied to eigenvalue problems. Polygonal and polyhedral meshes are advantageous to discretize domains of complicated shape reducing the overall number of elements needed.

A priori convergence analysis is presented for the method and tested on several numerical examples. Some of the numerical examples use non-convex elements that could be considered pathological in the finite element context.

Further, adaptive techniques are presented for DGCFEM and applied to complicated domains [3]. The mesh-adaptivity is based on a residual error estimator specific for DGCFEM. The robustness and accuracy of the adaptive techniques are supported by numerical examples. Interestingly, the convergence rate of the *hp*-adaptive technique is exponential also for polygonal meshes.

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HP-ADAPTIVE CELATUS ENRICHED DISCONTINUOUS GALERKIN METHODS FOR SECOND-ORDER ELLIPTIC SOURCE PROBLEMS

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A new method to enrich discontinuous Galerkin (DG) finite element spaces with non-polynomial functions is presented [1]. The new approach is called "celatus" that in Latin means "hidden from view" in order to emphasise that the enrichment is done without adding any non-polynomial function to the finite element DG space. Rather, the approximation of the non-smooth part of the solution is done solving an optimisation problem aiming to minimize the value of the a posteriori error estimator. In this way, many issues with standard enriched methods are avoided, among which there is the worsening of the condition of the linear system. The optimisation problem is constructed in such a way to try to capture the non-smooth part of the solution outside the finite element space. Smaller is the portion of the non-smooth part of the solution in the finite element space, smaller is the value of the error estimator since polynomial finite element methods have difficulties to approximate non-smooth functions. The resulting method converges very fast, even faster than standard hp-adaptive methods.

As for all enriched methods, the best performances can be obtained if the span of the enriched functions contains the non-smooth part of the solution to approximate. Therefore, some prior knowledge about the considered problem is necessary. However, compared to other enriched methods, the celatus method is more robust because if the enrichment fails to capture the non-smooth part of the solution, the hp-adaptivity steps in and a good approximation of the solution is computed anyway.

In the presentation, the method is applied to second-order elliptic source problems with re-entering corners. A series of numerical examples, some of them with multiple re-entering corners, is presented.

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ADAPTIVE CRACK TIP TRACKING AND FRACTURE SIMULATION USING COUPLED FE MESHES AND PD GRIDS

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Bond-Based Peridynamics (PD) is a nonlocal method for solid mechanics introduced by Silling [S. A. Silling, "Reformulation of elasticity theory for discontinuities and long-range forces," J. Mech. Phys. Solids, vol. 48, no. 1, pp. 175 209, 2000]. The PD theory has two properties that are very attractive for fracture problems: i) its formulation is based on an integrodifferential equation that avoids the use of spatial derivatives and ii) fracture is simulated by the consecutive breaking of bonds. As such, no special treatment is required for the discontinuous displacement fields that appear and circumvent the need for additional external phenomenological criteria to define crack nucleation and propagation.

However, implementation of the PD theory can be restrictive, particularly for large scale simulations due to its high computational cost [F. Han, G. Lubineau, and Y. Azdoud, "Adaptive coupling between damage mechanics and peridynamics: a route for objective simulation of material degradation up to complete failure," J. Mech. Phys. Solids, vol. 94, pp. 453 472, 2016]. A possible strategy to overcome this limitation is to combine finite element (FE) meshes with PD grids. This strategy tries to combine the efficiency and robustness of FE with the ability of PD to simulate fracture. However, as reported in the relevant literature, spurious reflections appear when pulses cross the coupling interface [J. Fish,*Multiscale methods: bridging the scales in science and engineering*. Oxford University Press on Demand, 2010].

In the present study a methodology is presented for the simulation of fracture using coupled FE meshes with PD grids. The difference between the proposed method and similar approaches in the literature, e.g. [M. Zaccariotto, D. Tomasi, and U. Galvanetto, "An enhanced coupling of PD grids to FE meshes," Mech. Res. Commun., vol. 84, pp. 125 135, 2017] and [T. Ni, M. Zaccariotto, Q.-Z. Zhu, and U. Galvanetto, "Static solution of crack propagation problems in Peridynamics," Comput. Methods Appl. Mech. Eng., vol. 346, pp. 126 151, 2019] is that the proposed method has the ability to adaptively relocate the position of the PD domain, following the crack propagation. Thus, no *a priori* knowledge of the crack path is required. Additionally, the use of XFEM enrichment for elements that are cut by the crack body allows for an adaptive relocation without remeshing the FEs [T. L. Anderson, Fracture mechanics: fundamentals and applications. CRC press, 2017]. The method is applied to the simulation of static and dynamic problems and the results are compared with similar numerical and experimental studies.

NUMERICAL METHODS FOR MAXWELL'S EQUATIONS WITH RANDOM POLARIZATION

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Electromagnetic wave propagation in complex dispersive media is governed by the time dependent Maxwell's equations coupled to equations that describe the evolution of the induced macroscopic polarization, so-called Auxiliary Differential Equations (ADE). We consider "polydispersive" materials represented by distributions of dielectric parameters in a polarization model. The work focuses on the novel computational framework for such problems introduced in [1], involving Polynomial Chaos Expansions as a method to improve the modeling accuracy of the ADE model and allow for easy simulation using standard numerical methods. We discuss generalizations of the approach and stability and dispersion analyzes of the resulting fully discrete schemes.

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MODEL-ADAPTIVE DISCONTINUOUS GALERKIN SCHEMES FOR COMPRESSIBLE FLUID FLOWS

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We study numerical schemes for compressible fluid flows with a focus on using discretizations of different models in different parts of the computational domain. The underlying principle is that most (physical) processes can be described by a variety of models that differ in their levels of complexity and detail. One example is fluid flows in bounded domains where the viscosity of the fluid is certainly the same throughout the domain but in many cases it only needs to be accounted for close to boundaries. Another example is fluid mixtures where models can either account for chemical reactions or can assume chemical equilibrium. In most of these cases, the more detailed model is numerically much more expensive than the less accurate model and, for constructing efficient numerical schemes, it seems desirable to use the complex model only where is is necessary and the simpler model wherever it is sufficient. The obvious difficulty in this approach is how to decide which model to use in an objective and automatizable manner. We suggest to approach this question by deriving a posteriori error estimates for modelling errors, i.e., estimators for the difference between solutions to both models.

For the numerical implementation of this approach, which can be seen as dynamical and heterogeneous domain decompositions, different models need to be solved on different parts of the computational domain and they need to be coupled at their boundaries. Discontinuous Galerkin schemes are a well-established tool for simulations of compressible fluid flows which allow us to discretize the different models in a systematic way and which provide the flexibility to properly couple the different models. Finally, efficient numerical simulations do not only require model adaptation but also mesh adaptation. In order to enable simultaneous model and mesh adaptation we extend our error estimates such that it also accounts for discretization errors.

MULTILEVEL QUASI-MONTE CARLO METHODS FOR RANDOM ELLIPTIC EIGENVALUE PROBLEMS

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Motivated by uncertainty quantification for the neutron diffusion criticality problem, we will study an elliptic eigenvalue problem with coefficients that depend on infinitely many stochastic parameters. The stochasticity in the coefficients causes the eigenvalues and eigenfunctions to also be stochastic, and so our goal is to compute the expectation of the minimal eigenvalue. In practice, to approximate this expectation one must: 1) truncate the stochastic dimension; 2) discretise the eigenvalue problem in space (e.g., by finite elements); and 3) apply a quadrature rule to estimate the expected value.

In this talk, we will present a multilevel Monte Carlo method for approximating the expectation of the minimal eigenvalue, which is based on a hierarchy of finite element meshes and truncation dimensions. To improve the sampling efficiency over Monte Carlo we will use a quasi-Monte Carlo rule to generate the sampling points. Quasi-Monte Carlo rules are deterministic (or quasi-random) quadrature rules that are well-suited to high-dimensional integration and can converge at a rate of $1/N$, which is faster than the rate of $1/\sqrt{N}$ for Monte Carlo. Also, to make each eigenproblem solve on a given level more efficient, we utilise two-grid scheme from to obtain the eigenvalue on the fine mesh from the coarse eigenvalue (and eigenfunction) with a single linear solve.

A FAST DIRECT SOLVER FOR SCATTERING PROBLEMS IN QUASI-PERIODIC LAYERED MEDIUM

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Being able to accurately and efficiently solve quasi-periodic scattering problems involving multi-layered medium is important for the design of composite materials. This talk presents a fast direct solver for the linear system that results from discetizing a robust integral equation. The direct solver scales linearly with respect to the number of discretization points and the precomputation is able to be reused for all right hand sides.

HP-VERSION BOUNDARY ELEMENTS FOR THE WAVE EQUATION

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We discuss *hp* approximations on quasi-uniform meshes to the time-dependent wave equation by boundary element methods on quasi-uniform meshes. The wave equation is here considered in the exterior domain outside a screen or outside a polyhedral domain. For inhomogeneous boundary problems, the solution exhibits singularities from the edges and corners. In this talk we focus on circular and polygonal flat screens as prototype geometries, as they pose the greatest numerical challenges. Based on the analysis of the singularities by Plamenevskii and coauthors, we discuss the approximation by piecewise polynomials of tensor product type in space and time. Quasi-optimal approximation rates are obtained. As in the time-independent case, the p version converges at twice the rate of the h-version. Numerical experiments confirm the theoretical analysis for h and p versions.

ANALYSIS AND DISCRETIZATION OF COUPLED 1D-3D FLOW MODELS

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Coupled 1D-3D flow models are used for a variety of applications, such as modeling fluid flow through vascularized tissue, modeling the flow of water and nutrients through soil embedded with a root system, and modeling the interaction between a well and reservoir. Veins, arteries, roots and wells all have in common that their radius is negligible compared to their length and the size of the domain as a whole. For this reason, we idealize them as being 1D geometries. The 1D structures are then endowed with a 1D flow equation, and coupled to the 3D flow equation by the use of a line source.

The main challenge associated with the coupled 1D-3D flow model is that the line source makes the solution singular. This complicates both the analysis and approximation of the problem. In this talk, we show that the solution admits a splitting into two parts: (i) a term that explicitly captures the singularity and (ii) some smooth remainder. Via this splitting, we can then subtract the singularity. This yields a reformulated model in which all variables are smooth. The solution can then be approximated using any standard numerical method. We conclude by showing numerical experiments relevant for biomedical applications.

HIGH ORDER EXACT SEQUENCES OF COMPOSITE FINITE ELEMENT APPROXIMATIONS BASED ON GENERAL MESHES WITH INTERFACE CONSTRAINTS

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Guidelines are given for a general construction of high order exact sequences of finite element spaces in $H^1(\Omega)$, $\mathbf{H}(\mathrm{curl}, \Omega)$, $\mathbf{H}(\mathrm{div}, \Omega)$, and $L^2(\Omega)$ based on conformal meshes $\mathcal{T} = \{\Omega_e\}$, each subdomain Ω_e being assumed to be a polyhedron, which may be non-convex. At each space level, the approach is to consider composite polynomial approximations $V(\Omega_e)$ based on local partitions $\mathcal{T}^e = \{K\}$, formed by elements K having usual geometry, and on trace spaces Λ_c piecewise defined over a partition of the mesh skeleton, the only requirement being that the functions in Λ_c should be embedded in the space formed by the traces of the local approximation spaces $V(\Omega_e)$ over $\partial\Omega_e$. The construction of subspaces $V_c(\Omega_e) \subset V(\Omega_e)$ only keeps the coarser trace components of $V(\Omega_e)$ constrained by Λ_c, but the components having vanishing traces may be richer in different extents: with respect to internal mesh size, internal polynomial degree, or both. Projection-based interpolants commuting the de Rham diagram are expressed as the sum of linearly independent contributions associated with vertices, edges, faces, and volume, according to the kind of traces appropriate to the space under consideration. The implementation of such constrained space configurations are similar to the ones adopted in h-p adaptive contexts, using hierarchies of shape functions for classic polynomial spaces of arbitrary degree, and a data structure allowing the identification of trace and internal shape functions of different degrees, and procedures for shape function constraints in two or three dimensions. These kinds of space approximations have been recently used for H^1-conforming and mixed formulations of Darcy's flows: a) using combined tetrahedral-hexahedral-pyramidal-prismatic meshes [1], and b) in multiscale hybrid mixed settings [2].

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STRUCTURE-AWARE TAYLOR TIME STEPPING FOR TENT PITCHING SCHEMES

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Many ideas have been put forth to advance numerical solutions of wave and other hyperbolic problems in time through local operations in spacetime regions. Tent-shaped spacetime regions appear to be natural for solving hyperbolic systems because one can ensure causality by constraining the height of the tent pole. Specifically, the domain of dependence of all points within a tent can be guaranteed to be contained within the tent by constraining the tent pole height. Moreover, a spacetime simulation region can be covered by advancing fronts of such tents. Building on this idea, we have introduced new schemes, called Mapped Tent Pitching (MTP) schemes, which proceed by transforming tents into domains where space and time are separated, allowing standard methods to be used within tents. This technique also allows, for the first time, the use of fully explicit schemes within tents. After highlighting certain difficulties that arise with naive use of standard explicit Runge-Kutta time stepping algorithms in this context, we propose an alternative structure-aware Taylor time-stepping technique. New explicit methods are thus built that allow variable time steps and local refinements without compromising high-order accuracy in space and time. They lead to highly parallel algorithms, which utilize modern computer architectures extremely well.

NONLINEARY PRECONDITIONED FETI METHOD

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We consider the Finite Element approximation of the solution to nonlinear elliptic partial differential equations such as the ones encountered in (quasi)-static mechanics, in transient mechanics with implicit time integration, or in thermal diffusion. Non-overlapping domain decomposition methods (DDM) offer an interesting framework for the distribution of the resolution. We focus on methods allowing independent nonlinear computations on the subdomains, sometimes called "nonlinear relocalization techniques".

Nonlinear counterparts to classical non-overlapping DDM have been proposed: nonlinear primal (Dirichlet) and mixed (Robin) approach [Philippe Cresta, Olivier Allix, Christian Rey, and St phane Guinard. Nonlinear localization strategies for domain decomposition methods: Application to post-buckling analyses. Computer Methods in Applied Mechanics and Engineering, 196(8):1436 1446, 2007], dual approach [Julien Pebrel, Christian Rey, and Pierre Gosselet. A nonlinear dual-domain decomposition method: Application to structural problems with damage. International Journal for Multiscale Computational Engineering, 6(3), 2008], and nonlinear FETI-DP and BDDC [Axel Klawonn, Martin Lanser, and Oliver Rheinbach. Nonlinear FETI-DP and BDDC Methods. SIAM Journal on Scientific Computing, 36(2):A737 A765, 2014]. The latter methods were improved and assessed at a large scale in [Axel Klawonn, Martin Lanser, Oliver Rheinbach, and Matthias Uran. Nonlinear FETI-DP and BDDC methods: A unified framework and parallel results. SIAM J. Sci. Comput., 39(6):C417 C451, 2017]. A global framework for primal/dual/mixed approaches was also proposed [Camille Negrello, Pierre Gosselet, Christian Rey, and Julien Pebrel. Substructured formulations of nonlinear structure problems – influence of the interface condition. International Journal for Numerical Methods in Engineering, 2016] and the impedance of the mixed approach was improved [Camille Negrello, Pierre Gosselet, and Christian Rey. A new impedance accounting for short and long range effects in mixed substructured formulations of nonlinear problems. International Journal for Numerical Methods in Engineering, 2017].

Our objective is to double the intensity of the local independent nonlinear computations by modifying the condensed problem to be solved. The method can be interpreted as proposing a nonlinear preconditioner [Peter R Brune, Matthew G Knepley, Barry F Smith, and Xuemin Tu. Composing scalable nonlinear algebraic solvers. SIAM Review, 57(4):535 565, 2015] to the nonlinear DDM.

It appears that this idea applies particularly easily to the dual approach, under an hypothesis equivalent to infinitesimal strain in mechanics. When applying a Newton algorithm to this nonlinear preconditioned condensed system, one alternates a sequence of two independent nonlinear local solves (one Neumann problem and one Dirichlet problem separated by one all-neighbor communication) and an interface tangent solve which exactly has the structure of a linear preconditioned FETI problem. Academic assessments show that the sequence of two local nonlinear solves can reduce the need of global Newton

iterations and thus the number of calls to the communication-demanding Krylov solver.

This work benefited from the support of the project SEMAFOR ANR-14-CE07-0037 of the French National Research Agency (ANR).

TWO-GRID FINITE ELEMENT GALERKIN APPROXIMATION OF EQUATIONS OF MOTION ARISING IN OLDROYD FLUIDS OF ORDER ONE WITH NON-SMOOTH INITIAL DATA

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We consider a two-grid finite element method for the equations of motion describing Oldroyd fluid of order one, see [J.G. Oldroyd, Non-Newtonian flow of liquids and solids, Rheology:Theory and Applications, Vol I (Ed. F.R. Eirich), Academic Press, NY, 1956, pp 653-682]. This viscoelastic fluid equation can also be considered as an integral perturbation of Navier-Stokes' equations. The numerical method involves solving the non-linear parabolic integro-differential equation on a coarse grid. And a linearized equation, linearized based on time-dependent Stokes type problem, is solved on a fine grid. We have obtained optimal rate of convergence for velocity in H^1-norm and for pressure in L^2-norm. Analysis has been carried out for non-smooth initial data. And error estimates are shown to be uniform under uniqueness condition.

PARALLEL CONTROLLABILITY METHODS FOR THE HELMHOLTZ EQUATION

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The Helmholtz equation is notoriously difficult to solve with standard iterative methods, increasingly so, in fact, at higher frequencies. Controllability methods instead transform the problem back to the time-domain, where they seek the time-harmonic solution of the corresponding time-dependent wave equation. Two different approaches are considered here based either on the first (mixed) or second-order formulation of the wave equation. Both are extended to general boundary-value problems governed by the Helmholtz equation and lead to robust and inherently parallel algorithms. Numerical results illustrate the accuracy, convergence and strong scalability of controllability methods for the solution of high frequency Helmholtz equations with up to a billion unknowns on massively parallel architectures.

FINITE-ELEMENT AND BOUNDARY-ELEMENT SIMULATIONS FOR HIGH-INTENSITY FOCUSED ULTRASOUND MODELLING

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High-intensity focused ultrasound (HIFU) is a promising non-invasive, non-radioactive technology for the ablation of tumours. By focusing energy on a small target region the tissue temperature in the target region can be elevated such that with sufficient treatment time the tissue is destroyed. Challenges in planning HIFU treatments in the abdomen include the presence of a large number of scatterers, nonlinear effects and the presence of transport mechanisms for heat.

In this talk, I will compare a range of different finite-element and boundary-element formulations for the non-linear wave equation in practically relevant HIFU scattering scenarios. These include classical implicit and explicit time-stepping schemes, high-order methods, and convolution quadrature. We aim to isolate the main challenges in such high-frequency, non-linear wave simulations and identify the most fruitful directions towards the development of accurate methods that are fast enough to be clinically relevant, and which will hopefully support patient treatment planning in the future.

The presented methods are implemented in the open source FEniCS (`https://fenicsproject.org`) and Bempp (`https://bempp.com/`) libraries.

FEAST ITERATION APPLIED TO PERTURBED PARTIAL DIFFERENTIAL OPERATORS

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Filtered subspace iteration with Rayleigh-Ritz eigenvalue extraction is a recently reviewed method in the form of the FEAST algorithm. In this talk we present a method motivated by the FEAST iteration and apply it directly on the operator level. The core of the algorithm is a numerical resolvent calculus based on contour quadratures coupled with a perturbation analysis of the resolvent evaluation motivated by the results in Numerical Linear Algebra. We prove convergence rate which depends on the properties of the filter (even in the presence of perturbations). Perturbations which we consider can originate both from the projection/truncation of infinite dimensional operators (necessary to evaluate resolvents) or from the uncertainty in the parameters of the underlying problem. This is a joint work with J. Gopalakrishnan and J. Ovall.

DISCONTINUOUS SKELETAL METHODS FOR THE OBSTACLE PROBLEM

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Discontinuous-skeletal methods are introduced and analyzed for the elliptic obstacle problem in two and three space dimensions. The methods are formulated in terms of face unknowns which are polynomials of degree $k = 0$ or $k = 1$ and in terms of cell unknowns which are polynomials of degree $l = 0$. The discrete obstacle constraints are enforced on the cell unknowns. A priori error estimates of optimal order (up to the regularity of the exact solution) are shown. Specifically, for $k = 0$, the method employs a local linear reconstruction operator and achieves an energy-error estimate of order h, where h is the mesh-size, whereas for $k = 1$, the method employs a local quadratic reconstruction operator and achieves an energy-error estimate of order $h^{\frac{3}{2}-\epsilon}$, $\epsilon > 0$. Numerical experiments in two and three space dimensions illustrate the theoretical results

A POSTERIORI ERROR ANALYSIS OF TWO-STEP BACKWARD DIFFERENTIATION FORMULA FINITE ELEMENT APPROXIMATION FOR PARABOLIC INTERFACE PROBLEMS

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In this talk, we discuss a residual-based a posteriori error estimates via elliptic reconstruction for linear parabolic interface problems in a bounded convex polygonal domain in $\mathbb{R}^2$. The interfaces are assumed to be of arbitrary shape but are smooth for our purpose. The standard linear finite element spaces (allowed to change in time) are used in space whereas, the two-step backward differentiation formula (BDF-2) approximation is used for the time discretizations. The key ingredients in the a posteriori error analysis are the continuous piecewise quadratic space-time BDF-2 reconstruction and approximation results for Clément-type interpolation operator of Scott and Zhang. We use only the energy arguments to derive a posteriori error estimates with an optimal order in time and an almost optimal order in space in the $L^\infty(L^2)$-norm. Numerical results are reported to validate the theoretical findings.

NONREFLECTING BOUNDARY CONDITIONS FOR A MIXED DG DISCRETIZATION OF THE MAXWELL EQUATIONS

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Mixed discontinuous Galerkin methods are well suited to solving the Maxwell equations in complex structures, as they allow an efficient capturing of singularities at dielectric corners and also can provide a spurious free spectrum [1, 2]. In this work, we combine such a mixed DG discretization with a nonreflecting boundary condition. We use the Hagstrom-Warburton condition, since it has an a-priori error estimate and allows control over the error by adding an increasing number of wave directions that are exactly absorbed [3].

A distinctive feature of our work is that we use the Hagstrom-Warburton condition in a second order mixed DG formulation of the Maxwell equations. In our approach, we apply the condition separately to the two tangential components of the electric field, which results in a well-posed problem at the continuous level as shown by our Kreiss analysis. We have developed a DG discretization of the auxiliary equations of the boundary condition which is based on Bassi-Rebay type fluxes and contains additional stabilization terms. Our numerical tests with plane waves show that the discretization is stable, and converges with the optimal order.

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EIGENLOCKING ON THIN SHELLS OF REVOLUTION

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The finite element modelling of thin shells is known to be a very demanding task because of the many different ways parametric error amplification or locking phenomena can occur. Here we consider locking in connection with eigenvalue problems in shells, especially in inhibited pure bending shells or shells with clamped support. Our purpose is not to suggest ways for alleviating or circumventing eigenlocking, but to analyse, predict, and demonstrate its existence when the lowest eigenfrequency is computed. Here one has to account for the fact that unlike in second order problems, the lowest mode can have a higher multiplicity. Furthermore, it is possible that the lowest mode is part of such a narrow cluster that the only meaningful interpretation for convergence is to the cluster rather than to the mode itself. The concept of locking in parabolic shells was first identified in [1], but never fully demonstrated through numerical experiments. The results obtained for hyperbolic shells are new.

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SCALABILITY ANALYSIS OF AN INTEGRAL EQUATION FORMULATION OF THE MANY-BODY DIELECTRIC PROBLEM IN ELECTROSTATICS

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We consider the problem of calculating the electrostatic interaction between dielectric spheres embedded in a polarisable continuum. In order to solve this problem, E. Lindgren and co-workers have proposed in [E. Lindgren et al, An integral equation approach to calculate electrostatic interactions in many-body dielectric systems, Journal of Computational Physics, 2018, pp. 712-731] a numerical method based on a Galerkin discretisation of an integral equation formulation of this problem. The proposed method is general enough to treat any homogeneous dielectric medium containing an arbitrary number of spherical particles of any size, charge, dielectric constant and position in the three-dimensional space. Furthermore, numerical experiments indicate that the algorithmic complexity of the method scales linearly with respect to the number of particles thanks to the use of a modified Fast Multipole Method.

The current talk will present some results on the numerical analysis of this algorithm with a focus on proving that the method is indeed scalable with respect to the number of objects N in the problem. As a first step, we demonstrate that both the infinite-dimensional integral equation formulation and its Galerkin discretisation are well-posed with explicitly characterisable continuity and inf-sup constants. Our main result is to derive error estimates that do not explicitly depend on N. We show in addition that under suitable regularity assumptions, the numerical method exhibits exponential convergence. We also obtain an upper bound for the condition number of the stiffness matrix that does not explicitly depend on N and consequently show that under suitable assumptions, a Krylov subspace solver such as GMRES that is used to solve the underlying linear system converges to a given tolerance independent of N. We conclude the talk with a brief discussion about the efficient computation of the electrostatic forces.

NUMERICAL REALIZATION OF SHAPE OPTIMIZATION FOR UNSTEADY FLUID-STRUCTURE INTERACTION

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We consider shape optimization for unsteady fluid-structure interaction problems that couple the Navier-Stokes equations with non-linear elasticity equations. We focus on the monolithic approach in the ALE framework. It is obtained by transforming the time-dependent fluid domain to a fixed reference domain. Shape optimization by the method of mappings approach requires another transformation which maps the ALE reference domain to a nominal domain. This yields an optimal control setting and therefore can be used to drive an optimization algorithm with adjoint based gradient computation. The continuous formulation of the problem and the numerical realization are discussed. Numerical results for our implementation, which builds on FEniCS, dolfin-adjoint and IPOPT are presented.

SPACE-TIME METHODS FOR MAXWELL'S EQUATIONS

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We consider space-time variational formulations for the Maxwell equations. In particular we consider the vectorial wave equation for the electric field E including the spatial curl operator. As with the scalar wave equation we apply integration by parts both in time and space and discuss unique solvability of the resulting Galerkin-Petrov formulation under different assumptions on the given data. Although the numerical discretization in a 4D space-time setting seems to be ambitious at a first glance, it allows for an adaptive resolution simultaneously in space and time and for a parallel implementation.

THE FROSCH PACKAGE IN CARDIOVASCULAR SIMULATIONS

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FROSch (Fast and Robust Overlapping Schwarz), a framework for overlapping Schwarz preconditioners, has recently been integrated into Trilinos as part of the package ShyLU. It contains scalable preconditioners that are robust for a wide class of problems, e.g., from solid or fluid mechanics, and can be constructed in an algebraic way. In particular, the preconditioners can be constructed from the fully assembled matrix without an additional coarse triangulation, even for unstructured domain decompositions. Additional information about the geometry or the null space of the operator can further improve the convergence and robustness of the solvers.

This talk gives an overview of the FROSch code, its features, and user-interface and shows the parallel scalability and robustness of the solvers for different problems. In particular, the focus of this talk lies on the application of FROSch in large-scale simulations of blood flow in arteries and the deformation of arterial walls.

Based on joint work with Christian Hochmuth, Sivasankaran Rajamanickam, and Friederike Röver.

A PARALLEL, ADAPTIVE PHASE-FIELD FRACTURE CODE

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We present an open source, finite element code to simulate crack propagation using a quasi-static fracture model. The cracks are discretized using a phase-field approach, which allows merging and joining of cracks.

We employ an efficient numerical scheme based on an active set strategy formulated as a semi-smooth Newton method. We propose a strategy for adaptive mesh refinement that saves computational time and offers a convergent scheme.

To confirm these claims, we show benchmark results that show convergence of our adaptive scheme under mesh refinement and phase field parameter. Finally, we show the parallel scalability of the algorithm on thousands of processors.

- T. Heister, T. Wick:
  Parallel solution, adaptivity, computational convergence, and open-source code of 2d and 3d pressurized phase-field fracture problems.
  Proc. Appl. Math. Mech., 2018. doi:10.1002/pamm.201800353

- T. Heister, M. Wheeler, T. Wick:
  A primal-dual active set method and predictor-corrector mesh adaptivity for computing fracture propagation using a phase-field approach
  CMAME, Volume 290, 15 June 2015, Pages 466-495. doi:10.1016/j.cma.2015.03.009

MODELLING AND NUMERICAL SIMULATION OF ONE-COMPONENT TWO-PHASE FLOW WITH PARTIAL MISCIBILITY USING GENERALIZED SLIP BOUNDARY CONDITION

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We propose a diffuse interface model with the Van der Waals equation of state considering the slip effect at the interface. For numerical simulation of the proposed model, we introduce a numerical scheme that satisfies a discrete energy law which is consistent with energy law of the model. Numerical tests are carried out to verify the effectiveness of the proposed method.

ANDERSON LOCALIZATION OF SCHRÖDINGER EIGENFUNCTIONS

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The phenomenon of Anderson localization refers to the observation that waves in a sufficiently disordered medium show a strong localization effect. In this talk we want to investigate Anderson localization for the linear Schrödinger equation as a model problem. We will see how disorder changes the properties of the wave function, we point out important observations and try to formulate mathematical explanations for it. In essence, we will see that disorder causes large gaps in the spectrum of the Schrödinger operator and that the size of these gaps is immediately tied to the prominence of the localization effect.

QUANTUM CHEMISTRY IN ARBITRARY DIELECTRIC ENVIRONMENTS

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We have recently developed a multigrid solver for the generalized Poisson equation that can be used for arbitrary solute densities $\rho(\mathbf{r})$ obtained from an electronic structure calculation, by means of which the molecular density $\rho(\mathbf{r})$ and the dielectric polarization $\varphi(\mathbf{r})$ are iterated to mutual self-consistency.[1, 2] The generalized Poisson equation may include an arbitrary, spatially-varying dielectric function $\varepsilon(\mathbf{r})$ specified by the user, so that the method can describe anisotropic solvation environments such as the air/water interface. Borrowing ideas from polarizable continuum models, we have implemented nonequilibrium solvation corrections in which the solvent's optical dielectric constant is used to account for instantaneous re-polarization of the dielectric continuum evironment upon vertical excitation or ionization of the solute. We have used this code to compute accurate vertical ionization energies for small ions in bulk water and to examine whether these ionization energies are modified at the air/water interface. Particular attention is paid to whether the solvated electron, e^-(aq), is spectroscopically distinguishable at the interface as compared to the same species in bulk water.[1]

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A DPG METHOD FOR THE BI-LAPLACE EQUATION

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We study the bi-Laplace equation with homogeneous Dirichlet conditions and its approximation by the discontinuous Petrov–Galerkin method with optimal test functions (DPG method). To this end we develop ultraweak variational formulations that are well posed in spaces of natural regularity, assuming the right-hand side function to be L_2-regular. At the heart of the analysis are trace operators stemming from the bi-Laplacian. Resulting trace spaces are a little tricky to deal with, in one case it is not closed. It turns out that the right way to analyze this setting is to switch to trace operators and spaces known from the Kirchhoff–Love plate bending model, as analyzed in [2]. We present some numerical experiments that show convergence properties of our DPG schemes. The contents of this presentation is taken from [1].

We gratefully acknowledge financial support by CONICYT-Chile through FONDECYT projects 11170050 and 1190009.

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BOUNDARY ELEMENT METHODS FOR ACOUSTIC SCATTERING BY FRACTAL SCREENS

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We consider time-harmonic acoustic scattering by a planar screen, i.e. a subset of a two-dimensional hyperplane embedded in a three-dimensional propagation domain. In contrast to previous studies we allow the relative boundary of the screen to be arbitrarily rough - in particular, the screen could have fractal boundary (Koch snowflake), or itself be a fractal (Sierpinski triangle). Such problems are of interest in the study of fractal antennas in electrical engineering, light scattering by snowflakes/ice crystals in atmospheric physics, and in laser optics.

The fractal nature of the screen presents challenging questions concerning how boundary conditions should be enforced, and the appropriate function space setting. But progress is possible and there is interesting behaviour to be discovered: for example, a sound-soft screen with zero area (planar measure zero) can scatter waves provided the fractal dimension of the set is large enough [1,2]. Accurate computations are obviously challenging because of the need to capture the fine structure of the fractal. A natural approach to numerical simulation is via boundary element method approximations on sequences of smoother "prefractal" approximations. As well as presenting numerical results for such an approach, I will outline some of our recent theoretical results, and some outstanding open questions, regarding convergence analysis [3].

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HYBRID NUMERICAL-ASYMPTOTIC BOUNDARY ELEMENT METHODS FOR HIGH FREQUENCY TRANSMISSION PROBLEMS

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High frequency scattering is notoriously challenging for conventional boundary element methods based on piecewise polynomial approximation spaces, because of the large number of degrees of freedom required to capture the oscillatory solution. Hybrid numerical-asymptotic (HNA) methods aim to significantly reduce the dimension of the numerical approximation space by enriching it with oscillatory functions, carefully chosen to capture the high frequency asymptotic behaviour of the wave solution [1].

In this talk I will report some recent advances in HNA boundary element methods for transmission problems (involving penetrable, or dielectric scatterers), relevant, for example, to light scattering by atmospheric ice crystals. For scattering by penetrable convex polygons in two dimensions our algorithm presented in [2] achieves fixed accuracy with a frequency-independent number of BEM degrees of freedom, associated with oscillatory basis functions capturing corner-diffracted waves. Our current investigations suggest that to obtain good performance uniformly across all incident angles it is necessary to include basis functions capturing so-called "lateral" or "head" waves, which in the high frequency asymptotic theory correct for the phase mismatch between the internal and external diffracted waves.

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MULTI-TRACE BOUNDARY ELEMENT METHODS

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The scattering of acoustic or electromagnetic waves at a penetrable object composed of different homogeneous materials can be modelled by means of boundary integral equations (BIE) posed on the interfaces. This approach is widely used in numerical simulations and often relies on so-called first-kind single-trace BIE [3, Sect. 2]. Their boundary element Galerkin discretization gives rise to poorly conditioned linear systems, for which the otherwise successful operator (Calderón) preconditioning approach does not seem to be available.

As a remedy we propose new multi-trace boundary integral equations; whereas the single-trace BIE feature unique Cauchy traces on sub-domain interfaces as unknowns, the multi-trace idea takes the cue from domain decomposition and tears the unknowns apart so that *local* Cauchy traces are recovered. The benefit is the possibility of straightforward Calderón preconditioning.

Multi-trace formulations come in two flavors. A first variant, the *global multi-trace approach*, is obtained from the single-trace equations by taking a "vanishing gap limit" [3, Sect. 3]. The second variant is the *local multi-trace method* and is based on local coupling across sub-domain interfaces [1, Sect. 4]. Numerical experiments for acoustic scattering demonstrate the efficacy of Calderón preconditioning.

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SHAPE GRADIENTS IN FINITE ELEMENT EXTERIOR CALCULUS

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We blend two recent developments in numerical shape calculus under constraints imposed by second-order elliptic boundary value problems:

(I) The insight that the calculus of differential forms offers a powerful and unifying framework for computing shape derivatives in the sense of the velocity method [2, 1],

(II) The realization that shape gradients permit equivalent expressions based on either boundary expressions (Hadamard form) or volume integrals [4],

Hence, in the framework of exterior calculus we establish volume and boundary formulas for shape gradients. Subsequently, we generalize the duality techniques of [3] to show higher-order convergence of a Galerkin finite element approximation of the volume expressions based on discrete differential forms. This results covers the results of [3] as the case of 0-forms, and the case of shape gradients constrained by Maxwell's equations as the case of 1-forms.

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NUMERICAL ANALYSIS FOR THE OPTIMAL CONTROL OF SIMPLIFIED MECHANICAL DAMAGE PROCESSES

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In this talk we investigate a priori error estimates for the space-time Galerkin finite element discretization of an optimal control problem governed by a simplified damage model. The model equations are of a special structure as the state equation consists of a coupled PDE-ODE system. One difficulty for the derivation of error estimates arises from low regularity properties of solutions provided by this system. The state equation is discretized by a piecewise constant discontinuous Galerkin method in time and usual conforming linear finite elements in space. For the discretization of the control we employ the same discretization technique which turns out to be equivalent to a variational discretization approach. We provide error estimates both for the discretization of the state equation as well as for the optimal control. Numerical experiments are added to illustrate the proven rates of convergence.

ADAPTIVE ARBITRARY LAGRANGIAN-EULERIAN DISCONTINUOUS GALERKIN METHOD FOR HYPERBOLIC EQUATIONS INVOLVING $\delta-$ SINGULARITIES

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In this talk, we present and analyze an arbitrary Lagrangian-Eulerian discontinuous Galerkin (ALE-DG) method to solve one-dimensional hyperbolic equations involving δ-singularities over adaptive moving meshes. The L^2-norm and negative-order norm error estimates are proven for the ALE-DG approximation. More precisely, when choosing the piecewise kth degree polynomials approximation space, the convergence rate in L^2-norm for the scheme with the upwind flux over the region apart from the singularities is the $(k+1)$th order, the convergence rate in the $H^{-(k+1)}$ norm for the scheme with the monotone fluxes over the whole domain is the kth order, the convergence rate in the $H^{-(k+2)}$ norm for the scheme with the upwind flux over the whole domain can achieve the $(k+\frac{1}{2})$th order, and the convergence rate in the $H^{-(k+1)}(R\backslash R_T)$ norm for the upwind flux is the $(2k+1)$th order, where R_T is the pollution region at time T due to the singularities. Moreover, numerically the $(2k+1)$th order accuracy for post-processed solution in the smooth region can be obtained, which is produced by convolving the ALE-DG numerical solution with a suitable kernel consisted of B-splines. Numerical examples will be shown to demonstrate the accuracy and capability of the ALE-DG method for the hyperbolic equations involving δ-singularity over the adaptive moving meshes.

HIGH-ORDER DISCONTINUOUS GALERKIN METHODS ON POLYTOPIC GRIDS

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Numerical methods defined on computational meshes consisting of polytopic elements, which potentially contain many faces, have gained substantial traction in recent years for a number of important reasons. Firstly, flexibility, in terms of the shape of the elements admitted within a given mesh, is crucial in the context of the efficient approximation of localized geometrical features present in the underlying geometry. Indeed, the use of standard element shapes typically necessitates the exploitation of very fine computational meshes when the geometry possesses small details or microstructures. Furthermore, polytopic elements are naturally suited to applications in complicated/moving domains, for example, in solid mechanics, fluid-structure interaction, geophysical problems including earthquake engineering and flows in fractured porous media, and mathematical biology. Moreover, the ability to incorporate polytopic meshes offers a number of advantages also in the context of multilevel linear solvers, such as Schwarz-based domain decomposition preconditioners and multigrid.

In this talk, we present a survey of so-called composite/agglomerated discontinuous Galerkin finite element methods (DGFEMs) which employ general polytopic elements. In particular, we provide an overview of *hp* -version inverse estimates and approximation results for general polytopic elements, which are sharp with respect to element facet degeneration. On the basis of these results, *a priori* error bounds for the *hp*- DGFEM approximation of both second–order elliptic and first–order hyperbolic PDEs will be derived, cf. [1, 4]. Furthermore, the design of efficient quadrature rules for the numerical approximation of integrals of polynomial functions over general polytopic elements that do not require the explicit construction of a sub-tessellation into triangular/tetrahedral elements will be discussed, based on the work presented in our recent article [2]. Finally, we consider the application of these methods within Schwarz-type domain decomposition preconditioners; see [3] for further details.

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PREDICTING THE BALLISTIC RESPONSE OF ALUMINIUM SANDWICH PANELS.

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This paper presents research on developing of a predictive modelling capability for ballistic impact on an aluminium sandwich panels. A predictive modelling capability supports the design of capture and deorbit missions for large items of space debris such as satellites and rocket upper stages. A detailed explicit finite element model of the panel was built and results were compared with experimental data to investigate key modelling assumptions. The primary assumptions influencing the model behaviour were the strength and failure of the aluminium face sheets and the friction between projectile and panel. The model results showed good agreement with experimental results for an ogive nose projectile, but overestimated the exit velocity for a flat nose projectile where different behaviour of the honeycomb core is a modelling challenge.

ON THE INTEREST OF HIGH MEMORY BANDWIDTH ARCHITECTURES FOR PDE DISCRETIZATIONS WITH COMPACT SUPPORT

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The arithmetic intensity of PDE discretization schemes with compact support, in particular on unstructured meshes, is so low that on current architures these schemes are limited by the available bandwidth more than by the computational power. Over the last few years, a small number of high bandwidth memory (HBM) systems have become available. We will present performance results on one of these architectures, the NEC vector engine SX-Aurora Tsubasa, and compare it to the performance prediction of the roofline model.

INTERPOLATION PROPERTIES OF GENERALIZED PLANE WAVES FOR THE CONVECTED HELMHOLTZ EQUATION

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Trefftz methods are commonly used for wave propagation problems in frequency domain, and rely on basis functions that solve exactly the driving equation, such as classical plane waves. In order to take advantage of Trefftz methods for problems with variable coefficients, in which case there is usually no known exact solution of the PDE to discretize the Trefftz formulation, Generalized Plane Waves (GPWs) have been developed as approximated solutions to the given PDE.

We will discuss the design and interpolation properties of GPWs for the 3D convected Helmholtz equation, emphasizing the similarities with the 2D Helmholtz equation as well as the challenges arising from inhomogeneity and anisotropy of the 3D medium.

WAVE BLOW-UP THROUGH MIXING OF NEUMANN AND DIRICHLET BOUNDARY CONDITIONS

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This talk aims at showing a new and efficient approach for maximizing the transmission between two points at a chosen frequency in terms of the boundary conditions. The proposed approach makes use of recent results on the monotonicity of the eigenvalues of the mixed boundary value problem and on the asymptotic expansion of the Green s function to small changes in the boundary conditions.

More precisely, starting with a Dirichlet boundary condition, we search for a location on the boundary, in which we can apply a short Neumann boundary condition to get an increase in the transmission intensity. As it turns out, there exists a critical length for the Neumann boundary, which will make the transmission-wave blow up. Our algorithm tries to find that domain-depending length, and as we will show, the algorithm succeeds whenever the critical length is small enough.

The switching of the boundary condition from Dirichlet to Neumann can be performed through the use of the recently modeled concept of metasurfaces comprised of coupled pairs of Helmholtz resonators.

A variety of numerical experiments are presented to show the applicability and the accuracy of the proposed new methodology.

EIGENPROBLEM WITH LOW-REGULARITY SOLUTION FOR NUCLEAR REACTOR CORE MODELING

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The behaviour of a nuclear reactor core depends on the nuclear chain reaction, which is described by the neutron transport equation. This equation is a balance statement that conserves neutrons. It governs the neutron flux density, which depends on 7 variables: 3 for the space, 2 for the motion direction, 1 for the energy (or the speed), and 1 for the time. In the steady-state case, one must solve an eigenvalue problem. The energy variable is discretized using the multigroup theory (G groups). Concerning the motion direction, an inexpensive approach to approximate the transport equation is to solve the simplified PN equations ($\frac{N+1}{2}$ coupled diffusion equations). It can be shown that the basic building block which allows to solve the general multigroup simplified PN equations, is the so-called neutron diffusion equation ($G = 1$, $N = 1$), which reads as the following eigenproblem, set in a bounded domain Ω of $\mathbf{R}^3$:
Find $\phi \in H^1(\Omega), \lambda \in \mathbf{R}^+$ such that:

$$\left\{ \begin{array}{rcll} -\mathrm{div}\, D\, \mathbf{grad}\, \phi + \Sigma_a\, \phi & = & \lambda\, \nu \Sigma_f \phi & \text{in } \Omega \\ \phi & = & 0 & \text{on } \partial\Omega. \end{array} \right. \tag{1}$$

Above, the data D, Σ_a, ν and Σ_f denote respectively the diffusion coefficient, the macroscopic absorption cross section, the fission yield and the fission cross section. Note that the data D can be a tensor and the fission cross section can vanish in some area. Concerning the resolution of the eigenproblem (1), we look for the criticality factor: $1/\min_\lambda \lambda$, together with the associated ϕ which corresponds to the averaged neutron flux density. Special attention is paid to the case where the eigenfunctions ϕ can be of low regularity. Such a situation commonly arises in the presence of three or more intersecting material components with different characteristics, as it appears in reactor cores studies. Indeed, the nuclear reactor cores have often a cubic or parallelepipedic geometry and the cross sections are averaged in each square or rectangular cell. They may be constant or piecewise polynomial. They may differ from one cell to another by a factor of order 10.

We analyze matching and non-matching domain decomposition methods for the numerical approximation of the eigenproblem (1). The domain decomposition method can be non-matching in the sense that the meshes of the subdomains, and more generally

the finite elements spaces, may not fit at the interface between subdomains. We prove well-posedness of the discrete eigenproblems with the help of a uniform discrete inf-sup condition, and we provide optimal a priori convergence estimates. Numerical experiments illustrate the accuracy of the method.

DISCONTINUOUS GALERKIN FINITE ELEMENT APPROXIMATION TO FRACTIONAL ORDER VISCOELASTICITY PROBLEMS

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A viscoelastic problem is modelled with a Volterra type integro-differential equation. The kernel in the integral can be either exponentially decaying or of weakly singular type. For example, if the kernel is defined as $t^{-\alpha}$ for $0 < \alpha < 1$, it is weakly singular and the integral can be regared as having fractional order. We consider a fractional differential equation as the constitutive equation between the stress $\underline{\boldsymbol{\sigma}}$ and the strain $\underline{\boldsymbol{\varepsilon}}$ given by

$$\underline{\boldsymbol{\sigma}}(t) = \underline{\boldsymbol{D}}_0\underline{\boldsymbol{\varepsilon}}(t) + \frac{\underline{\boldsymbol{D}}_1\underline{\boldsymbol{\varepsilon}}(0)}{\Gamma(1-\alpha)}t^{-\alpha} + \frac{1}{\Gamma(1-\alpha)}\int_0^t (t-s)^{-\alpha}\underline{\boldsymbol{D}}_1\dot{\underline{\boldsymbol{\varepsilon}}}(s)ds$$

where $\alpha \in (0,1)$ and $\underline{\boldsymbol{D}}_0, \underline{\boldsymbol{D}}_1$ are positive definite fourth order tensors. The integral part indicates fractional integration of the order $1-\alpha$. To simplify and remain only fractional integral part in the constitutive equation, we assume a zero constant tensor $\underline{\boldsymbol{D}}_0$ and $\underline{\boldsymbol{\varepsilon}}(0) = \underline{\mathbf{0}}$ so that the model problem is given as

$$\rho\dot{\boldsymbol{w}}(t) - \nabla\cdot {}_0I_t^{1-\alpha}(\underline{\boldsymbol{D}}_1\underline{\boldsymbol{\varepsilon}}(\boldsymbol{w}(t))) = \boldsymbol{f}(t)$$

for the velocity $\boldsymbol{w}$, the body force $\boldsymbol{f}$ and the fractional integral operator ${}_0I_t^{1-\alpha}$. We can formulate semidiscrete and fully discrete problems by using finite element methods for spatial discretisation and the Crank-Nicolson finite difference method in time. The fractional integration is dealt with numerically, by using quadrature rules. Taking the weak singularity of the kernel $t^{-\alpha}$ at $t = 0$ into account, we replace $\boldsymbol{w}(t)$ by continuous piecewise linear interpolation with respect to time in order to take an advantage of the Crank-Nicolson finite difference scheme as well as overcome the weak singularity. Stability and error estimates theorems are presented and proved without using Grnwall's inequality. Numerical results using FEniCS will be given.

HIGHER ORDER TRACE FINITE ELEMENT METHODS FOR SURFACE VECTOR LAPLACE EQUATIONS

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In recent years there has been a strongly growing interest in the field of modeling and numerical simulation of surface fluids, in which Navier-Stokes type PDEs for (evolving) surfaces with fluidic properties are proposed. One crucial point in the development and analysis of finite element methods for surface Stokes equations is the numerical treatment of the constraint that the flow must be tangential to the surface ("tangent condition"). This constraint also occurs in the class of surface vector-Laplace problems, which only contain a velocity unknown and not a pressure variable. We present three different natural techniques for treating the tangent condition, namely a consistent penalty method, a simpler inconsistent penalty method and a Lagrange multiplier method. Instead of triangulating the surface directly, which is in the spirit of the surface finite element method (SFEM) for scalar surface PDEs, we use a trace finite element method (TraceFEM), where we use the finite element spaces of a background volume mesh in which the surface is embedded. From [1] we present the results of a detailed error analysis of the three methods that shows how the discretization error depends on relevant parameters such as the degree of the polynomials used for the approximation of the solution, the degree of the polynomials used for the approximation of the level set function that characterizes the surface, the penalty parameter and the degree of the polynomials used for the approximation of the Lagrange multiplier. Based on these results we will discuss the suitability of the three methods for higher order TraceFEM and present some numerical results.

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FAST CALDERÓN PRECONDITIONING FOR HELMHOLTZ BOUNDARY INTEGRAL EQUATIONS

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Calderón multiplicative preconditioners are an effective way to improve the condition number of first kind boundary integral equations yielding provable mesh independent bounds. However, when discretizing by local low-order basis functions as in standard Galerkin boundary element methods, their computational performance worsens as meshes are refined. This stems from the barycentric mesh refinement used to construct dual basis functions that guarantee the discrete stability of L^2-pairings. Based on coarser quadrature rules over dual cells and H-matrix compression, we propose a family of fast preconditioners that significantly reduce assembly and computation times when compared to standard versions of Calderón preconditioning for the three-dimensional Helmholtz weakly and hyper-singular boundary integral operators. Several numerical experiments validate our claims and point towards further enhancements.

ON NUMERICAL SIMULATIONS AND A POSTERIORI ANALYSIS FOR ALGEBRAIC FLUX CORRECTION SCHEMES

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Non-linear discretizations are necessary for convection-diffusion-reaction equations for obtaining accurate solutions that satisfy the discrete maximum principle (DMP). Algebraic stabilizations, also known as Algebraic Flux Correction (AFC) schemes, belong to the very few finite element discretizations that satisfy this property. The non-linearity of the system arises because of the presence of solution dependent limiters. Because of the non-linear nature of the problem, a new issue arises, which is the efficient solution of the system of equations.

The first part of the talk will address this issue and several methods will be discussed for solving the non-linear problem with a major focus on fixed point iterations and Newton's method. Different algorithmic components such as Anderson acceleration and dynamic damping will be discussed as well. The methods are compared on different parameters such as the number of iterations and computing time needed. Numerical examples are presented in 2d as well as 3d which will asses the different solvers.

The second part of the talk is devoted to the proposal of a new a posteriori error estimator for the AFC scheme. With a mild assumption on the interpolation error, we find a global upper bound in the energy norm of the system which is independent of the choice of limiters. Numerical results are presented in 2d with two different types of limiters.

NUMERICAL ANALYSIS OF SUBDIFFUSION WITH A TIME-DEPENDENT COEFFICIENT

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In the past few years, the numerical analysis of the subdiffusion equation has witnessed impressive progress. However, most works are concerned with the case of a time-independent diffusion coefficient, and the analysis techniques are not directly applicable to the case of a time-dependent coefficient. In this talk, we present some recent works on the error analysis for the case of a time-dependent coefficient, and illustrate the theory with numerical experiments.

PATHWAYS TO GEOMETRIC SOLID MECHANICS

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Describing materials sub-continuum structures with 3-complexes, known from algebraic topology, offers multiple advantages for modelling and simulation. For example, a set of grains forming a polycrystalline material is a 3-complex of 3-celles (volumes), 2-cells (faces), 1-cells (edges) and 0-cells (vertices). Sub-grains structures down to atomic lattices can be conceptualised in a similar way, providing an opportunity to work across length scales with a single computational framework. The discrete nature of such representations is attractive, because it allows for assigning different characteristics to individual or sets of k-cells in order to capture heterogeneity at particular length scales. For example, measurable features of variable sizes or properties of variable magnitudes can be readily incorporated. Importantly for mechanical analysis, discrete representations allow for capturing explicitly micro-crack initiation, growth and coalescence. Development of analysis on such 3-complexes is essential for unlocking the potential of such representations.

Discrete Exterior Calculus (DEC) offers an efficient way to analyse 3-complexes. Currently DEC uses the de Rham complex, known from algebraic and differential topology, with Hodge star operators to form discrete analogues of gradient, curl and divergence. This approach has been successfully applied to analysis of a number of physical problems with scalar principal unknown. The few attempts to describe elasticity with DEC are limited to 2D problems and have a common problem Hodge stars couple fully material constitutive laws with metric information. As a result, such descriptions are only applicable to truss structures, and these are more conveniently analysed with 1-complexes (graphs). This talk presents the on-going project Geometric Mechanics of Solids (GEMS), which aims at developing an efficient tool for analysis on 3-complexes with representing elasticity as critical first step.

The scene is set by a brief description of the DEC theory. Several DEC based-schemes with different Hodge star operators, implemented in in-house codes, are discussed. One line of enquiry is based on a discrete analogue of the Navier-Lame equation of linear elasticity using a scalar-valued discrete differential forms: 0,1,2,3-cochains (functions on 0,1,2,3-cells). While this formulation can be seen as intrinsic, prescribing boundary conditions requires mapping between co-chains and external vector fields. Finding unique mapping is challenging because both vector fields and cochains belong to infinite dimensional function spaces before the discretization is made.

Another line of enquiry is based on vector-valued co-chains, offering direct correspondence between external vector fields and 0-cochains. Main issue with this approach is the unwanted coupling of metric and constitutive information by the Hodge star, seen in the few past works on the topic. Discussed are options for decoupling by separating the deformation component from the rotation component of the discrete displacement/deformation gradient.

A third line of enquiry is based on analysis of sub-complexes, formed by existing 1-

cells, intended to measure length changes, and a set of complimentary 1-cells (3-complex dependent), intended to measure angle changes. Examples solved with this approach are demonstrated.

Final line of enquiry is inspired by the computational attractiveness of modern tools in geometry integration. Elasticity problems are a formulated by energy functional, which for quasi-static cases uses a generalization of the Biot strain measure. The deriving schemes minimised via variational methods are structure preserving. That opens up a wide range of possibilities for robust and efficient nonlinear elastic simulation, improving on state of the art methods in geometry discretization schemes on solid mechanics.

MATRIX-FREE MULTIGRID FOR PHASE-FIELD FRACTURE PROBLEMS

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Standard matrix-based FEM requires huge amounts of memory as the number of elements increases. This non neglectable drawback can be overcome by using matrix-free methods. Such methods do not require building and storing huge linear systems, instead they compute the necessary information on the fly. Hence, such approaches need far less memory than classical methods, which makes them the method of choice for very large problems. Without the matrix at hands, the number of available solvers is very limited, i.e., direct solvers and algebraic multigrid methods are no longer possible. A class of solvers that is very suitable in this case are geometric multigrid methods. These methods do not require explicit knowledge about the matrix entries and, thus, can be applied in a matrix-free fashion. In this talk, we present a framework for the matrix-free solution to a monolithic quasi-static phase-field fracture model. The equations of interest are nonlinear and need to satisfy a variational inequality. This imposes several challenges for the implementation, which will be discussed throughout the talk. Finally, several numerical examples are presented to show the applicability and parallel scalability of the matrix-free geometric multigrid solver.

GPU-ACCELERATED DISCONTINUOUS GALERKIN METHODS ON POLYTOPIC MESHES

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Discontinuous Galerkin finite element methods have received considerable attention during the last two decades. By combining advantages from both FEMs and FVMs they allow the simple treatment of complicated computational geometries, ease of adaptivity and stability for non-self-adjoint PDE problems. Greater flexibility comes at an increased computational cost if we compare DGFEMs directly with conforming FEMs, but this is a naive approach since it overlooks the key advantages of DGFEMs. Their greater mesh-flexibility allows for the handling of extremely general computational meshes, consisting of polytopic elements with arbitrary number of faces and different polynomial degree on each element. This can reduce both the higher number of degrees of freedom, regularly associated with them, and also the higher cost of computing numerical fluxes along faces. In this vein, we will present our results on a massively parallel implementation of a space-time time-stepping dG-method on CUDA-enabled graphics cards. In particular, we will showcase almost linear scalability of the assembly step with respect to the number of cores used. In turn, this can justify the claim that polytopic dG methods can be implemented extremely efficiently, as the additional assembly overhead of quadratures over polytopic domains is eliminated.

NUMERICAL APPROXIMATION OF SEMILINEAR SUBDIFFUSION EQUATIONS WITH NONSMOOTH INITIAL DATA

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We consider the numerical approximation of a semilinear fractional order evolution equation involving a Caputo derivative in time of order $\alpha \in (0,1)$. Assuming a Lipschitz continuous nonlinear source term and an initial data $u_0 \in \dot{H}^\nu(\Omega)$, $\nu \in [0,2]$, we discuss existence, stability, and provide regularity estimates for the solution of the problem. For a spatial discretization via piecewise linear finite elements, we establish optimal $L^2(\Omega)$-error estimates for cases with smooth and nonsmooth initial data, extending thereby known results derived for the classical semilinear parabolic problem. We further investigate fully implicit and linearized time-stepping schemes based on a convolution quadrature in time generated by the backward Euler method. Our main result provides pointwise-in-time optimal $L^2(\Omega)$-error estimates for both numerical schemes. Numerical examples in one- and two-dimensional domains are presented to illustrate the theoretical results.

CONVERGENCE STUDIES FOR A PML-FEM SOLVER IN WATER WAVE SCATTERING PROBLEMS

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The 'optimal' Perfectly Matched Layer (PML) by [A. Bermudez, L. Hervella-Nieto, A. Prieto, R. Rodriguez, 2010. Perfectly matched layers for time-harmonic second order elliptic problems, Arch. Comput. Methods 17, pp. 77-107] is an effective computational region truncation technique for time-harmonic wave scattering problems that are inherently defined in infinite domains. The PML model in question, proven optimal for the Helmholtz equation, features an unbounded absorbing function that requires no *a priori* tuning, as opposed to classical PML adaptations that are based on polynomial functions. In [R. Cimpeanu, A. Martinsson, M. Heil, 2015. A parameter-free perfectly matched layer formulation for the finite-element-based solution of the Helmholtz equation. J. Comput. Phys. 296, 329 347], extensive numerical studies suggest that the singular PML introduced by Bermudez et al. is highly efficient even at a thickness that is several orders of magnitude smaller than the examined principal wavelength, rendering it cost-effective compared to other boundary termination methods. Recently, a PML-FEM solver utilising linear triangles was proposed for water wave propagation problems in coastal regions, featuring scatterers such as shoals, seabed founded structures, etc. [A. E. Karperaki, T. K. Papathanasiou, K. A. Belibassakis, 2019. An optimized, parameter-free PML-FEM for wave scattering problems in the ocean and coastal environment, Ocean Eng. 179, pp. 307-324]. The field equation adopted in this work was the Modified Mild Slope equation [S. R. Massel, 1993. Extended refraction-diffraction equation for surface waves. Coast. Eng. 19, pp. 97 127.], which can be reformulated as a Helmholtz equation with variable coefficients.

In the present contribution, numerical experiments of the employed PML-FEM strategy are performed in order to verify the convergence characteristics, for problems with sufficient regularity, dictated by the underlying approximation error. Several problems, including scattering by an array of founded cylinders, relevant to coastal engineering and hydroacoustics, are analysed and the method is found to produce optimal convergence rates up to a certain point of refinement. Beyond that point however, round off errors become dominant, leading to inferior results and performance. The small thickness of the employed PML model, although highly appealing due to the reduction of degrees of freedom, can cause numerical issues during the implementation of Gauss quadrature for the numerical integration of stiffness and mass type matrices. In particular, since the equation coefficients are variable and the elements size is very small inside the layer, Gauss points and weights are not implemented appropriately, suffering misplacement due to inexact

calculations. The performed numerical experiments indicate that, given a consistent implementation and an appropriate refinement level, the singular PML-FEM solver operates with optimal convergence rates in a very wide range of incident wave frequencies and is therefore an effective simulation tool for coastal engineering applications.

STOCHASTIC GALERKIN MIXED FINITE ELEMENT APPROXIMATION FOR LINEAR POROELASTICITY WITH UNCERTAIN INPUTS

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Over the last couple of decades, mathematical models of fluid flow through deformable porous media have gained a lot attention due to their wide applicability in science and engineering. In particular, Biot's consolidation model arises in applications ranging from geoscience to medicine. In such applications, we encounter scenarios where there is uncertainty about the model inputs.

In this talk, we discuss a novel locking-free stochastic Galerkin mixed finite element method for the Biot consolidation model with uncertain Young's modulus and hydraulic conductivity field. After introducing a five-field mixed variational formulation of the standard Biot consolidation model, we discuss stochastic Galerkin mixed finite element approximation, focusing on the issue of well-posedness and efficient linear algebra for the discretized system. We introduce a new preconditioner for use with MINRES and establish eigenvalue bounds. Finally, we present specific numerical examples to illustrate the efficiency of our numerical solution approach.

ANALYSIS OF A SPACE–TIME HYBRIDIZABLE DISCONTINUOUS GALERKIN METHOD FOR THE ADVECTION–DIFFUSION PROBLEM ON TIME-DEPENDENT DOMAINS

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A viable candidate for the solution of partial differential equations on time-dependent domains is the space-time discontinuous Galerkin (DG) method, wherein the problem is fully discretized in space and time using discontinuous finite elements. The resulting scheme is well suited to handle moving and deforming domains but at a significant increase in computational cost in comparison to traditional time-stepping methods. Attempts to rectify this situation have led to the pairing of space-time DG with the hybridizable DG (HDG) method. The combination of the two methods retains the higher-order accuracy and geometric flexibility of space-time DG while mitigating the computational burden through the use of static condensation.

In this work, we introduce and analyze a space-time HDG method for the time-dependent advection-diffusion problem on moving domains. We discuss well-posedness of the discrete system, and we derive theoretical rates of convergence in a mesh-dependent norm.

A SPATIAL DISCONTINUOUS GALERKIN METHOD WITH RESCALED VELOCITIES FOR THE BOLTZMANN EQUATION

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In the talk we present a numerical method for the Boltzmann equation. It is a spectral discretization in the velocity and a discontinuous Galerkin discretization in physical space. To obtain uniform approximation properties in the mach number, we shift the velocity by the (smoothed) bulk velocity and scale it by the (smoothed) temperature, both extracted from the density distribution. The velocity trial functions are polynomials multiplied by a Maxwellian. Consequently, an expansion with a low number of trial functions already yields satisfying approximation quality for nearly equilibrated solutions. By a polynomial test space, density, velocity and energy are conserved on the discrete level. To stabilize the free flow operator we use upwind fluxes in phase space. Several numerical results are presented to justify our approach.

DOMAIN DECOMPOSITION IN COMPUTATIONAL HOMOGENIZATION WITH MILLION-WAY PARALLELISM

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The computational simulation of modern high-strength steel materials with micro structure is still a challenge. As a computational homogenization approach we consider the FE^2 method combined with efficient parallel domain decomposition methods of FETI-DP type. In the FE^2 approach, in each Gauss integration point of the macroscopic problem, a microscopic problem on a representative volume element (RVE) is solved. The microscopic problems are only coupled through the macroscopic level and can be solved all in parallel. Each of these microscopic problems itself will be solved using a parallel FETI-DP domain decomposition method. This approach is implemented in PETSc and uses efficient solver packages including BoomerAMG, MUMPS, and UMFPACK, resulting in the parallel computational homogenization software FE2TI. We present weak scalability results obtained using several hundred thousands of cores and more than a million MPI ranks.

ON ALGEBRAICALLY STABILIZED METHODS FOR CONVECTION-DIFFUSION PROBLEMS

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Most of the methods developed for the numerical solution of convection-dominated problems either do not suppress spurious oscillations in layer regions sufficiently, or introduce too much artificial diffusion and lead to a pronounced smearing of layers. Nevertheless, some of the algebraically stabilized methods seem not to suffer from these two deficiencies. These schemes are designed to satisfy the discrete maximum principle by construction (so that spurious oscillations cannot appear) and provide sharp approximations of layers.

Based on our previous research on algebraic flux corection schemes, we propose a new class of algebraically stabilized methods for convection–diffusion problems. We shall present a general existence and convergence theory and discuss the choice of limiters leading to the validity of the discrete maximum principle on arbitrary meshes. The theoretical findings will be illustrated by numerical results.

RECONSTRUCTION-BASED A-POSTERIORI ERROR ESTIMATION IN STRESS-BASED FEM FOR FRICTIONAL CONTACT PROBLEMS

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The use of stress-based finite element methods for the treatment of contact problems admits locking free performance in the incompressible limit as well as direct access to the surface forces at the contact zone. Consequently we are studying the application of the stress-based FEM described in [1] featuring next-to-lowest order Raviart-Thomas-Elements to the Signorini contact problem with Coloumb friction using a dual variational formulation similar to the one studied in [2].
Since frictional contact problems tend to feature singularities, adaptive refinement strategies are to be considered and reliable a-posteriori error estimation is needed. We therefore extend the a-posteriori error estimator in [5] to frictional contact and reconstruct a H^1-conforming displacement following the ideas in [3] and [4]. We prove reliablity of our error esitmator under similar assumptions as those made in [6] for uniqueness and test its efficiency by numerical experiments in two and three dimensions.

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A POSTERIORI ERROR ESTIMATION ON ANISOTROPIC MESHES

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Residual-type a posteriori error estimates in the maximum norm and the energy norm will be given for linear finite elements on anisotropic triangulations. The error constants are independent of the diameters and the aspect ratios of mesh elements and, in the case of a singularly perturbed equation, of the small perturbation parameter. Fully computable a posteriori error estimators and the efficiency of energy-norm error estimators on anisotropic meshes will also be addressed.

BARRIER FUNCTIONS IN THE ERROR ANALYSIS FOR FRACTIONAL-DERIVATIVE PARABOLIC PROBLEMS ON QUASI-GRADED MESHES

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An initial-boundary value problem with a Caputo time derivative of fractional order $\alpha \in (0,1)$ is considered, solutions of which typically exhibit a singular behaviour at an initial time. For this problem, building on [N. Kopteva, Error analysis of the L1 method on graded and uniform meshes for a fractional-derivative problem in two and three dimensions, Math. Comp., 2019], we give a simple and general numerical-stability analysis using barrier functions, which yields sharp pointwise-in-time error bounds on quasi-graded temporal meshes with arbitrary degree of grading. L1-type and higher-order discretizations in time are considered in combination with finite element spatial discretiztions. In particular, those results imply that milder (compared to the optimal) grading yields optimal convergence rates in positive time. Our theoretical findings are illustrated by numerical experiments.

STABLE AND CONVERGENT FULLY DISCRETE INTERIOR–EXTERIOR COUPLING OF MAXWELL'S EQUATIONS

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Maxwell's equations are considered with transparent boundary conditions, for initial conditions and inhomogeneity having support in a bounded, not necessarily convex three-dimensional domain or in a collection of such domains. The numerical method only involves the interior domain and its boundary. The transparent boundary conditions are imposed via a time-dependent boundary integral operator that is shown to satisfy a coercivity property. The stability of the numerical method relies on this coercivity and on an anti-symmetric structure of the discretized equations that is inherited from a weak first-order formulation of the continuous equations. The method proposed here uses a discontinuous Galerkin method and the leapfrog scheme in the interior and is coupled to boundary elements and convolution quadrature on the boundary. The method is explicit in the interior and implicit on the boundary. Stability and convergence of the spatial semi-discretisation are proven, and with a computationally simple stabilization term, this is also shown for the full discretization.

RECENT WORK ON TREECODES AND APPLICATIONS

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We review a recently developed kernel-independent treecode (KITC) algorithm based on barycentric Lagrange interpolation at Chebyshev points for fast summation of pairwise particle interactions [1]. This is joint work with Lei Wang (University of Wisconsin, Milwaukee) and Svetlana Tlupova (Farmingdale State College, Farmingdale).

Next we present an application of the KITC to accelerate the evaluation of the asymptotic correlation functions in 3D-RISM (Reference Interaction Site Model) for computation of thermodynamic properties and solvent structure of solvated biomolecules [2]. The 3D-RISM/KITC is demonstrated for a solvated tubulin (1TVK) with 13456 atoms on a grid of dimensions $320 \times 256 \times 256$ computed on 64 cores. This is joint work with Leighton Wilson (University of Michigan, Ann Arbor) and Tyler Luchko (California State University, Northridge).

Finally we present a boundary element method for the interaction energy of charged dielectric spheres immersed in solvent. Accuracy is improved by singularity subtraction and Richardson extrapolation, and the BEM is applied to demonstrate the like-charge attraction of asymmetric dielectric spheres. This is joint work with Zecheng Gan (University of Michigan, Ann Arbor) and Weihua Geng (Southern Methodist University, Dallas).

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OPTIMIZED SCHWARZ ALGORITHMS FOR DDFV DISCRETIZATION

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We introduce a new non-overlapping optimized Schwarz method for anisotropic diffusion problems. Optimized Schwarz methods are ideally suited for solving anisotropic diffusion problems since they can take into account the underlying physical properties of the problem at hand throught the transmission conditions. We present a discretization of the algorithm using discrete duality finite volumes (DDFV for short), which are ideally suited for anisotropic diffusion problem on general meshes. We present here the case of high order transmission conditions in the framework of DDFV. We prove convergence of the algorithm for a large class of symmetric transmission operators, including the discrete Ventcell operator. We also illustrate with numerical simulations that the use of high order transmission conditions (the optimized Ventcell conditions) leads to more efficient algorithms than the use of first order Robin transmission conditions, especially in case of strong anisotropic operators.

ON FAST ITERATIVE SOLVERS FOR PROBLEMS IN STRUCTURAL MECHANICS

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The prestressed concrete structure of civil engineering buildings can be modeled as a problem in linear elasticity for which one-, two- and three-dimensional finite elements are coupled by multi-point constraints. Multi-point constraints describe linear relationships between degrees of freedom and are introduced in the discrete system. Enforcing these constraints by Lagrange multipliers results in a symmetric indefinite matrix with a 2x2 block structure. In practice, these systems are very difficult to solve since they become quickly too large for direct solvers and common iterative methods work only poorly on them.
In this talk, we present a new iterative solver that is based on the Golub-Kahan bidiagonalization (GKB) method, which has been widely used in solving least-squares problems and in the computation of the singular value decomposition of rectangular matrices. The algorithm is applied to matrices that are generated by code_aster, an open-source finite element software developed at the French electricity utility company EDF. We show that the GKB method has excellent convergence properties for this problem class and that, for a good choice of some parameter, the number of iterations depends only weakly on the discretization size. This generalized GKB algorithm has also been implemented in PETSc and we present its scalability on practical problems. In particular, as a linear system of the size of the (1,1)-block has to be solved in each iteration of the GKB method, we compare the performance of direct and iterative methods for the solution of this inner linear system.

ON AN EFFICIENT PARALLEL IMPLEMENTATION OF ADAPTIVE FETI-DP WITH LOAD BALANCING

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Domain decomposition methods such as FETI-DP (Finite Element Tearing and Interconnecting - Dual Primal) and BDDC (Balancing Domain Decomposition by Constraints) are highly scalable parallel solvers for large sparse systems obtained from the discretization of partial differential equations (PDEs).

However, the convergence behavior of FETI-DP and BDDC methods with a standard coarse space highly depends on the parameters of the underlying PDE. The convergence rate of both methods can deteriorate significantly if composite materials are considered. In such cases, problem-dependent (or adaptive) coarse spaces offer a remedy. In adaptive methods, difficulties arisen from highly heterogeneous materials are detected automatically by solving local generalized eigenvalue problems and an adaptive coarse space is set up. These methods are thus characterized by great robustness.

Though, for an efficient parallel implementation, different issues such as load imbalances and the solution of unnecessary eigenvalue problems have to be avoided and the eigenvalue solver has to be optimized to reduce the computational overhead in the set up phase. We will present details of the set up of the adaptive method to implement the coarse space enrichment efficiently in a parallel context.

We will present weak and strong scaling results to show the good parallel scalability of our method.

A LOCALLY CONSERVATIVE PARTICLE-MESH STRATEGY FOR HYPERBOLIC CONSERVATION LAWS

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In an attempt to reconcile the advantages of a Lagrangian method with those of an Eulerian method, hybrid particle-mesh methods make combined use of Lagrangian particles and an Eulerian mesh. Particularly, using Lagrangian particles to account for the advective transport entails the promise of ruling out numerical diffusion and avoiding stabilization of the advection term. Simultaneously, the Eulerian mesh admits an efficient discretization of constitutive relations.

Despite many successful applications, it is not surprising that such an approach tends to have difficulties in unifying accuracy and exact conservation. Most notably so, since information is repeatedly projected back-and-forth between a discrete set of Lagrangian particles and an Eulerian mesh field.

In this contribution, a particle-mesh interaction strategy on arbitrary meshes is presented in which the aforementioned issue is fundamentally overcome. Central to the presented approach is to cast the particle-mesh interaction as a PDE-constrained minimization problem in such a way that, from a mesh-perspective, the transported Lagrangian particle field satisfies a hyperbolic conservation law. Loosely stated, the constrained particle-mesh projection for a scalar-valued field ψ_p defined on the Lagrangian particles reads

$$\min_{\psi_h} J = \sum_p \frac{1}{2} \left(\psi_h(\mathbf{x}_p(t), t) - \psi_p(t)\right)^2 \tag{1}$$

such that a scalar hyperbolic conservation law is satisfied in a weak sense.

with ψ_h the state variable to be approximated in an appropriate function space. Furthermore, the summation over p runs over all particles in the domain of interest.

Starting from Eq. (1), the optimality system for the scalar-valued constrained particle-mesh projection is derived, and - by introducing a facet-based control variable - it is shown that a hybridized Discontinuous Galerkin (HDG) framework naturally provides the ingredients required for the optimality control. Several properties of the resulting particle-mesh projection are derived, including consistency and local conservation. Furthermore, an efficient solution strategy using *static condensation* is proposed. Key features of the constrained particle-mesh projection are highlighted for a number of scalar advection benchmarks, demonstrating high-order accuracy and the absence of numerical diffusion.

The presented approach is believed be useful for a range of applications. In particular, it is shown how the particle-mesh projections can serve as a building block for mass conservative density tracking in multi-phase flows. To give attendees a headstart to apply the presented work to their own challenges, core functionality is made available under an open-source license in LEoPart[2].

APOSTERIORI ANALYSIS OF HP-DISCONTINUOUS GALERKIN TIMESTEPPING FOR FULLY DISCRETIZED PARABOLIC PROBLEMS

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We derive aposteriori error bounds in time-maximum-space-squared-sums and time-mean-squares-of-spatial-energy norms for a class of fully-discrete methods for linear parabolic partial differential equations (PDEs) on the space-time domain based on hp-version discontinuous Galerkin time-stepping scheme combined with conforming spatial Galerkin finite element method. The proofs are based on a novel space-time reconstructions, which combines the elliptic reconstruction Georgoulis, Lakkis & Virtanen (2011), Lakkis & Makridakis (2006), and Makridakis & Nochetto (2003) of and the time reconstruction for discontinuous time-Galerkin schemes Makridakis & Nochetto (2006), Sch tzau & Wihler (2010) into a novel tool, allows for the user's preferred choice of aposteriori error estimates in space and careful analysis of mesh-change effects.

MULTILEVEL MONTE CARLO METHODS FOR BAYESIAN INVERSE PROBLEMS

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In this talk we will look at Bayesian static parameter estimation using multilevel Monte Carlo (MLMC) for partially observed diffusions.

COUPLED SIMULATION OF MAGNETO-MECHANICAL PROBLEMS USING HP FINITE ELEMENTS APPLIED TO MRI SCANNERS

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Magnetic resonance imaging (MRI) is a diagnosis tool available in most of major medical centres. Its importance in the medical industry is continuously increasing due to its application to a wide range of medical areas such as tumour detection and neuroimaging. MRI scanners utilise a set of superconducting coils to generate a uniform strong magnetic field, and a set of gradient coils to produce pulsed field gradients in order to generate an image. These gradient fields give rise to eddy currents in conducting components, as well as Lorentz forces leading to vibrations and deformations. As such it represents a coupled physics problem involving low frequency electromagnetism and mechanics. The resulting eddy (Ohmic) currents and mechanical vibrations are undesirable, as they can lead to imaging artefacts, patient discomfort and helium boil-off.

In this presentation we will present a new computational methodology [1] to solve the coupled three- dimensional magneto-mechanical problem of interest. Our approach employs a Lagrangian description of the problem [2] and an AC-DC splitting of the fields to linearise the problem [3]. Through a subtle treatment, this leads naturally to a staggered computational methodology and, to ensure accurate solutions, a *hp*-finite element discretisation is employed. The talk will describe the complete computational approach including the coupling, linearisation, H^1 and $H(curl)$-conforming finite element discrestisation used to discretise the mechanical and electromagnetic fields, respectively, and the preconditioning approach employed for the solution of the large system of complex linear equations. The success of our proposed methodology will be demonstrated by making comparisons with our group's axisymmetric software [3] and measured data as well as applying it to complex challenging three-dimensional industrial benchmark problems, which are not rotationally symmetric.

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NONPERIODIC MULTISCALE PROBLEMS: SOME RECENT NUMERICAL ADVANCES

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The Multiscale Finite Element Method (MsFEM) is a Finite Element type approach for multiscale PDEs, where the basis functions used to generate the approximation space are precomputed and are specifically adapted to the problem at hand. The computation is performed in a two-stage procedure: (i) a offline stage, in which local basis functions are computed, and (ii) a online stage, in which the global problem is solved using an inexpensive Galerkin approximation. Several variants of the approach have been proposed and a priori error estimates have been established.

We will review some recent progresses on the approach, aiming at:

- developping a more robust method, less sensitive to the geometry of the heterogeneities;
- understanding the approach in contexts more general than the classical purely diffusive context (such as the case of advection-diffusion equations in the regime when convection dominates over diffusion, and where stabilization-type methods may be needed);
- designing a posteriori error estimates, on the basis of which a strategy for adaptive discretization can be introduced.

This talk is based on joint works with L. Chamoin, C. Le Bris and F. Madiot.

Relevant references include [C. Le Bris, F. Legoll and F. Madiot, Multiscale Finite Element methods for advection-dominated problems in perforated domains, SIAM MMS, in press, arxiv preprint 1710.09331] and [L. Chamoin and F. Legoll, A posteriori error estimation and adaptive strategy for the control of MsFEM computations, CMAME 2018].

HIGHER ORDER UNFITTED FEM ON MOVING DOMAINS

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The methodology of unfitted finite element methods, i.e. methods which are able to cope with interfaces or boundaries which are not aligned with the grid, has been investigated for different problems in recent years. However, the development of numerical methods which are flexible with respect to the geometrical configuration, robust and *higher order accurate* at the same time is still challenging. One major issue in the design and realization of higher order finite element methods is the problem of accurate and stable numerical integration on time-dependent (level set) domains. We present two approaches which allow for a higher order accurate and robust numerical treatment of domains that are prescribed by level set functions. To obtain higher order accuracy in space we use an approach that is based on specifically tailored isoparametric mappings. We combine this approach with either a *space-time* discretization or a recently introduced *stabilized time stepping* based on more standard finite difference schemes. We introduce and compare the two approaches and present theoretical and numerical results.

FINITE ELEMENT METHODS FOR THE CURL-CURL EQUATION WITH MIXED BOUNDARY CONDITIONS

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The curl-curl equation is a model problem in theoretical and numerical electromagnetism. The largest share of the literature on the curl-curl equation treats only essential and natural boundary conditions. However, the curl-curl equation with *mixed boundary conditions* shows surprising qualitative features that are not present in the case of classical essential or natural boundary conditions. We study their impact on the design of mixed finite element methods with weakly imposed divergence constraints and their adaptive theory.

The nullmodes of the variational formulation, the *harmonic vector fields*, relate to algebraic topology. The harmonic vector fields are curl-free and divergence-free and satisfy homogeneous tangential and normal boundary conditions along complementary boundary parts. The dimension of this nullspace is the first Betti number of the domain relative to the essential boundary part. The nullspace of the variational formulation is a qualitative feature that should be replicated by any mixed finite element method.

Commuting projection operators from the continuous de Rham complex onto the finite element de Rham complex are central to the theoretical analysis of the mixed finite element method. A uniformly L^2-bounded *commuting projection* for the case of mixed boundary conditions has been derived recently, involving tools from Lipschitz topology and geometric measure theory.

Whereas the *Falk-Winther interpolant* commutes with the differential operators and satisfies local bounds, it has only been studied for the case of natural boundary conditions. Our uniformly bounded commuting projection facilitates extending the Falk-Winther interpolant to the case of mixed boundary conditions.

These projection operators appear in the analysis of adaptive mixed finite element methods. On the one hand, this talk describes the tools by which we can extend Demlow's adaptive procedure for the computation of harmonic vector fields to the case of mixed boundary conditions. On the other hand, this talk introduces several new results in the adaptive theory of finite element exterior calculus. We derive efficient a posteriori error estimates for several error components in the Hodge-Laplace equation, avoiding the obstacles faced by prior error estimators, and establish quasi-optimal convergence of our adaptive procedure.

FILTERING FOR DISCONTINUOUS GALERKIN METHOD: CHALLENGING THE ASSUMPTION OF UNIFORMITY

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Previous investigations into accuracy enhancement for a discontinuous Galerkin solution demonstrated that there are many ways to approach obtaining higher-order accuracy in the solution, for example, the post-processing technique. For the discontinuous Galerkin method, the order of accuracy without filtering (or say post-processing) is $k+1$. For the filtered solution, it is $2k+1$. Additionally, the filtering introduces higher levels of smoothness into the new approximation. However, previous investigations were mainly limited to uniform meshes (or nearly uniform meshes) consideration, which is highly restrictive for practical application. In this talk, we discuss the challenges and difficulties for nonuniform meshes. Additionally, we present several common techniques of for nonuniform meshes will be introduced. Moreover, we purpose a new technique which considers the mesh structure as a parameter when dealing the nonuniform meshes. A comparison is made among these techniques through numerical examples. Furthermore, the application of the new purposed technique for triangular meshes is also included.

EDGE MULTISCALE METHODS FOR ELLIPTIC PROBLEMS WITH HETEROGENEOUS COEFFICIENTS

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In this paper, we proposed two new types of edge multiscale methods to solve Partial Differential Equations (PDEs) with high-contrast heterogeneous coefficients: Edge Spectral Multiscale Finte Element Method (ESMsFEM) and Wavelet-based Edge Multiscale Finite Element Method (WEMsFEM). Their convergence rates for elliptic problems with high-contrast heterogeneous coefficients are demonstrated in terms of the coarse mesh size H, the number of spectral basis functions and the level of the wavelet space ℓ, which are verified by extensive numerical tests.

OPTIMAL CONTROL IN A BOUNDED DOMAIN FOR WAVE PROPAGATING IN THE WHOLE SPACE: COUPLED THROUGH BOUNDARY INTEGRAL EQUATIONS

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This paper is concerned with an optimal control problem in a bounded-domain Ω_0 under the constraint of a wave equation in the whole space. The problem is regularized and then reformulated as an initial-boundary value problem of the wave equation in a bounded domain $\Omega \supset \overline{\Omega}_0$ coupled with a set of boundary integral equations on $\partial\Omega$ taking account of wave propagation through the boundary. The well-posedness and stability of the reformulated problem are proved. A fully discrete finite element method is proposed for solving the reformulated problem. In particular, the wave equation in the bounded domain is discretized by an averaged central difference method in time, and the boundary integral equations are discretized in time by using the convolution quadrature generated by the second-order backward difference formula. The finite and boundary element methods are used for spatial discretization of the wave equation and the boundary integral equations, respectively. The stability and convergence of the numerical method are also proved. Finally, the spatial and temporal convergence rates are validated numerically in 2D.

DEVELOPMENT AND ANALYSIS OF FINITE ELEMENT AND FOURTH-ORDER FINITE DIFFERENCE METHODS FOR AN EQUIVALENT BERENGER'S PML MODEL

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In this paper, we continue our study of the equivalent Berenger's PML model formulated by Bécache and Joly in 2002. Here we will focus on developing and analyzing both finite element and high-order finite difference methods for solving the model. Numerical stability similar to the continuous model for both methods are established. Numerical examples implementing both methods are presented.

RIGOROUS EIGENVALUE ESTIMATION AND ITS APPLICATION IN COMPUTER-ASSISTED SOLUTION PROOF FOR THE NAVIER–STOKES EQUATION

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The explicit eigenvalue bounds for differential operators play an important role in the field of computer-assisted proof. For example, to provide mathematically correct solution verification for no-linear partial differential equations, e.g., the Navier–Stokes equation, there appears many quantities reducing to the eigenvalue problem of differential operators. A brief list includes the Poincare constant, the constant in trace theorem, the interpolation error constants, etc.

In this talk, I will first review recently developed numerical methods with the aim of explicit bounds of eigenvalues, especially the ones based on the finite element methods. Particularly, the method proposed in [1] will be mainly introduced, due to its generality in solving various eigenvalue problems, including the ones of the Laplacian [1], the biharmonic [3, 2], the Stokes [4], the Steklov operators [5]. As a direct application of explicit eigenvalue bounds, the case of the solution verification for stationary Navier–Stokes equation in 2D and 3D domains will be introduced [6].

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HYBRID SPECTRAL AND TIME DOMAIN NONLINEAR MAXWELL SOLVER

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In this talk, we report our recent progress on the development of a hybrid spectral and time domain method for solving Maxwell equations in complex media. Our goal is to be able to accurately model the electromagnetic wave propagation in general nonlinear media over a distance longer than hundreds or thousands of wavelengths. We apply the unidirectional pulse propagation equation (UPPE) to propagates the optical wave in spectral domain. The UPPE is derived from the Maxwell equations by assuming that the backward-scattered field can be neglected. In the region where we want to consider the backward-scattered field, we apply the finite difference time domain (FDTD) method. The FDTD method is a full vector Maxwell solver in time domain. To test the performance of our method, we simulate the optical pulse propagation in complex media with Lorentz dispersion and Kerr nonlinearity.

ALGEBRAIC FLUX CORRECTION FOR ADVECTION PROBLEMS AND ITS EXTENSION TO SYMMETRIC TENSOR FIELDS

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The work to be presented in this talk extends the algebraic flux correction (AFC) methodology to advection(-reaction) equations and symmetric tensor fields [3]. The new theoretical results are used to design bound-preserving finite element methods for steady and unsteady model problems. The proposed approaches add algebraically defined artificial diffusion operators to the Galerkin discretization. Then limited antidiffusive fluxes are incorporated into the residual of the resulting low order method to remove redundant diffusivity and to improve the accuracy of the approximation.

In the case of the steady state advection problem with a scalar solution, convergence with order $\frac{1}{2}$ is shown by adapting an a priori error estimate derived in [1]. Existence of a unique solution is proved under suitable assumptions. Furthermore, sufficient conditions for the validity of generalized discrete maximum principles (DMPs) are formulated. In addition to guaranteeing boundedness of the function values in terms of weakly imposed boundary conditions, they provide local L^∞ estimates for subsets of degrees of freedom. These DMP results are extended to the transient advection equation discretized in time by the θ-scheme. A priori time step restrictions are derived for $\theta \in [0, 1)$. The analysis of the forward Euler time discretization implies that bound-preserving approximations of higher order can be obtained without solving nonlinear systems if explicit strong stability preserving (SSP) Runge-Kutta time integrators are employed. Based on the results of theoretical studies, new definitions of correction factors are proposed which potentially facilitate the development of more efficient solvers and/or implementations.

Using the concept of Löwner ordering, the scalar AFC framework is extended to the numerical treatment of symmetric tensor quantities. In tensorial versions of the methods under consideration, antidiffusive fluxes are limited to constrain the eigenvalue range of the tensor field by imposing discrete maximum principles on the extremal eigenvalues [2]. This criterion is shown to be an appropriate frame invariant generalization of scalar maximum principles. It leads to a family of robust property-preserving limiters based on the same design principles as their scalar counterparts.

The potential of the presented methods is illustrated by numerical examples.

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A UNIFORM PARALLEL FRAMEWORK TO LARGE-SCALE FINITE ELEMENT SIMULATIONS OF 3D WAVE-TYPE EQUATIONS

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In many engineering areas such as nondestructive testing of materials and structures investigation of ultrasonic waves is of a great importance. In the talk we first recall the finite element approximation theory of the initial-boundary-value problem for the wave-type equations such as acoustics, elastodynamics, or Maxwell equations. We support the expected convergence rates with 3d numerical experiments. Further we describe a uniform framework for parallel implementation of matrix-vector product and inner-product regardless of the used type of 3d elements, e.g. Lagrange or Nédélec. The linear systems arising within an implicit time-discretization scheme are preconditioned by proper smoothers. Finally, we present parallel scalability of our approach up to a billion equations and hundreds of computational cores. We observe only a modest grow of conjugate gradient iterates regardless of a missing coarse problem, which makes the method convenient for solution to engineering problems at large scale.

DUALITY-BASED MODEL ADAPTIVITY FOR MULTISCALE FINITE ELEMENT METHODS

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A large class of modeling problems in Physics and Engineering is of multiscale character, meaning, that relevant physical processes act on highly different length scales. This usually implies high computational cost for a full resolution of the problem. One way to avoid such a full resolution are multiscale schemes, where, generally speaking, an effective model is solved on a coarse scale with upscaled, effective parameters. Those paramaters are determined with the help of localized sampling problems on a fine scale.

Multiscale schemes introduce significant complexity with respect to sources of error, not only are there discretization errors on a coarse and fine scale, but also a model error introduced by the modeling assumption. This makes suitable a posteriori strategies necessary.

In this talk different model adaptation strategies for the Variational Multiscale Method (VMM) and the Heterogeneous Multiscale Method (HMM) are examined and a general framework for model adaptation (based on the HMM) is introduced. The framework is derived within the setting of "goal-oriented" adaptivity given by the so-called Dual Weighted Residual (DWR) method.

Based on the framework a sampling-adaptation strategy is proposed that allows for simultaneous control of discretization and model errors with the help of classical refinement strategies for mesh and sampling regions. Further, a model-adaptation approach is derived that interprets model adaptivity as a minimization problem of a local model-error indicator.

PARALLEL SOLVERS WITH ADDITIVE SCHWARZ PRECONDITIONING FOR HIGH-ORDER TRANSPORT PROBLEMS

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In this talk we present several fast solvers for high-order transport problems, based on the Additive Schwarz Preconditioner for DG methods published by P Antonietti and P Houston 2011 [1] in conjunction with the work by F Mukhamedov in 2018 [2]. Our variant uses optimized basis functions to reduce the block size in the sparse-block system for the high-order DG method, by reducing the non-zero entries caused by the penalty terms without negative impact on the condition number. In addition we describe a suitable data structure, compatible with Additive Schwarz Preconditioner to minimise the communication costs, which makes use of the optimised basis functions. Our third variant of the solver replaces the block-inverse for the coarse grid subspace with a suitable Multigrid method, without penalty for the interations numbers, reducing the computational costs further, while keeping the minimised communication costs. We will present numerical results achieved on a cluster system, showing the scalability of the method, for two-dimensional and three-dimensional problems.

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NUMERICAL UPSCALING OF PERTURBED DIFFUSION PROBLEMS

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We consider elliptic partial differential equations with rapidly varying diffusion coefficient. In particular we study problems where the coefficient can be represented as a perturbation of a reference coefficient. We develop an efficient numerical method for solving multiple perturbed problems by reusing local computations, performed with the reference coefficient. The proposed method is based on the Petrov–Galerkin Localized Orthogonal Decomposition (PG-LOD) method which is a generalized finite element method with multiscale shape functions in the trial space. We focus on two types of perturbations. First, local defects which we treat by recomputation of multiscale shape functions. Second, global mappings of a reference coefficient for which we apply the domain mapping method. We show several numerical examples illustrating out theoretical findings.

THE NONCONFORMING VIRTUAL ELEMENT METHOD FOR ELLIPTIC PROBLEMS

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We present the nonconforming Virtual Element Method (VEM) for the numerical treatment of elliptic problems. This formulation works on very general unstructured meshes in 2D and 3D for arbitrary order of accuracy. The connection with the conforming VEM is discussed and examples of applications, e.g., the Poisson and Stokes equations as well as general diffusion problems (advection-diffusion-reaction equations) are presented. Numerical experiments verify the theory and validate the performance of the proposed method.

PHASE FIELD FRACTURE MODELLING OF HYDROGEN EMBRITTLEMENT

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Hydrogen embrittlement is arguably one of the most challenging problems in traditional solid mechanics. Hydrogen is ubiquitous, diffuses rapidly through the crystal lattice, and drastically reduces the ductility and fracture toughness of metals. The sensitivity to hydrogen damage increases with the yield strength and hydrogen related failures are now pervasive in the energy, defence, transport, and construction sectors. The prevention and modelling of hydrogen-induced fracture requires capturing multiple micro-mechanical and chemical phenomena across a wide range of scales. We take advantage of recent developments in variational methods for fracture to develop a novel phase field formulation for hydrogen assisted cracking. The model builds upon a coupled mechanical and hydrogen diffusion response, driven by chemical potential gradients, and a hydrogen-dependent fracture energy degradation law grounded on first principles calculations. The coupled problem is solved in an implicit time integration scheme, where displacements, phase field order parameter and hydrogen concentration are the primary variables. We showcase the capabilities of the model by addressing engineering case studies with complex loading conditions and crack trajectories. It is found that phase field formulations for fracture are particularly suitable to capture material degradation due to hydrogen. The finite element code developed can be downloaded from www.empaneda.com/codes.

THE TREFFTZ VIRTUAL ELEMENT METHOD

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Recently, an evolution of the virtual element method (VEM), called the Trefftz VEM, has been introduced [1, 2, 3, 4]. The main idea of this class of methods is that they are not based on standard polynomial-based approximation spaces, but rather on "problem–dependent" approximation spaces, consisting of functions which typically belong to the kernel of the differential operator appearing in the PDE under consideration.

The advantage of this approach over standard methods is that the computational cost in order to achieve a given accuracy is highly reduced. Importantly, using a filtering-and-orthogonalization technique, which is, to the best of our knowledge, not applicable in other settings, by using the Trefftz VEM, one can get convergence rates in terms of the dimension of the approximation spaces that are asymptotically better than those achieved by using other effective technologies, such as the Trefftz discontinuous Galerkin method.

In this talk, we present an overview and recent advancements in Trefftz VEM.

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VARIATIONAL TIME DISCRETISATIONS OF HIGHER ORDER AND HIGHER REGULARITY

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Starting from the well-known discontinuous Galerkin (dG) and continuous Galerkin-Petrov (cGP) methods we will present a two-parametric family of time discretisation schemes which combine variational and collocation conditions. The first parameter corresponds to the ansatz order while the second parameter is related to the global smoothness of the numerical solution. Hence, higher order schemes with higher order regularity can be obtained by adjusting the family parameters in the right way.

All members of the considered family show the same stability properties as either dG or cGP. Furthermore, the considered schemes provide a cheap post-processing to achieve better convergence orders in integral-based norms. In addition, the post-processing could be used for adaptive time-step control.

Error estimates and numerical results will be given.

A DISCONTINUOUS GALERKIN APPROXIMATION TO THE ELASTODYNAMICS EQUATION ON POLYGONAL AND POLYHEDRAL MESHES

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The study of direct and inverse wave propagation phenomena is an intensive research area and one important field application includes large-scale seismological problems and ground-motion induced by seismic events. From the mathematical perspective, the physics governing these phenomena can be modeled by means of the elastodynamics system. From the numerical viewpoint, a number of distinguishing challenges arise when tackling such kind of problems, and reflect onto the following features required to the numerical schemes: accuracy, geometric flexibility and scalability.

In recent years, high order Discontinuous Galerkin (DG) methods have became one of the most promising tool in computational seismology. Indeed, thanks to their local nature, DG methods are particularly apt to treat highly heterogeneous media, or in soil-structure interaction problems, where local refinements are needed to resolve the different spatial scales.

In this work we propose and analyze a high-order DG finite element method for the approximate solution of wave propagation problems modeled by the elastodynamics equations on computational meshes made by polygonal and polyhedral elements. We analyze the well posedness of the resulting formulation, prove hp-version error a-priori estimates, and present a dispersion analysis, showing that polygonal meshes behave as classical simplicial/quadrilateral grids in terms of dispersion properties. The theoretical estimates are confirmed through various two-dimensional numerical verifications.

HP-FEM FOR THE SPECTRAL FRACTIONAL LAPLACIAN IN POLYGONS

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For the spectral fractional Laplacian in polygons we present two types of discretizations that converge at an exponential rate. The first one is based on the Caffarelli-Silvestre extension, which realizes the non-local fractional Laplacian as a Dirichlet-to-Neumann map of a (degenerate) elliptic boundary value problem (BVP). This BVP is amenable to a discretization by high order finite element method (hp-FEM). Exponential convergence of the hp-FEM can be achieved if the underlying meshes are suitably refined towards the edges of the polygon so as to resolve the boundary singularities and towards the vertices in order to capture the corner singularities. The second discretization is based on the so-called "Balakrishnan" formula, an integral representation of the inverse of the spectral fractional Laplacian. The discretization of the integral leads to a collection of BVPs, which can be discretization by hp-FEM. Again, the use of meshes that are refined towards the vertices and the boundary leads to exponential convergence.

AFEM FOR THE FRACTIONAL LAPLACIAN

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For the discretization of the integral fractional Laplacian $(-\Delta)^s$, $0 < s < 1$, based on piecewise linear functions, we present and analyze a reliable weighted residual *a posteriori* error estimator. In order to compensate for a lack of L^2-regularity of the residual in the regime $3/4 < s < 1$, this weighted residual error estimator includes as an additional weight a power of the distance from the mesh skeleton. We prove optimal convergence rates for an h-adaptive algorithm driven by this error estimator in the framework of [Carstensen, Feischl, Page, Praetorius, axioms of adaptivity, CAMWA 2014]. Key to the analysis of the adaptive algorithm are novel local inverse estimates for the fractional Laplacian.

A DIVERGENCE FREE GALERKIN NUMERICAL SCHEME FOR DOUBLE-DIFFUSION EQUATIONS IN POROUS MEDIA

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A stationary Navier-Stokes-Brinkman model coupled to a system of advection-diffusion equations serves as a model for so-called double-diffusive viscous flow in porous media in which both heat and a solute within the fluid phase are subject to transport and diffusion. The solvability analysis of these governing equations results as a combination of compactness arguments and fixed-point theory. In addition an $\boldsymbol{H}(\mathrm{div})$-conforming discretisation is formulated by a modification of existing methods for Brinkman flows. The well-posedness of the discrete Galerkin formulation is also discussed, and convergence properties are derived rigorously. Computational tests confirm the predicted rates of error decay and illustrate the applicability of the methods for the simulation of bacterial bioconvection and thermohaline circulation problems.

ANALYSIS OF LOCAL DISCONTINUOUS GALERKIN METHODS WITH GENERALIZED NUMERICAL FLUXES FOR LINEARIZED KDV EQUATIONS

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In this talk, we analyze the local discontinuous Galerkin method using generalized numerical fluxes for linearized Korteweg–de Vries equations. The LDG scheme utilizes three independent weights in generalized numerical fluxes for convection and dispersion terms so that it provides more flexibility. By using inherent relations of three different numerical viscosity coefficients resulting from numerical fluxes, we first show a *uniform* stability for the auxiliary variables and the prime variable as well as its time derivative. To derive optimal error estimates of LDG methods with generalized fluxes for high order wave equations, a suitable design of the numerical initial condition with optimal convergence properties for all variables is vital. To this end, we then define and analyze a special numerical initial condition, which is nothing but the LDG approximation with the same numerical fluxes to the corresponding steady–state equation. Thus, optimal error estimates of order $k+1$ are obtained by using an energy analysis in combination with some particularly designed generalized Gauss–Radau projections, where k is the highest polynomial degree of discontinuous finite element space. The central numerical fluxes in the LDG scheme are also discussed. Numerical experiments are given to demonstrate the theoretical results.

NUMERICAL RESOLUTION THROUGH OPTIMIZATION OF $\det(\mathrm{D}^2 U) = F(U)$

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Several problems in geometry lead to equations of the form

$$g(\nabla u)) \det(\mathrm{D}^2 u) = a(u), \tag{1}$$

where $g : \mathbf{R}^d \to \mathbf{R}$ is a probability density and $a : \mathbf{R} \to \mathbf{R}$ decays sufficiently fast at infinity:

- For $a(t) = \exp(-t)$ this equation is related to the moment measure problem studied in [D. Cordero-Erausquin, B. Klartag, Journal of functional analysis, **268** (12), 3834–3866, 2015];
- For $a(t) = t^{-d+2}$ this equation appears in the construction of $(d-1)$-dimensional affine hemispheres in convex geometry [B. Klartag, arXiv:1508.00474, 2015].

As in optimal transport, one can define a Brenier solution to equation (1) as a convex function $u : \mathbf{R}^d \to \mathbf{R} \cup \{+\infty\}$ which satisfies $\nabla u_{\#} a(u) = \mu$, where μ is the measure on $\mathbf{R}^d$ with density g with respect to the Lebesgue measure. When $a(t) = \exp(-t)$ or $a(t) = t^{-d+2}$, Brenier solutions to (1) maximize a concave functional similar to the one appearing in Kantorovich duality. We will show that this leads to efficient numerical methods when the measure μ is finitely supported. In the moment measure case, we will deduce the convergence of a Newton algorithm from a discrete version of the differential Brascamp-Lieb inequality.

THE UNSTEADY, INCOMPRESSIBLE STOKES EQUATIONS WITH COMPATIBLE DISCRETE OPERATOR SCHEMES

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We investigate the extension of Compatible Discrete Operator schemes (CDO) [1] to the unsteady, incompressible Stokes equations.

CDO is a unifying framework on low-order mimetic schemes which preserve at the discrete level the structural properties of the PDEs, such as conservation laws and mathematical relations involving differential operators, while still ensuring competitive computational performances. General, polytopal and nonmatching meshes can be considered. Several discretizations are possible according to the mesh entities on which the main unknowns are defined. For the problem at hand, a full 3D face-based discretization has been selected, hence making the method close to the Hybrid High-Order method [2] for $k = 0$. A divergence operator relying on the Green theorem ensures the velocity-pressure coupling. Concerning the viscosity part, the scheme hinges on a stabilized gradient reconstruction which is piecewise constant on the sub-cell pyramids. Cell-based degrees of freedom are used as well, but eliminated before the assembly stage by means of static condensation.

In order to deal with the velocity-pressure coupling in the time-dependent case, several methods can be considered. In addition to the fully-coupled monolithic one, two well-known segregated approaches can be taken into account: the Augmented Lagrangian-Uzawa (ALU) and the Artificial Compressibility (AC) methods. Both schemes involve at least one user-parameter but, in the unsteady case, differently from the ALU, which consists in an iterative procedure, the AC framework has the advantage of requiring only one pressure update for the lowest-order time discretization, hence ensuring superior performances. Moreover, higher order time schemes can be devised as shown in [3]. The price to pay for this benefit is a non-divergence-free velocity: in fact, the method itself hinges on a small perturbation of the incompressibility constraint. We then explore the effects of such a velocity when it is used in a pure convection problem to transport a passive tracer.

Results concerning the latest developments towards the Navier-Stokes equations will be presented as well.

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A MULTILEVEL ALGEBRAIC ERROR ESTIMATOR AND THE CORRESPONDING ITERATIVE SOLVER WITH p-ROBUST BEHAVIOR

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In this work, we consider conforming finite element discretizations of arbitrary polynomial degree $p \geq 1$ of the Poisson problem. We propose a multilevel a posteriori estimator of the algebraic error. We prove that this estimator is reliable and efficient (represents a two-sided bound of the error), with a constant independent of the degree p. We next design a multilevel iterative algebraic solver from our estimator and we show that this solver contracts the algebraic error on each iteration by a factor bounded independently of p. Actually, we show that these two results are equivalent. The p-robustness results rely on the work of Schöberl *et al.* [IMA J. Numer. Anal., 28 (2008), pp. 1–24] for one given mesh. We combine this with the design of an algebraic residual lifting constructed over a hierarchy of nested, unstructured simplicial meshes, in the spirit of Papež *et al.* [HAL Preprint 01662944, 2017]. This includes a global coarse-level lowest-order solve, with local higher-order contributions from the subsequent mesh levels. These higher-order contributions are given as solutions of mutually independent Dirichlet problems posed over patches of elements around vertices. This residual lifting is the core of our a posteriori estimator and determines the descent direction for the next iteration of our multilevel solver. Its construction can be seen as one geometric V-cycle multigrid step with zero pre- and one post-smoothing by damped additive Schwarz. Numerical tests are presented to illustrate the theoretical findings.

ISOGEOMETRIC ANALYSIS FOR COMPRESSIBLE FLOWS IN COMPLEX INDUSTRIAL GEOMETRIES

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In this talk, we present our Isogeometric Analysis (IGA) framework for the numerical analysis of rotary positive displacement pumps and, in particular, twin-screw compressors. IGA was introduced by Hughes et al. in [2] as an extension of the finite element method to higher-order spline function spaces that can represent curved geometries more accurately.

Our approach is based on the overall philosophy that an efficient simulation and, at a later stage, optimization requires the co-design of all components involved in the pipeline, that is, the geometry model and the simulation tools. We present a fully automated algorithm [1] for generating time sequences of analysis-suitable multi-patch parameterizations of counterrotating twin-screw rotor profiles that do not involve topology changes over time and fully exploit the computational potential of modern high-performance computing platforms. The algorithm is based on elliptic grid generation principles and adopts a mixed variational formulation that makes it possible to handle multi-patch parameterizations and parameterizations with C^0 spline basis functions directly.

The second part of the talk describes our isogeometric flow solver [3] which, following our co-design philosophy, makes use of auto-generated compute kernels to achieve optimal computational efficiency for each individual patch. Within individual patches, the convective term of the Galerkin discretization is stabilized by algebraic flux-correction techniques [5] that have been generalized to high-order B-splines in order to suppress the generation of unphysical oscillations in the vicinity of shocks and discontinuities. The coupling of patches is realized via a discontinous Galerkin formulation, which reduces the amount of data that needs to be communicated to a minimum. The isogeometric flow solver has been realized within the open-source IGA library G+Smo [4].

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A PRIORI ERROR ESTIMATES FOR A FRACTURE CONTROL PROBLEM

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An optimal control problem governed by a time-discrete fracture propagation process is considered. The nonlinear fracture model is treated once as a linearized one, while the original nonlinear model is dealt with afterwards. The discretization of the problem in both cases is done using a conforming finite element method. Regarding the linearized case, in contrast to many works on discretization of PDE constrained optimization problems, the particular setting has to cope with the fact that the linearized fracture equation is not necessarily coercive. A quasi-best approximation result will be shown in the case of an invertible, though not necessarily coercive, fracture equation. Based on this, a priori error estimates for the control, state,and adjoint variables will be derived. The discretized nonlinear fracture model will be analyzed as well, which leads to a quantitative error estimate, while we avoid unrealistic regularity assumptions.

SURROGATE POLYNOMIALS IN MATRIX-FREE APPROACHES FOR LOW-ORDER FEM

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It has been noted for some time that the classical finite element procedure of discretising the PDE problem, assembling the global system matrix, storing it in some sparse matrix format and employing the latter in the solution process of the associated linear system is posing a bottleneck for performance in the context of large-scale applications. This is due to the huge disparity in the time required to perform floating point operations on current architectures and the time required for transferring the required operands through the memory system. Implementations following this paradigm are typically, what is denoted as, memory bound and, thus, only reach a meagre percentage of the theoretical peak performance of the systems.

Hence, matrix-free approaches, which do not explicitly store the system matrix, but facilitate the evaluation of a matrix-vector-product (MVP), are attracting considerable attention, especially in the light of upcoming exascale supercomputers. Computing the cell-wise MVP contributions by fusing them with the local integral evaluations has proven very successful for higher-order FE discretisations.

We are going to present a different idea which is based on the use of polynomial approximations of entries of local element matrices. This surrogate matrix methodology can provide significant performance advantages in the case of locally structured meshes. This approach can be seen as a variational crime and can be analysed accordingly. In our presentation we will mostly focus on numerical convergence and scaling results for problems ranging from the variable coefficient Poisson to the generalised Stokes problem of geodynamic convection demonstrating the applicability and efficiency of this approach. Our largest simulation, used to investigate the dynamic topography in models with lateral viscosity variations, employs a global mesh resolution of 1.5 km resulting in a trillion ($\mathcal{O}(10^{12})$) degrees of freedom.

ELECTROMAGNETIC TRANSMISSION PROBLEMS: WAVENUMBER-EXPLICIT BOUNDS

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We consider the time-harmonic Maxwell's equations with rough, possibly discontinuous, permittivity ϵ and magnetic permeability μ. Under a natural assumption on ϵ and μ, which excludes ray trapping, we prove bounds on the solution in terms of the data, with these bounds explicit in all parameters. The L^2 norms of the electric and the magnetic fields are bounded by the L^2 norm of the source term, independently of the wavenumber. The range of problems covered includes, e.g., the scattering by a penetrable star-shaped Lipschitz obstacle.

Such explicit bounds are key to developing frequency-explicit error analysis for numerical methods such as FEM and BEM. The "shape-robustness" allows to quantify how variations in the shape of the obstacle affect the solution and makes the bounds particularly suitable for uncertainty quantification (UQ) applications. Our bounds are obtained using identities first introduced by Morawetz (essentially integration by parts).

WEAKLY SYMMETRIC STRESS RECONSTRUCTION AND A POSTERIORI ERROR ESTIMATION FOR HYPERELASTICITY

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By extending the techniques in [1] for the linear elastic case, an algorithm to reconstruct a H(div)-conforming weakly symmetric stress tensor for the non-linear hyperelastic case is presented. This work builds upon [2] where a local weakly symmetric stress reconstruction is derived for arbitrary conforming finite elements in linear elasticity. The reconstructed stress tensor is used as an a posteriori error estimator. Numerical results for the incompressible hyperelastic case are presented.

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OPTIMIZING THE DESIGN OF THIN FILM SOLAR CELLS

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We describe an ongoing project to develop a flexible and rigorously justified software tool for optimizing the design of thin film solar cells [1]. We use the differential evolution algorithm (DEA) [3] to optimize the efficiency of a solar cell design. To evaluate the efficiency there are two steps:

Photonic model Maxwell's equations need to be solved in the solar cell to find the generation rate of electrons and holes. We restrict ourselves to the case when Maxwell's equations decouples into s-polarized and p-polarized waves that satisfy different Helmholtz equations.

To solve these Helmholtz equations rapidly we use the Rigorous Coupled Wave Analysis (RCWA) method [4], that is based on using Fourier series in the horizontal (quasi-periodic) direction. Since the technique is meshless, it is easy to change both the geometry of the device and the material parameters for each simulation. We prove convergence of RCWA [2].

Electron transport We use the drift-diffusion model to simulate electron transport in the semiconductor layers of the device. This model involves the density of electrons and holes in the device as well as the static electric field generated by these entities. Using the Hybridizable Discontinuous Galerkin (HDG) scheme [5], we can discretize the system using appropriate piecewise polynomials for each unknown in the system. The resulting system of nonlinear equations is solved by Newton's method, and by using different biasing voltages the optimal efficiency for a given design can be computed. Convergence is proved for a related time domain problem.

We have used the above algorithm to optimize a representative solar cell. Future work will include investigating more novel designs, and implementing a full three dimensional model.

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RIGOROUS COUPLE WAVE ANALYSIS OF ONE DIMENSIONAL DIFFRACTION GRATINGS

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Rigorous Coupled Wave Analysis (RCWA) is a technique for approximating the electromagnetic field in a diffraction grating. It is widely used to obtain rapid solutions for heterogeneous gratings where the relative permittivity varies periodically in one direction. This semi-analytical approach expands all the electromagnetic field phasors as well as the relative permittivity as Fourier series in the spatial variable along the direction of periodicity, and also replaces the relative permittivity with a stairstep approximation along the direction normal to the direction of periodicity. Thus, there is error due to Fourier truncation and also due to the approximation of grating permittivity.

We study the convergence properties of RCWA for s- and p-polarized monochromatic incident light on a one dimensional grating. We prove that the RCWA is a Galerkin scheme, which allows us to employ techniques borrowed from the Finite Element Method to analyze the error.

Fo s-polarization an essential tool is a Rellich identity that shows that certain continuous problems have unique solutions that depend continuously on the data with a continuity constant having explicit dependence on the relative permittivity. We prove that for s-polarization the RCWA converges with an increasing number of retained Fourier modes and with a finer approximation of the grating interfaces. Numerical results show that our convergence results for increasing the number of retained Fourier modes are seen in practice, while our estimates of convergence in slice thickness are pessimistic.

For p-polarization the analysis via a Rellich identity is much more delicate. However, for a grating consisting of absorbing media, we prove convergence both with an increasing number of retained Fourier modes and with a finer approximation of the grating interfaces. Our analytical results suggest a slow rate of convergence depending on the singularities occurring in the solution due to material interfaces.

MULTIGRID PRECONDITIONERS FOR FINITE ELEMENT AND DG DISCRETISATIONS: APPLICATIONS IN GEOPHYSICAL FLUID DYNAMICS

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Numerical weather- and climate- prediction models rely on algorithmically optimal time-integrators and fast linear solvers. Modern codes have to make efficient use of massively parallel computer hardware and deliver forecasts under very tight time constraints. Semi-implicit integrators allow the separate treatment of fast and slow atmospheric waves and permit larger model timesteps. However, they require the repeated solution of very large, ill-conditioned sparse systems of equations which is only possible with algorithms such as the multigrid method. In operational configurations, systems with $10^9 - 10^{12}$ unknowns have to be solved within in a few seconds.

Advanced discretisations, such as mimetic Finite Elements and Discontinuous Galerkin (DG) approaches are currently implemented for next-generation operational models. This includes, for example, the UK Met Office's forecast model "LFRic" and the "NUMA" code developed in the US. Those discretisations offer flexibility on non-trivial grids, allow the exact conservation of physical quantities and can increase data-locality. By using sum-factorisation techniques, higher-order discretisations also permit the efficient utilisation of modern chip architectures with a poor bandwidth-to-FLOP ratio. The design of good multigrid solvers is, however, very challenging since the traditional Schur-complement reduction to a system in pressure space is hampered by non-diagonal mass-matrices and artificial diffusion terms.

In this talk I will discuss the implementation of bespoke multigrid solvers in operational weather- and climate models and describe some recent progress on solvers for hybridised DG methods. In addition to discussing the design of the algorithms, I will comment on the implementation and performance portability: being able to run and maintain the model on different architectures and massively parallel supercomputers is an increasingly important aspect.

AN ADAPTIVE NESTED SOURCE TERM ITERATION FOR RADIATIVE TRANSFER EQUATIONS

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In this talk, we present a new approach to the numerical solution of radiative transfer equations with certified a posteriori error bounds. We formulate a fixed-point iteration in a suitable, infinite dimensional function space that is guaranteed to converge with a fixed error reduction per step. The numerical scheme is then based on approximately realizing this outer iteration within dynamically updated accuracy tolerances that still ensure convergence to the exact solution. To gurantee that these error tolerances are met, we employ rigorous a posteriori error bounds based on a Discontinuous Petrov–Galerkin (DPG) scheme. These a posteriori bounds are also used to generate adapted angular dependent spatial meshes to significantly reduce overall computational complexity. The scheme also requires the evaluation of the global scattering operator at increasing accuracy at every iteration and its computation is accelerated through low-rank approximation and matrix compression techniques. We will illustrate the theoretical findings with numerical experiments involving non-trivial scattering kernels.

This is a joint work with Wolfgang Dahmen (University of South Carolina) and Felix Gruber (RWTH Aachen).

FIRST-ORDER SYSTEM LEAST SQUARES METHODS FOR SEA ICE MODELS

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In this talk a viscoplastic sea ice model is considered. Sea ice is modeled as a generalized Newtonian compressible fluid, which satisfies a power law. The nonlinearity caused by the power law for the viscosity is severe and requires careful treatment. The talk considers a first-order system least squares method (FOSLS), where the velocity, ice height, ice concentration and the stress are used as variables. This approach leads to a nonlinear system of partial differential equations and for the least-squares finite element method to a non-quadratic minimization problem.

The talk addresses the numerical challenges that arise while solving this system. After deriving a proper linearization and discussing fitting approximation spaces, numerical experiments will be presented. The talk also examines the advantages of adaptive refinement in this setting.

A MOVING GRID FINITE ELEMENT METHOD APPLIED TO A MECHANOBIOCHEMICAL MODEL FOR 3D CELL MIGRATION

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I will present the development, analysis and numerical simulations of a biophysical model for 3D cell deformation and movement, which couples biochemical reactions and biomechanical forces.

The mechanobiochemical model considers the actin filament network as a viscoelastic and contractile gel. The mechanical properties are modelled by a force balancing equation for the displacements, the pressure and contraction forces are driven by actin and myosin dynamics, and these are in turn modelled by a system of reaction-diffusion equations on a moving cell domain.

The biophysical model consists of highly non-linear partial differential equations whose analytical solutions are intractable. To obtain approximate solutions to the model system, we employ the moving grid finite element method. The numerical results are supported by linear stability theoretical results during the early stages of cell migration. Numerical simulations show both simple and complex cell deformations in 3-dimensions that include cell expansion, cell protrusion and cell contraction.

The computational framework sets a strong foundation that allows the study of more complex and experimentally driven reaction-kinetics involving actin, myosin and other molecular species that play an important role in cell movement and deformation.

COMPUTATIONAL SOLUTIONS FOR FRACTIONAL DIFFUSION EQUATIONS

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VIRTUAL ELEMENT METHODS FOR NONLINEAR PROBLEMS

E. Natarajan

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In this talk, we discuss and analyze new conforming virtual element methods (VEMs) for the approximation of nonlinear problems on convex polygonal meshes in two spatial dimension. The spatial discretization is based on polynomial and suitable nonpolynomial functions. The discrete formulation of both the proposed schemes is discussed in detail, and the unique solvability of the resulted schemes is discussed. A priori error estimates for the proposed schemes in H^1 and L^2 norms are derived under the assumption that the source term f is Lipschitz continuous. Some numerical experiments are conducted to illustrate the performance of the proposed scheme and to confirm the theoretical convergence rates.

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MORLEY FEM FOR A DISTRIBUTED OPTIMAL CONTROL PROBLEM GOVERNED BY THE VON KÁRMÁN EQUATIONS

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Consider the distributed optimal control problem governed by the von Kármán equations that describe the deflection of very thin plates defined on a polygonal domain of $\mathbb{R}^2$ with box constraints on the control variable. The talk discusses a numerical approximation of the problem that employs the Morley nonconforming finite element method to discretize the state and adjoint variables. The control is discretized using piecewise constants. A priori error estimates are derived for the state, adjoint and control variables under minimal regularity assumptions on the exact solution. Error estimates in lower order norms for the state and adjoint variables are derived. The lower order estimates for the adjoint variable and a post-processing of control leads to an improved error estimate for the control variable. Numerical results confirm the theoretical results obtained.

This is a joint work with Sudipto Chowdhury and Devika Shylaja.

HIGH–ORDER SPECTRAL SIMULATION OF GRAPHENE RIBBONS

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The plasmonics of graphene and other two-dimensional materials has attracted enormous attention in the past decade. Both the possibility of exciting plasmons in the terahertz to midinfrared regime, and the active tunability of graphene has generated a great deal of excitement. Consequently there is significant demand for robust and highly accurate computational schemes which incorporate such materials. We describe an algorithm which models the graphene layer with a surface current that is applicable to a wide class of two-dimensional materials. We reformulate the governing volumetric equations in terms of surface quantities using Dirichlet-Neumann operators, which can be numerical simulated in an efficient, stable, and accurate fashion using a novel High-Order Perturbation of Envelopes methodology. We demonstrate an implementation of this algorithm to study absorbance spectra of TM polarized plane-waves scattered by a periodic grid of graphene ribbons.

NUMERICAL BUCKLING ANALYSIS OF CIRCULAR CYLINDRICAL SHELLS

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Elastic buckling of thin shells is a mysterious phenomenon. The critical load of the real shell is known to be very sensitive to small geometric imperfections and deviations in boundary conditions which are difficult to take into account in linear or nonlinear stability theory. As a result, theoretical and experimental results do not agree well in many loading scenarios. In any case, even the linear stability theory provides us useful information regarding the buckling behaviour of thin shells. Moreover, it serves as a first step in the analysis of geometric nonlinearities arising from large deformations. In this work, the buckling problem of circular cylindrical shells is analysed from the point of view of finite element analysis. In particular, the asymptotic behaviour of the buckling modes for thin shells and the associated numerical problem of locking are discussed.

ON THE SPECTRAL GEOMETRY OF STEKLOV EIGENVALUE PROBLEMS

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Spectral geometry concerns the study of the interplay between geometric properties of a domain and the spectrum of pseudodifferential operators defined on these domains. Of particular interest in the design of optical and photonic devices is the question of spectral optimization. In this talk, we consider some theoretical and computational questions which arise in the spectral geometry of the Steklov eigenvalue problem for the Laplacian and the Lamé operators. We present discretization methodologies based on both a finite element method, and a boundary integral strategy.

FEMS FOR FRACTIONAL DIFFUSION: A SURVEY

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Fractional diffusion is a non-local diffusion process that accounts for long-range interactions. We review three finite element methods that build on different definitions of the fractional Laplacian in bounded domain. The first method is the integral formulation and deals with singular non-integrable kernels. The second method is a PDE approach that applies to the spectral definition and exploits the extension to one higher dimension. The third method is a discretization of the Dunford-Taylor formula. We discuss pros and cons of each method, error estimates, and document their performance with a few numerical experiments. We conclude with extensions to several nonlinear fractional diffusion problems.

THE GRADIENT FLOW STRUCTURE OF AN EXTENDED MAXWELL VISCOELASTIC MODEL

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An extended Maxwell viscoelastic model is studied from mathematical and numerical points of view. It is shown that the model has a gradient flow structure with respect to a viscoelastic energy. A P1/P0 finite element scheme is presented and its stability in the sense of energy is proved by using a corresponding discrete gradient flow structure. The talk is given based on the following paper.

[1] M. Kimura, H. Notsu, Y. Tanaka and H. Yamamoto. The gradient flow structure of an extended Maxwell viscoelastic model and a structure-preserving finite element scheme. *Journal of Scientific Computing*, Vol.78(2019), pp.1111–1131.

QUANTUM CALCULATIONS IN SOLUTION WITH DOMAIN DECOMPOSITION POLARIZABLE CONTINUUM MODEL

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Polarizable continuum solvation models (PCSM) nowadays have become a standard tool in computational chemistry to include solvation in a wide range of applications, usually coupled with quantum mechanical (QM) methods.[3] However, recent developments in algorithms made QM methods applicable to systems large enough that the cost associated with solving the PCSM equations can become the computational bottleneck.

In order for PCSM to be applicable to large and very large molecular problems, an efficient and robust numerical strategy has to be devised. In recent years, we have proposed a completely new formulation of PCSM that is not based on the numerical solution of an integral equation as in traditional methods, but on a domain-decomposition (dd) strategy. This new formulation has been applied first to PCSM in the conductor-like approximation (ddCOSMO)[1] and then to the dielectric scheme (ddPCM).[2]

In this work, we present the first implementation of ddPCM for a solute described at a quantum mechanical level of theory. We start by discussing the ideas behind the ddPCM method and then how it is coupled to Hartree-Fock, Density Functional Theory and semi-empirical methods. In particular, we discuss how to compute the solvation effect on properties and excitation energies of the solute. Finally, we discuss the timings and scaling of the new implementation and we compare it with a previous, state-of-the-art, implementation of a PCSM.

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A PARALLEL SPACE-TIME BOUNDARY ELEMENT METHOD FOR THE HEAT EQUATION

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We present a parallel boundary element solver for space-time boundary integral equations of the heat equation. The related system matrix is huge, but it allows for additional parallelization with respect to time. The related space-time boundary mesh is decomposed into submeshes and the system matrix is decomposed into related blocks. These blocks are distributed among computational nodes by an algorithm based on a cyclic decomposition of complete graphs to achieve load balance. In addition, we employ vectorization and threading in shared memory to ensure intra-node efficiency. We present scalability experiments to evaluate the performance of the proposed parallelization techniques and observe almost optimal speedup.

DISCRETIZATION ERRORS IN FILTERED SUBSPACE ITERATION FOR SELF-ADJOINT OPERATORS

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In recent years, a variety of contour-integral based methods for approximating targeted clusters of eigenvalues, together with their corresponding invariant subspaces, have been proposed and analyzed for finite rank operators (matrices). One particularly popular approach in this vein is the so-called FEAST method, which is essentially a subspace iteration scheme employing a rational function of the operator that "filters" its spectrum in the sense that the eigenvalues of interest of the original operator become the dominant eigenvalues of the filtered operator, while their corresponding invariant subspaces remain the same. Analyses of such methods for matrices, regardless of whether or not they arise from discretizing an infinite rank (unbounded) operator, have focused on *iterative error*, i.e. how rapidly the approximate eigenvalues and invariant subspace converge to the corresponding true eigenvalues and invariant subspace *of the matrix* with respect to the number of iterations.

The focus of our study is on *discretization error*. In other words, if subspace iteration is applied using a discretized version of the filtered operator, how well do the computed eigenvalues and invariant subspace returned by this iteration approximate the corresponding true eigenvalues and invariant subspace *of the original (unbounded) operator* with respect to discretization parameters? We provide a general framework for analyzing filtered subspace iteration for (unbounded) selfadjoint operators that addresses discretization error in approximating both the invariant subspace and the collection of eigenvalues, highlighting a small set of practically-verifiable abstract assumptions that, if satisfied, guarantee convergence with respect to discretization parameters. Because our analysis is carried out on the level of Hilbert spaces, we naturally achieve convergence results in norms appropriate to such settings. We illustrate our key results on one or, if time permits, two types of discretizations of second-order elliptic operators, providing numerical experiments to gauge the sharpness of our results.

TREFFTZ FINITE ELEMENTS ON MESHES CONSISTING CURVILINEAR POLYGONS

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We consider finite element methods in 2D employing meshes consisting of quite general curvilinear polygons. These methods are in the spirit of Trefftz methods for second order linear elliptic equations, in that the local finite element spaces are defined implicitly in terms of local Poisson problems involving polynomial data. Immediately one must decide what should be meant by "polynomial space on a curve", and perhaps the two most natural choices are: polynomials with respect to arclength or other natural parameter related to the curve, or restrictions of polynomials in 2D to the curve. We discuss why the latter space is preferred, and indicate how to work with it in practice. Having made this choice, we introduce a natural interpolation operator, and establish convergence results with respect to mesh size. Several numerical examples, some for which every element has at least one curved edge, illustrate these convergence results in practice.

The proposed method is strongly related to both Virtual Element Methods (VEM) and Boundary Element Based Finite Element Methods (BEM-FEM) in terms of how the local spaces are defined—with the possible exception of how we define what it means to be polynomial on an edge. In terms of how we use the spaces in practice, our approach is much closer to BEM-FEM in the sense that we use local bases much more directly, evaluating quantities needed for quadrature approximation of local stiffness matrices via integral equation techniques. In our case, these integral equations are solved using Nyström methods, which are better-suited to handling curvilinear polygons than BEM.

FIRESHAPE: A SHAPE OPTIMIZATION TOOLBOX FOR FIREDRAKE

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Fireshape is a shape optimization toolbox for the finite element library Firedrake. Fireshape can tackle optimization problems constrained by boundary value problems and offers the following features: decoupled discretization of control and state variables, automatic derivation of shape derivatives and adjoint equations, different metrics to define shape gradients, and numerous optimization algorithms. The shape optimization knowledge required to use this library is minimal.

Fireshape is available at https://github.com/fireshape/fireshape

ON THE EQUATION OF MOTION ARISING IN THE OLDROYD MODEL: THEORETICAL AND COMPUTATIONAL ISSUES

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Newton's model of incompressible viscous fluid is described by the wellknown Navier-Stokes equations. This has been a basic model for describing flow at moderate velocities of majority of viscous incompressible fluids encountered in practice. However, models of viscoelastic fluids have been proposed in the mid twentieth century which take into consideration the prehistory of the flow and are not subject to Newtonian flow. One such model was proposed by J.G. Oldroyd and hence, it is named after him. The equation of motion in this case gives rise to the following integro-differential equation

$$\frac{\partial u}{\partial t} + u \cdot \nabla u - \mu \Delta u - \int_0^t \beta(t-\tau)\Delta u(x,\tau)\, d\tau + \nabla p = f(x,t),\ x \in \Omega, t > 0, (*)$$

and incompressibility condition

$$\bigtriangledown . u = 0, \quad x \in \Omega, t > 0$$

with initial condition

$$u(x,0) = u_0, u = 0,\ x \in \partial\Omega, t \geq 0.$$

Here, Ω is a bounded domain in $R^d (d = 2, 3)$ with boundary $\partial\Omega, \mu > 0$ and the kernel $\beta(t) = \gamma exp(-\delta t)$, where both γ and δ are positive constants. With a brief discussion on existential analysis, we, in this talk, concentrate on the finite element Galerkin method for the above system under realistically assumed regularity on the exact solutions. Since the problem (*) is an integral perturbation of the Navier-Stokes equations, we would like to discuss '*how far the results on finite element analysis for the Navier-Stokes equations can be carried over to the present case.*'

A PRIORI ERROR ESTIMATES FOR A CLASS OF HYDROELASTIC FINITE ELEMENTS

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Hydroelastic modelling of pontoon type Very Large Floating Structures (VLFSs) under long wave excitation has been a subject of study since the pioneering work of F. John [F. John, 1949. On the motion of floating bodies I. Communications on pure and applied mathematics, Vol. 2, pp. 13-57] and [F. John, 1950. On the motion of floating bodies II. Communications on pure and applied mathematics, Vol. 3, pp. 45-100]. Due to the significant applications of this coupled partial differential equation system in coastal engineering, many methods of solution have been proposed. Initially, analysis was typically conducted in the frequency domain for the case of harmonic waves [J. J. Stoker, 1957. Water Waves: the mathematical theory with applications, Interscience Publishers, Inc., New York, 1957]. Hydroelastic interactions in the time domain have been studied recently by I. V. Sturova [I. V. Sturova, 2009. Time-dependent response of a heterogeneous elastic plate oating on shallow water of variable depth. J. Fluid Mech. 637, 305-325] and Papathanasiou et al. [T. K. Papathanasiou, A. Karperaki, E. E. Theotokoglou, K. A. Belibassakis, 2014. A higher order FEM for time-domain hydroelastic analysis of large floating bodies in an inhomogeneous shallow water environment, Proc. R. Soc. A, 471: 20140643], among others. Sturova (2009) developed a solution technique based on eigenfunction expansions, using the modes of the dry flexible plate. Papathanasiou et al. (2014), developed high-order finite elements for the same Initial Boundary Value problem (IBVp).

In this study the effectiveness of the finite element procedure will be studied in terms of *a priori* energy norm error estimates. After a brief recapitulation of the governing equations and their variational form, error estimates for the semi-discrete system (vertical method of lines) are derived. The basic feature of the proposed finite elements is the combination of Hermite and Lagrange type interpolations. The error estimation procedure adopted is based on energy balance and stability results derived in Papathanasiou et al. (2014) and application of the Deny-Lions Lemma. Optimal convergence rate schemes, for cases of sufficiently smooth solutions, are pursued. The absence of dissipation mechanisms in the model under consideration dictates the introduction of time integration schemes with energy preserving properties at the discrete level. A time stepping method with this characteristic is considered for the fully discrete scheme. Numerical results are studied for verification of the predicted asymptotic error behaviour. Particular emphasis is given to the possible loss of solution regularity in cases of finite draft. This important feature of the hydroelastic configuration could potentially cause convergence rate reduction due to the introduction of finite jumps in the bathymetry function.

NEARBY PRECONDITIONING FOR MULTIPLE REALISATIONS OF THE HELMHOLTZ EQUATION, WITH APPLICATION TO UNCERTAINTY QUANTIFICATION

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Let $\mathbf{A}^{(j)}$, $j = 1, 2$, be the Galerkin matrices corresponding to the h-FEM discretisation of the Helmholtz equations

$$\nabla \cdot (A^{(j)} \nabla u^{(j)}) + k^2 n^{(j)} u^{(j)} = -f, \quad j = 1, 2$$

in the exterior of some bounded set with Dirichlet boundary conditions. In this work we answer the following question: when is $\mathbf{A}^{(1)}$ a good left- or right-preconditioner for $\mathbf{A}^{(2)}$? More precisely, we ask: How small must $\|A^{(1)} - A^{(2)}\|_{L^\infty}$ and $\|n^{(1)} - n^{(2)}\|_{L^\infty}$ be (in terms of k-dependence) for GMRES applied to either $(\mathbf{A}^{(1)})^{-1}\mathbf{A}^{(2)}$ or $\mathbf{A}^{(2)}(\mathbf{A}^{(1)})^{-1}$ to converge in a k-independent number of iterations for arbitrarily large k?

We prove that, if

$$k\|A^{(1)} - A^{(2)}\|_{L^\infty} \text{ and } k\|n^{(1)} - n^{(2)}\|_{L^\infty} \text{ are both sufficiently small} \tag{1}$$

then $\mathbf{A}^{(1)}$ is a good preconditioner for $\mathbf{A}^{(2)}$ when using *weighted* GMRES, and numerical experiments show the conditions (1) are sharp. Moreover, numerical experiments show that the conditions (1) are sharp for standard GMRES, but to prove $\mathbf{A}^{(1)}$ is a good preconditioner for $\mathbf{A}^{(2)}$ for standard GMRES we require a slightly stronger condition on $A^{(1)}$ and $A^{(2)}$ than that in (1).

Our motivation for tackling this question comes from calculations in uncertainty quantification (UQ) for the Helmholtz equation with *random* coefficients A and n. Such a calculation requires the solution of many deterministic Helmholtz problems, each with different A and n. The answer to the question above dictates to what extent a previously-calculated preconditioner of one of the Galerkin matrices can be used as a preconditioner for other Galerkin matrices. The extent to which one can reuse preconditioners reduces the cost of the UQ calculation.

VARIOUS MATHEMATICAL APPROACHES TO MECHANICAL SIMULATIONS IN WOUND HEALING PROCESSES

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Deep tissue injuries often result in contractions of skin due to mechanical pulling forces exerted by skin cells in the dermal layer. If contractions are morbid, then they are referred to as contractures. Contractures cause disabilities to the patients, by, for instance, loss of mobility of a joint. By the use of modelling, we aim at understanding the mechanisms behind the formation of a contracture and we aim at predicting which wound is likely to develop a contracture and which treatments can be employed to minimize the likelihood of a contracture. We used the immerse boundary approach based on a superposition of Dirac Delta functions to describe the forces exerted by individual skin cells. The use of this superposition of Delta functions results in a numerical solution that is not in H1. Therefore we investigate alternative finite element methodologies, such as the mixed finite element method, next to standard Galerkin finite element techniques. Next to the mixed finite element method, we also analysed an approach based on Green's fundamental functions and an approach based on formulating the surface forces at the cell by means of a force boundary condition. The simulations and results will eventually contribute to modelling the contractions of the wound.

A MULTISCALE METHOD FOR H(CURL)-PROBLEMS

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In this talk I will present a method for computing numerical approximations to H(curl)-problems with multiscale coefficients. Problems of this type typically occur when simulating electromagnetic wave propagation with Maxwell's equations in heterogeneous media, such as photonic crystals and other metamaterials.

The method is based on the local orthogonal decomposition (LOD) technique first introduced by Målqvist and Peterseim (2014). This talk focuses on how to generalize the LOD technique to the H(curl)-setting and we will see that linear convergence is obtained in H(curl)-norm, independently of the variations in the coefficients. In addition, numerical examples of the convergence in both two and three dimensions will be presented.

FINITE ELEMENT ANALYSIS OF A COUPLED SYSTEM OF VARIATIONAL INEQUALITIES MODELING BIOFILM GROWTH AT THE PORESCALE

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We consider a nonlinear system of diffusion-reaction PDEs for the evolution of biofilm and nutrient. Biofilm is a collection of microbial cells embedded in a protective extracellular polymer substance (EPS). While the model for biomass-nutrient dynamics is well-known, we consider the process at a micro-scale at which one recognizes a free boundary between the biofilm and the surrounding fluid through which nutrient and individual cells migrate. The model is motivated by the available micro-CT imaging data of the porescale invaded by microbial growth.

The coupled PDE system involves thus a freee boundary modeled by a variational inequality. We describe the model and its Finite Element discretizations and present convergence proof and experiments both in the Galerking and mixed finite element setting.

FINITE ELEMENT ERROR ESTIMATES IN L^2 FOR REGULARIZED DISCRETE APPROXIMATIONS TO THE OBSTACLE PROBLEM

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In this talk, we consider the standard obstacle problem in a convex and polygonally/ polyhedrally bounded domain. For the forcing term and the obstacle we assume for simplicity that they are arbitrarily smooth. As main result, we derive quasi-optimal error estimates in L^2 for a sequence of numerical approximations to the obstacle problem based on a regularization approach. More precisely, we obtain second order convergence in L^2 (up to logarithmic factors) with respect to the mesh size. The meshes are assumed to be quasi-uniform. The main ingredient for proving the quasi-optimal estimates is the structural and commonly used assumption that the obstacle is inactive on the boundary of the domain. No discrete maximum principle is required.

For instance, estimates of this kind may be needed when estimating the finite element error for optimal control problems subject to the obstacle problem.

SOME CONTRIBUTIONS OF THE NUMERICAL SIMULATION FOR WAVES PROPAGATION IN COMPLEX MEDIA

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In this talk, I will present two numerical methods we have widely used to obtain nice physical results regarding wave propagation in complex heterogeneous media: the moment or volume integral method [3] and the coupled dipoles method [4]. For both I will present the advantages and limitations in term of accuracy and requested computing resources. Two physical systems will be considered as illustrations: near-field optics of semi-continuous metallic films [2] and light propagation in disordered clouds of correlated dipolar nanoparticles [5, 1]. With these examples, I will show the important contribution of the numerical simulation in the understanding and control of wave propagation in strongly scattering media.

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A HYBRID HIGH-ORDER METHOD FOR INCREMENTAL ASSOCIATIVE PLASTICITY WITH SMALL DEFORMATIONS

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We devise and evaluate numerically a Hybrid High-Order (HHO) method for incremental associative plasticity with small deformations [2]. HHO methods were initially introduced in [3] for linear elasticity and in [4] for diffusion problems. For a recent work on HHO methods for hyperelasticity, we refer to [1]. The HHO method uses as discrete unknowns piecewise polynomials of order $k \geq 1$ on the mesh skeleton, together with cell-based polynomials that can be eliminated locally by static condensation. The HHO method supports polyhedral meshes with non-matching interfaces and is free of volumetric locking. The HHO method has also the following salient features compared to discontinuous Galerkin methods: the integration of the behavior law is performed only at cell-based quadrature nodes and the tangent matrix arising in the Newton's method is symmetric. Moreover, the principle of virtual work is satisfied locally with equilibrated tractions. We evaluate the proposed HHO method on two- and three-dimensional test cases from the literature and we compare the results produced by the HHO method to the analytical solution whenever available or to numerical results obtained using the industrial software *code_aster* with conforming and mixed finite elements.

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HYBRID HIGH-ORDER DISCRETIZATIONS COMBINED WITH NITSCHE'S METHOD FOR CONTACT WITH TRESCA FRICTION IN SMALL STRAIN ELASTICITY

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We present the extension of two primal methods to weakly discretize contact and Tresca friction conditions in small strain elasticity, that were previously devised and studied for Dirichlet and scalar Signorini conditions [1]. Both methods support polyhedral meshes with nonmatching interfaces and are based on a combination of the Hybrid High-Order (HHO) method [2, 3] and Nitsche's method [4]. The HHO method uses as discrete unknowns piecewise polynomials of order $k \geq 1$ on the mesh skeleton, together with cell-based polynomials that can be eliminated locally by static condensation. Since HHO methods involve both cell unknowns and face unknowns, this leads to different formulations of Nitsche's consistency and penalty terms, either using the trace of the cell unknowns (cell version) or using directly the face unknowns (face version). The face version uses equal order polynomials for cell and face unknowns, whereas the cell version uses cell unknowns of one order higher than the face unknowns. Error estimates are proven to be optimal only for the cell version and robust at the quasi-incompressible limit only for the face version. Numerical experiments confirm the theoretical results, and also reveal optimal convergence and robustness for both the cell and face versions.

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TENSOR-PRODUCT DISCRETIZATION FOR THE SPATIALLY INHOMOGENEOUS AND TRANSIENT BOLTZMANN EQUATION IN TWO DIMENSIONS

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In this talk we present a numerical method for the spatially inhomogeneous and nonlinear Boltzmann equation for the variable hard spheres model. The distribution function is discretized by a tensor-product ansatz by combining Maxwellian modulated Laguerre polynomials in velocity with continuous, linear finite elements in the spatial domain. The advection problem in phase space is discretized through a Galerkin least squares technique and yields an implicit formulation in time. The discrete collision operator can be evaluated with an asymptotic effort of $\mathcal{O}(K^5)$, where K is the number of velocity degrees of freedom in a single direction. Numerical results in 2D are presented for rarefied gases with different Mach and Knudsen numbers.

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NUMERICAL ANALYSIS OF A POROUS ELASTIC MODEL FOR CONVECTION ENHANCED DRUG DELIVERY

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In this work we are concerned with the numerical analysis of a piecewise linear FEM for a coupled system of partial differential equations that arise, for example, in the mathematical modeling of porous elastic convection enhanced drug delivery (CED). The system consists of a parabolic equation, an elliptic equation, and a wave-type equation. CED is a drug delivery method that uses catheters to deliver therapeutic agents directly into target sites. This procedure is particularly useful in the treatment of diseases of the central nervous system, since it allows to bypass the blood-brain barrier, a physiological barrier that prevents many therapeutic agents to diffuse from the blood vessels to the brain. The main result of this work is a convergence result that shows that our piecewise linear FEM is second order convergent with respect to a discrete L^2-norm when the solution belongs to H^3. Numerical experiments illustrating the theoretical finds and the behavior of a particular CED model will be shown.

A POSTERIORI ERROR ESTIMATES FOR THE ALLEN-CAHN PROBLEM

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We derive a posteriori error bounds in $L_4(0,T;L_4(\Omega))$-norm for fully-discrete approximations of the Allen-Cahn equation in two and three dimensions. The Allen-Cahn equation is a singularly perturbed parameter-dependent parabolic semi-linear PDE and was originally introduced to describe the phase separation process of a binary alloy at a fixed temperature. In particular, we consider the lowest order discontinuous Galerkin time-stepping method with conforming finite elements in space. For this method, we prove conditional a posteriori error estimates that depend *polynomially* upon ϵ^{-1}, with ϵ denoting the characteristic interface length. The derivation relies crucially on the availability of a spectral estimate for the linearised Allen-Cahn operator about the approximating solution in conjunction with a continuation argument and a variant of the elliptic reconstruction that allows us to control the error. The key idea of the proof involves a carefully constructed test function that results to estimation of the $L_4(0,T;L_4(\Omega))$-norm error via an energy argument with very attractive ϵ-dependence of the conditional estimates. Interestingly, the new a posteriori error analysis appears to improve the polynomial dependence of energy-norm and $L_\infty(0,T;L_2(\Omega))$ a posteriori error bounds from the literature for the two-dimensional problem. The new a posteriori analysis is valid for the case of a smoothly developing interface, but also for the case of topological changes occurring in the interface development.

GOAL-ORIENTED ERROR ESTIMATION WITHIN THE GENERALIZED MULTISCALE FINITE ELEMENT METHOD

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We will discuss recent results in the use of goal-oriented adaptivity within the Generalized Multiscale Finite Element Method (GMsFEM). Standard finite element approximations of multiscale problems can be prohibitively computationally expensive due to the need to resolve fine scales throughout the domain to achieve an accurate approximation. To reduce the computational complexity, multiscale methods can be used to generate a collection of basis functions based on local fine-scale data by which a global approximation to the PDE solution can be formed. Goal-oriented adaptivity can be used in this context to select which local neighborhoods to enrich with either precomputed (offline) basis functions or adaptively constructed online basis functions. We will discuss how such goal-oriented strategies can be designed and implemented for Darcy flow problems for flux-based quantities-of-interest based on a mixed-formulation or pressure-based quantities-of-interest based on a standard formulation. Numerical results will demonstrate the efficacy of the methods, and some of the differences between the multiscale and standard goal-oriented adaptive strategies.

PHASE FIELD MODELLING FOR DISSOLUTION AND PRECIPITATION

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We consider a model for precipitation and dissolution in a porous medium. The ions transported by a fluid through the pores can precipitate at the pore walls. The mineral formed in this way can dissolve, increasing the amount of dissolved ions in the fluid. These processes lead to changes in the flow domain, which are not known a-priori but depend on the concentration of the solute.

One possible approach is to consider the fluid and mineral phases as different phases, separated by an interface that moves in time depending on the model unknowns. Here we discuss an alternative approach, based on a phase field variable having a smooth, diffuse transition of non-zero width from the fluid into the mineral phase. The evolution of the phase field variable is determined through the Allen-Cahn equation.

We first show that as the width of the diffuse transition zone approaches zero, the sharp-interface formulation is recovered. Then, considering a periodically perforated domain mimicking a porous medium, we employ homogenization techniques to derive an upscaled model, valid at the Darcy scale. This involves solving so-called cell problems, providing the effective diffusion and permeability matrices that are depending on the phase field variable.

Finally, we extend this approach to non-periodic media, and propose an adaptive upscaling procedure. Coupled with a linearisation scheme, this becomes an efficient numerical homogenisation scheme for simulating such multi-scale processes involving freely moving interfaces at the micro-scale.

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MORLEY FINITE ELEMENT METHOD FOR AN ELLIPTIC DISTRIBUTED OPTIMAL CONTROL PROBLEM WITH POINTWISE STATE AND CONTROL CONSTRAINT

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We design and analyze a Morley finite element method for an elliptic distributed optimal control problem with pointwise state and control constraints on convex polygonal domains. The constrained minimization problem is analyzed by reducing it into a fourth order variational inequality and convergence of the state error is established in the H2-like energy norm. The key ingredients of the analysis are constraint preserving properties of the interpolation operator and the enriching map. We also discuss post-processing methods to obtain the approximation of the control from the discrete state. Numerical results are presented to illustrate the theoretical findings.

APPROXIMATION OF HIGH ORDER HOMOGENISED EQUATIONS FOR WAVE PROPAGATION

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Over the last few years, the long time homogenization of the wave equation has been the subject of considerable study. While the standard homogenized equation describes the effective behavior of the waves at short times, this model fails to capture macroscopic dispersion effects that appear at long times. To describe the dispersion, the effective model must include additional operators of higher order. In this talk, we present a practical way to construct effective equations of arbitrary order in periodic media [1], with a focus on their numerical approximation. In particular, we exhibit an important structure hidden in the definition of the effective tensors of arbitrary order which leads to two new results: the first result ensures a substantial reduction of the computational cost to approximate the effective tensors; the second result proves that this calculation naturally benefits from a high accuracy.

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ADAPTIVE BEM WITH INEXACT PCG SOLVER YIELDS ALMOST OPTIMAL COMPUTATIONAL COSTS

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In our talk, we will sketch our recent work [Führer et al., Numer. Math. 141, 2019]. We consider the preconditioned conjugate gradient method (PCG) with optimal preconditioner in the frame of the boundary element method (BEM) with adaptive mesh-refinement. As model problem serves the weakly-singular integral equation $V\phi = f$ associated with the Laplace operator. Given an initial mesh $\mathcal{T}_0$, adaptivity parameters $0 < \theta \leq 1$ and $\lambda > 0$, counter $j = 0$ (for the mesh-sequence $\mathcal{T}_j$) and $k = 0$ (for the PCG steps per mesh $\mathcal{T}_j$), as well as a discrete initial guess $\phi_{00} \approx \phi$ on $\mathcal{T}_0$ (e.g., $\phi_{00} = 0$), our adaptive strategy reads as follows:

(i) Update counter $(j, k) \mapsto (j, k + 1)$.

(ii) Do one PCG step to obtain ϕ_{jk} from $\phi_{j(k-1)}$.

(iii) Compute refinement indicators $\eta_j(T, \phi_{jk})$ for all elements $T \in \mathcal{T}_j$.

(iv) If $\lambda^{-1} \|\phi_{jk} - \phi_{j(k-1)}\|^2 > \eta_j(\phi_{jk})^2 = \sum_{T\in\mathcal{T}_j} \eta_j(T, \phi_{jk})^2$, continue with (i).

(v) Otherwise determine marked elements $\mathcal{M}_j \subseteq \mathcal{T}_j$ such that $\theta\, \eta_j(\phi_{jk})^2 \leq \sum_{T\in\mathcal{M}_j} \eta_j(T, \phi_{jk})^2$.

(vi) Refine all $T \in \mathcal{M}_j$ to obtain the new mesh $\mathcal{T}_{j+1}$.

(vii) Update counter $(j, k) \mapsto (j + 1, 0)$ and continue with (i).

For *a posteriori* error estimation, we employ the weighted-residual error estimator. If the final ϕ_{jk} on each mesh $\mathcal{T}_j$ is the exact Galerkin solution, then linear convergence of adaptive BEM, even with optimal algebraic rates, has been proved independently in [Feischl et al., SIAM J. Numer. Anal. 51, 2013] and [Gantumur, Numer. Math. 124, 2013]. As a novel contribution, we now extend this result to adaptive BEM with inexact PCG solver.

We prove that the proposed adaptive algorithm does not only lead to linear convergence of the error estimator (for arbitrary $0 < \theta \leq 1$ and $\lambda > 0$) with optimal algebraic rates (for $0 < \theta, \lambda \ll 1$ sufficiently small), but also to almost optimal computational complexity, if $\mathcal{H}^2$-matrices (resp. the fast multipole method) are employed for the effective treatment of the discrete integral operators. In particular, we provide an additive Schwarz preconditioner which can be computed in linear complexity and which is optimal in the

sense that the condition numbers of the preconditioned systems are uniformly bounded (see [Feischl et al., Calcolo 54, 2017] in the context of the hypersingular integral equation).

MULTISCALE MODEL REDUCTION AND ITS APPLICATIONS TO GOAL-ORIENTED ERROR CONTROL.

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In this talk, we present a model reduction technique based on the Generalized Multiscale Finite Element Method (GMsFEM) and investigate its applications on the goal-oriented error control. We introduce two different adaptive approaches (namely, offline and online) for Darcy s flow model and the mixed formulation. The idea is to include more degrees of freedoms based on a class of well-designed error indicators, depending on the information of residuals, during the adaptive iteration. Analytical properties and numerical performances of these approaches are discussed.

A DOMAIN DECOMPOSITION METHOD FOR THE POISSON–BOLTZMANN SOLVATION MODEL IN QUANTUM CHEMISTRY

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A particular domain decomposition method, called ddLPB, is developed for solving the Poisson–Boltzmann solvation model in quantum chemistry. In this method, the domain (solute molecule) is decomposed into (atomic) balls and the global Poisson–Boltzmann equation is transformed into a system of coupled subequations restricted in these balls. As a consequence, each local subequation can be solved explicitly, using the Galerkin spectral method with spherical harmonics as basis functions. Based on the local solvers, the coupling conditions among the subequations are then discretized, which derives a global linear system that can be solved by linear solvers. A series of numerical experiments will be presented to show the robustness and the efficiency of this new method.

A FRAMEWORK FOR APPLYING THE DWR METHOD ON VARIATIONAL INEQUALITIES

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In this talk, we consider variational inequalities of first and second kind including a smooth nonlinear differential operator. We rewrite the variational inequalities with the help of nonlinear complementarity (NCP) functions as a nonlinear problem. However, due to the nonsmoothness of the NCP functions, the resulting problem is not smooth and we have potentially to assume additional properties of the analytic solution to do the reformulation. We want to apply the dual weighted residual (DWR) method to estimate the discretization error in a user defined quantity of interest. The classic DWR approach, see, for instance, [1], relies on the fact that the semi linearform defining the problem is optimally three times directional differentiable. Due to the nonsmoothness of our formulation, we cannot directly apply the classic DWR approach, where the problem is linearized on the basis of the directional derivative of the underlying semi linearform. Instead, we use the active sets provided by the NCP functions to do the linearization w.r.t. them, while the differential operator is treated in the classic way. The arising dual problem is closely connected to the linear system of equations, which has to be solved in the last step of a semi smooth Newton method applied to the original problem. We derive an error identity, which consists in the primal residual and the dual residual plus a remainder term. The remainder term includes the error due to the linearization and is usually of higher order in the error. Hence, it is neglected. The primal residual and the dual residual are weighted by the dual and the primal discretization error, respectively. Thus, their evaluation has to be approximated numerically using suitable techniques. Finally, the error estimate is localized to the mesh cells by a filtering approach to utilize it in an adaptive strategy. A comparatively simple example, Signorini's problem, for the application of this framework is discussed first, cf. [3]. Then, the more complex case of frictional contact is considered, cf. [2]. Finally, we give an outlook on elasto-plastic problems and thermoplastic contact problems.

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EFFICIENT SIMULATION OF LINEAR AND NONLINEAR POROELASTICITY

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Poroelasticity, i.e. fully coupled porous media flow and mechanics has many societal important applications including geothermal energy, enhanced oil recovery or CO_2 storage. A typical mathematical model for poroelasticity is the quasi-static, linear Biot model, see e.g. [3]. Nevertheless, the linearity assumption is not valid in many practical situations and extension of the model should be considered.

In this work we present efficient numerical schemes for the linear and nonlinear Biot models [1]. The Bulk modulus (Lame coefficient) and the fluid compressibility are nonlinear functions satisfying certain assumptions. We use the L-scheme, see e.g. [4, 5] or the Newton method for linearization, either monolithically or combined with a fixed stress type splitting [2, 3, 6]. Additionally, the optimisation of the stabilisation parameter in the fixed-stress scheme will be discussed [7].

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IMPACT ANALYSIS AS AN INTEGRAL PART OF THE DESIGN PROCESS

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During the design and certification process for its products, Rolls-Royce has a need to solve various impact and non-linear structural dynamic problems. These include bird/ice ingestion, fan blade-off, core engine blade-off and response of aerofoils to tip rubbing to name but a few. The standard Finite Element package used during this process is LS-Dyna; suitably modified by Rolls-Royce in-house routines.

This lecture will provide some insight into the philosophy employed by Rolls-Royce in the analysis of impact and non-linear structural dynamic events and will also discuss the necessary rigour and attention to detail that is required to use Finite Elements routinely and robustly in a reliable predictive manner. Reference will be made where appropriate to test/analysis comparisons to demonstrate the points made.

Comment will be made as to progress made over recent years to develop the use of the software and large-scale computing to replace test and enable a smoother engine development process and eventual certification; this includes the prospect of certification of products by analysis only. In addition, a look forward to the likely future requirements for impact and non-linear structural dynamic analyses over the next few years is made.

NUMERICAL SOLUTION OF TWO DIMENSIONAL TUMOUR GROWTH WITH MOVING BOUNDARY

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The two-phase tumour growth problem in two dimensions is a coupled system of a hyperbolic, elliptic and parabolic partial differential equations that respectively model volume fraction, velocity and pressure of tumour cells, and nutrient concentration within the tumour tissue. We present a numerical technique that overcomes the challenges associated with the time-dependent boundary of a growing tumour. The hyperbolic equation is extended to a fixed domain, which encompasses all time-dependent domains up-to a fixed time, without applying any domain transformation. This extension correctly embeds the dynamics of the moving boundary. A finite volume - finite element method is used to solve the system where the tumour boundary is recovered by locating the discontinuity in the volume fraction of the tumour cells. The new method overcomes the re-meshing issues associated with numerically solving similar moving boundary problems. The ability of the current technique to predict the evolution of irregularly shaped tumours, and thus relaxing the assumption of radially symmetric growth in previous works, is a novelty and an advantage.

A SPACE–TIME HYBRIDIZABLE DISCONTINUOUS GALERKIN METHOD FOR THE NAVIER–STOKES EQUATIONS

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Recently there has been much interest in exactly divergence-free and $H(\text{div})$-conforming finite element methods for incompressible flows due to their improved accuracy compared to other finite element methods, see for example the review paper [1]. In this talk we present a finite element method for the Navier–Stokes equations that maintains these properties even on time-dependent domains.

In particular, we present a space–time hybridizable discontinous Galerkin (HDG) discretization of the Navier–Stokes equations. Space-time finite element methods have excellent properties when discretizing partial differential equations on time-dependent domains. For example, they automatically satisfy the geometric conservation law, are higher-order accurate in space and time, and allow for *hp*-adaptivity in space and/or time [2].

In a space–time discretization, the Navier–Stokes equations are discretized on a $(d+1)$-dimensional space–time domain. By partitioning the space–time domain into $(d+1)$-dimensional space–time simplices, we can apply a divergence-free and $H(\text{div})$-conforming HDG method to the space–time formulation of the Navier–Stokes equations [3]. The resulting scheme automatically takes into account the domain deformation, and is divergence-free and $H(\text{div})$-conforming in $(d+1)$-dimensional space–time. We will present the derivation of the scheme and some numerical examples.

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HP-FEM FOR THE FRACTIONAL HEAT EQUATION

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In this talk, we present an approximation scheme for the following time dependent fractional diffusion problem on a bounded domain $\Omega \subseteq \mathbb{R}^d$:

$$u_t + (-\Delta)^s u = f, \qquad u(0) = u_0, \quad \text{and} \quad u|_{\partial\Omega} = 0$$

with a parameter $s \in (0,1)$. In order to localize the non-local operator $(-\Delta)^s$, we employ the so-called Caffarelli-Silvestre extension, which yields an equivalent $d+1$-dimensional local problem.

This kind of problem exhibits two sources of singularities, which need to be taken into account for the numerical scheme: The extended problem is degenerate for $y \to 0$, where y is the extended variable, and for $t \to 0$, the parabolic problem may suffer from startup singularities due to incompatibilities of the data with the boundary condition on u.

For discretization, we consider a hp-type finite element discretization in space and an hp-DG method for the time variable. We provide an abstract framework to analyze the convergence of the method. For the one dimensional setting (i.e., $d = 1$), we rigorously prove exponential convergence of the fully discrete scheme without imposing a compatibility condition on the data.

FAST BOUNDARY ELEMENT METHODS FOR COMPOSITE MATERIALS

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In this talk, we discuss numerical solutions to the problems in the field of solid mechanics by combining the Boundary Element Method (BEM) with interpolation by means of radial basis functions, [1]. The main task is to find an approximation to a particular solution of the corresponding elliptic system of partial differential equations. To construct the approximation, the differential operator is applied to a vector of radial basis functions. The resulting vectors are linearly combined to interpolate the function on the right-hand side. The solubility of the interpolation problem is established. Additionally, stability and accuracy estimates for the method are given. A fast numerical method for the solution of the interpolation problem is proposed. These theoretical results are then illustrated on several numerical examples related to the Lamé system.

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EFFICIENT MOLECULAR SURFACE CONSTRUCTION WITHIN AND BEYOND THE CONTINUUM SOLVATION FRAMEWORK: THE NANOSHAPER EXAMPLE

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The progress of powerful experimental techniques such as Cryo-Electron Microscopy represents a remarkable opportunity but also a significant challenge for computational techniques, which aim at extracting useful information and predicting the behavior of biomolecular systems. While pioneering attempts to perform molecular dynamics simulation at this scale by means of super-computers have been made, there still is the compelling need for enabling tools and approaches able to routinely analyze this kind of structures, identifying, for instance, interaction hot spots or new target regions for next generation drug discovery. In this context, the construction and analysis of the Molecular Surface (MS) can play a significant role. MS, in the Solvent Excluded Surface definition, has been widely used as a separation between high from low dielectric regions preliminary to the solution of the Poisson-Boltzmann equation. However, the range of its application is significantly larger. Here, I will describe the development of NanoShaper,[1] a tool for building and analyzing the molecular surface of systems at the nanoscale, as well as a number of its applications, ranging from pocket identification to hydration analysis in molecular dynamics trajectories, until its integration with the widely used VMD software utility [2].

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FE ERROR ESTIMATES FOR SEMILINEAR PARABOLIC CONTROL PROBLEMS IN THE ABSENCE OF THE TIKHONOV TERM

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We study the FE discretization of a semilinear parabolic optimal control problem without the Tikhonov term. A priori error estimates for the FE discretization are derived based on a specific second-order sufficient optimality condition. This error estimate can be significantly improved for optimal controls with bang-bang structure. The theoretical results are illustrated by numerical experiments.

A NON-LINEAR PETROV-GALERKIN METHOD FOR CONVECTION-DOMINATED PROBLEMS

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We consider the numerical approximation of partial differential equations whose solutions may contain sharp features, such as interior and boundary layers. One of the main challenges of designing a numerical method for these types of problems is that these sharp features can lead to non-physical oscillations in the numerical approximation, often referred to as Gibbs phenomena.

The idea we are pursuing is to consider the approximation problem as a residual minimization in dual norms in L^q-type Sobolev spaces, with $1 < q < \infty$. We then apply a non-standard, non-linear Petrov-Galerkin discretization, proposed in [1], that is applicable to reflexive Banach spaces such that the space itself and its dual are strictly convex. Similar to discontinuous Petrov-Galerkin methods [2], this method is based on employing optimal test functions. Replacing the intractable optimal test space by a suitable computable approximation gives rise to a non-linear inexact mixed method for which optimal a priori estimates hold. This generalizes the Petrov-Galerkin framework developed in the context of discontinuous Petrov-Galerkin methods to more general Banach spaces. For the convection-diffusion equation, this yields a generalization of the approach described in [3] from the L^2-setting to the L^q-setting.

A key advantage of considering a more general Banach space setting is that in some cases the oscillations in the numerical approximation vanish as q tends to 1, as we will demonstrate using a few simple numerical examples.

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CONVERGENCE OF ADAPTIVE STOCHASTIC GALERKIN FEM FOR ELLIPTIC PARAMETRIC PDES

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We present an adaptive stochastic Galerkin finite element method for a class of parametric elliptic boundary value problems. The adaptive algorithm is steered by a reliable and efficient *a posteriori* error estimator, which can be decomposed into a two-level spatial estimator and a hierarchical parametric estimator [2]. The structure of the estimated error is exploited by the algorithm to perform a balanced adaptive refinement of the spatial and parametric discretizations. The adaptive algorithm is proved to be convergent in the sense that the estimated error converges to zero [1]. Numerical experiments underpin the theoretical findings and show that the proposed adaptive strategy helps to mitigate the 'curse of dimensionality' which usually afflicts the numerical approximation of parametric PDEs.

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NUMERICAL METHODS BASED ON STAGGERED GRIDS FOR COUPLED STOKES AND DARCY FLOWS

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The marker and cell (MAC) method, a finite volume or finite difference method based on staggered grids, has been one of the simplest and most effective numerical schemes for solving the Stokes and Navier-Stokes equations. The superconvergence on uniform grids for Stokes equations has been observed since 1992 but numerical analysis was not obtained completely. In this talk we will present the second order superconvergence for both velocity and pressure for the MAC scheme for Stokes and Navier-Stokes equations. Then we will present the MAC scheme for coupled Stokes and Darcy problems, and then the second order superconvergence. Numerical experiments using the MAC scheme show agreement of the numerical results with theoretical analysis. Some corresponding and extended results will also be mentioned.

This work is jointed with Xiaoli Li, Yue Sun.

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USING TIME AVERAGED WAVES IN MULTISCALE COMPUTATIONS

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We introduce the operator that maps initial data of a wave equation to the local average in time of the corresponding wave solution around the initial time point. This operator is easy to evaluate numerically by standard wave solvers and it has some interesting properties for multiscale computations. It approximates a projection operator on the lowest eigenmodes of the elliptic operator in the wave equation. Moreover, by the finite speed of propagation of waves, it is a local operator. In this talk we will discuss how it can be used in the numerical solution of PDEs with strongly varying coefficients.

A STABLE AND CONSERVATIVE DG DISCRETIZATION FOR COUPLED SHALLOW WATER–DARCY FLOW

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Interaction between surface flow and subsurface systems is important for a variety of environmental and industrial applications. Mathematical models for such coupled surface/subsurface flows generally express the conservation of mass and momentum, and pose substantial challenges for mathematicians and computational scientists due to the complexity of interface driven processes that are coupled, non-linear, and evolving on various spatial and temporal scales.

We propose a coupled surface/subsurface flow model that relies on hydrostatic (shallow water) equations with free surface in the free flow domain and on the Darcy model in the subsurface part. The interface conditions are motivated by the continuity of the normal flux, the continuity of the total head (different terms of the total head are neglected in the Darcy and the shallow water models, respectively), and a standard friction law. The model is discretized using the local discontinuous Galerkin method and implemented within the fully-vectorized MATLAB / GNU Octave toolbox FESTUNG. Moreover, a discrete energy stability analysis for the coupled system is provided.

THE VIRTUAL ELEMENT METHOD FOR CURVED POLYGONS: STATE OF THE ART AND PERSPECTIVES

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In the past couple of years there have been several attempts to take advantage of the flexibility of VEM in order to deal with elements with curved boundaries. In this talk I will present the pros and cons of the various approaches and discuss their relationship with classical FEM.

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EXPLOITING UNDERLYING APPROXIMATION PROPERTIES IN THE DISCONTINUOUS GALERKIN METHOD FOR IMPROVED TROUBLE CELL INDICATION

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Nonlinear hyperbolic equations are often used to describe the behaviour of a quantity of interest in many areas such as climate modeling, shallow water equations, and computational fluid dynamics. Solutions of these equations may develop discontinuities or shocks. The discontinuous Galerkin (DG) method allows for great flexibility in creating accurate and efficient simulations. However, near a discontinuity or shock, solutions may develop non-physical spurious oscillations. Areas where these occur are called "troubled cells". To counteract these oscillations, typically some stabilization is used such as limiting, filtering, or artificial dissipation. To ensure these techniques are only applied in necessary regions, an accurate troubled cell indicator is needed.

In this presentation we discuss how to exploit the underlying approximation space of the DG method. Specifically, the use of multiwavelets [1] for troubled cell indication. We explain how the DG coefficients easily relate to the multiwavelet decomposition [2]. This decomposition is written as a sum of a global average and finer details on different levels. Using such a decomposition allows the multiwavelet expansion to act as a troubled-cell indicator, where the averages of this contribution are computed on each element, [3, 4]. Additionally, we will discuss the performance of this indicator which typically relies on a problem-dependent parameter. Optimal performance of these indicators should produce an approximation that is free of spurious oscillations. In general, many tests are required to obtain this optimal parameter for each problem. However, to avoid choosing parameters, it is possible to combine the underlying approximation properties with techniques from statistics such as Tukey's boxplot approach [5]. This allows for investigating sudden increases or decreases of the indicator value with respect to the neighboring values and hence, indication basically reduces to detecting outliers. This allows for an automated algorithm that can easily be applied to various troubled-cell indication variables.

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CONTINUOUS AND DISCONTINUOUS GALERKIN METHODS FOR FRACTIONAL ORDER VISCOELASTICITY

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A problem modelling fractional order viscoelasticity, is considered. Well-posedness of the model problem is studied within the framework of the semigroup theory of linear operators and the Galerkin approximation method. Spatial semidiscretization of the problem is formulated by means of finite element method, and full discretization of the problem is studied using continuous and discontinuous Galerkin methods. Stability estimates and optimal order a priori error estimates are proved.

FINITE ELEMENT APPROXIMATION OF THE ISAACS EQUATION

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We propose and analyze a two-scale finite element method for the Isaacs equation. The fine scale is given by the mesh size h whereas the coarse scale ε is dictated by an integro-differential approximation of the partial differential equation. We show that the method satisfies the discrete maximum principle provided that the mesh is weakly acute. This, in conjunction with weak operator consistency of the finite element method, allows us to establish convergence of the numerical solution to the viscosity solution as $\varepsilon, h \to 0$, and $\varepsilon \geq C(h|\log h|)^{1/2}$. In addition, using a discrete Alexandrov Bakelman Pucci estimate we deduce rates of convergence, under suitable smoothness assumptions on the exact solution.

WAVENUMBER-EXPLICIT ANALYSIS FOR HIGH-FREQUENCY MAXWELL EQUATIONS

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In our talk we consider the Maxwell equations in the frequency domain, discretized by Nédélec-*hp*-finite elements. We develop a stability and convergence analysis which is explicit with respect to the wave number k, the mesh size h, and the local polynomial degree p. It turns out that, for the choice $p \gtrsim \log(k)$, the discretization does not suffer from the so-called pollution effect. This is known for high-frequency acoustic scattering. However, the analysis of Maxwell equations requires the development of twelve additional theoretical tools which we will introduce and explain how they are employed to prove the stability and convergence of our method.

VARIABLE ORDER, DIRECTIONAL $\mathcal{H}^2$-MATRICES FOR HELMHOLTZ PROBLEMS WITH COMPLEX FREQUENCY

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The sparse approximation of high-frequency Helmholtz-type integral operators has many important physical applications such as problems in wave propagation and wave scattering. The discrete system matrices are huge and densely populated; hence their sparse approximation is of outstanding importance. In our talk we will generalize the directional $\mathcal{H}^2$-matrix techniques from the "pure" Helmholtz operator $Lu = -\Delta u + z^2 u$ with $z = -ik, k$ real, to general complex frequencies z with $\mathrm{Re}(z) > 0$. In this case, the fundamental solution decreases exponentially for large arguments. We will develop a new admissibility condition which contain $\mathrm{Re}(z)$ and $\mathrm{Im}(z)$ in an explicit way and introduce the approximation of the integral kernel function on admissible blocks in terms of frequency-dependent directional expansion functions. We present an error analysis which is explicit with respect to the expansion order and with respect to the real and imaginary part of z. This allows us to choose the variable expansion order in a quasi-optimal way depending on $\mathrm{Re}(z)$ but independent of, possibly large, $\mathrm{Im}(z)$. The complexity analysis is explicit with respect to $\mathrm{Re}(z)$ and $\mathrm{Im}(z)$ and shows how higher values of $\mathrm{Re}(z)$ reduce the complexity. In certain cases, it even turns out that the discrete matrix can be replaced by its nearfield part.

Numerical experiments illustrate the sharpness of the derived estimates and the efficiency of our sparse approximation.

MULTILEVEL BEST LINEAR UNBIASED ESTIMATORS

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We present a general variance reduction technique to accelerate the estimation of an expectation of a scalar valued quantity of interest. We reformulate the estimation as a linear regression problem and show that the derived estimators are variance minimal within the class of linear unbiased estimators. We further decrease the cost of the estimation by solving a sample allocation problem and analyze the asymptotic complexity of the resulting estimater, which we call Sample Allocation Optimal Best Linear Unbiased Estimator, using Richardson extrapolation. We provide theoretical results that show that our framework improves upon other sampling based estimation techniques like Monte Carlo, Multilevel Monte Carlo and Multifidelity Monte Carlo. The results are illustrated by a numerical example where the underlying model of the quantity of interest is a partial differential equation.

FAST AND PARALLEL RUNGE-KUTTA APPROXIMATION OF SUBDIFFUSION EQUATIONS

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A highly parallel algorithm for the numerical solution of inhomogeneous linear time-fractional differential equations of the type

$$D_t^\alpha u(t) = Au(t) + f(t) \text{ for } t \in (0,T) \text{ and } u(0) = 0$$

is presented. Here D_t^α is a (Caputo) fractional derivative, and $(A, D(A))$ a closed, densely defined, sectorial linear operator in some Banach space defined on $D(A)$.

The algorithm requires the solution of $\mathcal{O}(\log(1/h)\log(1/\varepsilon))$ linear systems in parallel, where h is the time step size required to resolve the inhomogeneity f and ε is the required accuracy. Additionally the solution of $\mathcal{O}(N\log(1/h)\log(1/\varepsilon))$ scalar linear inhomogeneous differential equations $\dot{y}(t) = \lambda y(t) + f(t)$ on certain time intervals is needed. The basic ingredients of the algorithm are the variation of constants formula, the Cauchy integral representation for the approximation of the operator exponential and the discretization of contour integrals using $\mathcal{O}(\log(1/h))$ contours with $\mathcal{O}(\log(1/\varepsilon))$ quadrature points each. Details of the basic algorithm can be found in [M. Fischer, Fast and Parallel Runge–Kutta Approximation of Fractional Evolution Equations. SIAM Journal on Scientific Computing 41:2, 2019, A927-A947].

In the numerical example the operator A will be the Laplacian with appropriate boundary conditions, discretized by the finite element method.

SPACE-TIME FINITE ELEMENT METHODS FOR PARABOLIC INITIAL-BOUNDARY VALUE PROBLEMS WITH NON-SMOOTH SOLUTIONS

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We consider locally stabilized, conforming finite element schemes on completely unstructured simplicial space-time meshes for the numerical solution of parabolic initial-boundary value problems with variable coefficients that may be discontinuous in space and time. Discontinuous coefficients, non-smooth boundaries, and changing boundary conditions, non-smooth initial conditions, and non-smooth right-hand sides can lead to non-smooth solutions. For instance, in electromagnetics, permanent magnets cause line-delta-distributions in the source term of the right-hand side in 2D quasi-magnetostatic simulations of electrical machines. We present new a priori estimates under the assumption of local maximal parabolic regularity that includes low-regularity solutions arising from non-smooth data such as mentioned above. In order to avoid reduced convergence rates appearing in the case of uniform mesh refinement, we also consider adaptive refinement procedures based on residual a posteriori error indicators. The huge system of space-time finite element equations, that is positive definite, but non-symmetric, is then solved by means of the Generalized Minimal Residual Method preconditioned by algebraic multigrid. In particular, in the 4d space-time case that is 3d in space, simultaneous space-time adaptivity and parallelization can considerably reduce the computational time. The space-time finite element solver was implemented with the library MFEM. We present numerical examples with different features. The numerical results nicely confirm our theoretical findings. The parallel version of the code shows an excellent parallel performance.

NUMERICAL EVALUATION OF INTEGRAL OPERATORS WITHIN SPACE-TIME METHODS FOR THE WAVE EQUATION

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We discuss the development of a space-time boundary element method for the 3d wave equation. Classical approximation methods use a product ansatz in space and time. In contrast, we present a discretization method that is not based on such a separation, but treats the time variable as a further spatial coordinate. This idea leads to arbitrary discretizations of the operator equations in the 3+1-dimensional space-time cylinder.

Boundary element methods are based on surface potentials, which are known as *retarded* layer potentials in the context of the wave equation. Due to the use of these potentials, only a discretization of the lateral boundary of the space-time cylinder, which is a 3d hypersurface in 4d, is necessary. This boundary is decomposed into an unstructured mesh of tetrahedral elements and standard piecewise polynomial trial spaces are used to approximate the surface densities.

To implement boundary element methods, an accurate and robust algorithm for the evaluation of the underlying integral operators is vital. First, an integral representation of retarded layer potentials which genuinely fits the space-time setting is discussed. In particular, these operators integrate along the intersection of the boundary of the backward light cone and the lateral boundary of the space-time cylinder. Second, a numerical integration scheme for the pointwise evaluation of retarded layer potentials is presented. Moreover, we comment on a tentative approach for the evaluation of bilinear forms arising in typical variational formulations of boundary integral equations of the wave equation. Numerical examples close the talk.

MULTILEVEL UNCERTAINTY QUANTIFICATION WITH SAMPLE-ADAPTIVE MODEL HIERARCHIES

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Sample-based multilevel uncertainty quantification tools, such as multilevel Monte Carlo, multilevel quasi-Monte Carlo or multilevel stochastic collocation, have recently gained huge popularity due to their potential to efficiently compute robust estimates of quantities of interest (QoI) derived from PDE models that are subject to uncertainties in the input data (coefficients, boundary conditions, geometry, etc). Especially for problems with low regularity, they are asymptotically optimal in that they can provide statistics about such QoIs at (asymptotically) the same cost as it takes to compute one sample to the target accuracy. However, when the data uncertainty is localised at random locations, such as for manufacturing defects in composite materials, the cost per sample can be reduced significantly by adapting the spatial discretisation individually for each sample. Moreover, the adaptive process typically produces coarser approximations that can be used directly for the multilevel uncertainty quantification. In this talk, I will present two novel developments that aim to exploit these ideas.

In the first part I will present Continuous Level Monte Carlo (CLMC), a generalisation of multilevel Monte Carlo (MLMC) to a continuous framework where the level parameter is a continuous variable. This provides a natural framework to use sample-wise adaptive refinement strategy, with a goal-oriented error estimator as our new level parameter. We introduce a practical CLMC estimator (and algorithm) and prove a complexity theorem showing the same rate of complexity as for MLMC. Also, we show that it is possible to make the CLMC estimator unbiased with respect to the true quantity of interest. Finally, we provide two numerical experiments which test the CLMC framework alongside a sample-wise adaptive refinement strategy, showing clear gains over a standard MLMC approach with uniform grid hierarchies.

In the second part, I will show how to extend the sample-adaptive strategy to multilevel stochastic collocation (MLSC) methods providing a complexity estimate and numerical experiments for a MLSC method that is fully adaptive in the dimension, in the polynomial degrees and in the spatial discretisation.

This is joint work with Gianluca Detommaso (Bath), Tim Dodwell (Exeter) and Jens Lang (Darmstadt).

A STUDY OF LIGHT-MATTER INTERACTION AT THE NANOSCALE: THEORETICAL AND NUMERICAL CONSIDERATIONS

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Nanophotonics is the area of physics that tries to exploit the interaction of light with nanoscaled structures. By using metallic nanostructures, one is able in particular to obtain impressive exaltation of light and subwavelength confinement. This opens up new possibilities for controlling and enhancing optical wave-matter interactions and leads to a lot of interesting applications such as (to cite but a few) efficient design of nanolasers, nanoantennas, solar cells or biosensing.

In this domain, numerical modelling is fundamental in order to envisage any expensive experimental scenario. The deep understanding of the phenomenon itself is also essential for physicists. A precise study of the possible models are thus essential. The modelling relies on the accurate description of the propagation of an optical wave in a dispersive metallic medium. At the scales and frequencies considered, several effects have to be taken into account. In particular, a correct characterization of the response of the electrons in the metal to the applied electromagnetic field is crucial and can lead to new models. In this work, we propose to focus on a model that incorporates some quantum effects. It consists of a linear coupling between the time domain Maxwell's equations and a linearized hydrodynamic model with a quantum pressure term. Both theoretical and numerical interesting challenges emerge from this PDE model.

We are especially interested in providing a complete study in this context: from theoretical issues of well-posedness and stability, to the development of adapted and efficient numerical algorithms (here we choose to use a discontinuous Galerkin numerical framework) and the study of their academic properties, to finally, efficient numerical simulations on realistic test cases. We will go through several results that we recently obtained for this particular model.

NONCONFORMING HP-FE/BE COUPLING ON UNSTRUCTURED MESHES BASED ON NITSCHE'S METHOD

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We construct and analyze an *hp*-FE/BE coupling on non-matched meshes, based on Nitsche's method. Both, the mesh size and the polynomial degree are changed to improve accuracy. Nitsche's method leads to a positive definite formulation, thus, unlike the mortar method, it does not require the *Babuška-Brezzi* condition for stability. The method is stable provided the stabilization function is larger than a certain threshold reliant on mesh parameters at the interface. We obtain an *explicit* bound for the threshold and derive *a priori* error estimates for quasi-uniform and geometrically refined meshes. Our analysis can be easily extended to the case of pure FE or pure BE decomposition of the domain as well as to the case of more than two subdomains. The problem in a bounded domain is considered in detail, but the case of an unbounded BE subdomain and a bounded FE subdomain follows with similar arguments. Several numerical examples are given for quasi-uniform discretizations in both subdomains as well as *hp*-versions with analytic and singular solutions.

SECOND ORDER DIRECTIONAL SHAPE DERIVATIVES OF INTEGRALS ON SUBMANIFOLDS

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We compute first and second order shape sensitivities of integrals on smooth submanifolds using a variant of shape differentiation. The result is a quadratic form in terms of one perturbation vector field that yields a second order quadratic model of the perturbed functional. We discuss the structure of this derivative, derive domain expressions and Hadamard forms in a general geometric framework, and give a detailed geometric interpretation of the arising terms.

LOCALIZED MODEL REDUCTION FOR MULTI-SCALE PDE-CONSTRAINED OPTIMIZATION

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We consider optimization where the constraint involves solving an elliptic multi-scale problem. The computational demand of such tasks easily exceeds existing resources, if standard approximation methods are employed for the approximation of the underlying PDE. Model order reduction (MOR) methods for parameterized partial differential equation (pPDEs), such as the Reduced Basis (RB) method, allow to quickly obtain approximate solutions or derived quantities, which is achieved by a decomposition of the computation into an expensive offline and a cheap online part. If employed as a surrogate approximation for the underlying pPDE, MOR methods have the potential to significantly speed up the optimization. However, standard global (in a spatial as well as parametric sense) MOR methods that construct a single reduced space for the whole parameter range of the underlying pPDE may still induce a tremendous offline computational burden for multi-scale or large scale problems.

A possible remedy is to consider localized methods, both in parameter- as well as physical space. In the context of the latter, localized RB methods combine ideas from domain decomposition methods, numerical multi-scale methods and RB methods to obtain a (parameter) global surrogate model spanned by spatially localized reduced spaces. As a particular example, the localized RB multi-scale method equipped with error control w.r.t. the true solution allows to adaptively enrich these local reduced spaces [2]. In the context of PDE-constrained optimization, such adaptive localized MOR methods have the potential to adapt the reduced model during the optimization, as required (see also [3, 1]).

We will demonstrate recent advances of localized RB methods in the context of PDE-constrained optimization, in particular regarding error control and adaptivity.

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MULTILEVEL QUADRATURE FOR ELLIPTIC PROBLEMS ON RANDOM DOMAINS BY THE COUPLING OF FEM AND BEM

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Elliptic boundary value problems which are posed on a random domain can be mapped to a fixed, nominal domain. The randomness is thus transferred to the diffusion matrix and the loading. While this domain mapping method is quite efficient for theory and practice, since only a single domain discretisation is needed, it also requires the knowledge of the domain mapping.

However, in certain applications the random domain is only described by its random boundary, i.e. the domain mapping is only known for the boundary, while the quantity of interest is defined on a fixed, deterministic subdomain. In this setting, it thus becomes necessary to extend the domain mapping from the boundary to the whole domain, such that the domain mapping is the identity on the fixed subdomain.

To overcome the necessity of computing the extension, we therefore couple the finite element method on the fixed subdomain with the boundary element method on the random boundary. We verify the required regularity of the solution with respect to the random perturbation field for the use of multilevel quadrature, derive the coupling formulation, and show by numerical results that the approach is feasible.

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REFINED A POSTERIORI ERROR ESTIMATION FOR CLASSICAL AND PRESSURE-ROBUST STOKES FINITE ELEMENT METHODS

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Recent works showed that pressure-robust modifications of mixed finite element methods for the Stokes equations outperform their standard versions in many cases. This is achieved by divergence-free reconstruction operators and results in pressure independent velocity error estimates which are robust with respect to small viscosities. In this paper we develop a posteriori error control which reflects this robustness. The main difficulty lies in the volume contribution of the standard residual-based approach that includes the L2-norm of the right-hand side. However, the velocity is only steered by the divergence-free part of this source term. An efficient error estimator must approximate this divergence-free part in a proper manner, otherwise it can be dominated by the pressure error. To overcome this difficulty a novel approach is suggested that uses arguments from the stream function and vorticity formulation of the Navier–Stokes equations. The novel error estimators only take the curl of the right-hand side into account and so lead to provably reliable, efficient and pressure-independent upper bounds in case of a pressure-robust method in particular in pressure-dominant situations. This is also confirmed by some numerical examples with the novel pressure-robust modifications of the Taylor–Hood and mini finite element methods.

A PRIORI AND A POSTERIORI ERROR ESTIMATES FOR A STABILIZED PRIMAL-HYBRID HP-FINITE ELEMENT METHOD

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In this talk a stabilized primal-hybrid *hp*-method is introduced which approximatively ensures continuity conditions across element interfaces and avoids the enrichment of the primal discretization space as usually required to fulfill some discrete inf-sup condition. A priori as well as a posteriori error estimates are presented for this method. The stabilized primal-hybrid *hp*-method is also applied to a model contact problem since the method admits the definition of pointwise constraints. In numerical experiments convergence properties and the applicability of the a posteriori error estimates to drive *h*- and *hp*-adaptive schemes are discussed.

WEAKLY IMPOSING BOUNDARY CONDITIONS ON THE BOUNDARY ELEMENT METHOD USING A PENALTY METHOD

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In recent years, Nitche's method has become increasingly popular within the finite element community as a method for weakly imposing boundary conditions. Inspired by this, we propose a penalty-based method for weakly imposing boundary conditions within boundary element methods.

We consider boundary element methods where the Calderón projector is used for the system matrix and boundary conditions are weakly imposed using a particular variational boundary operator. Regardless of the boundary conditions, both the primal trace variable and the flux are approximated.

Due to using the full Calderón projector, the number of unknowns—and hence the computational cost—is higher for problems such as those with pure Dirichelt conditions. As such, we focus on more complex boundary conditions: mixed Dirichlet–Neumann, Robin, and Signorini contact conditions. The focus of this talk is on Laplace's equation, although the imposition method is also applicable to other problems.

The theory is illustrated by a series of numerical examples using the software library Bempp.

VARIATIONAL SMOOTH INTERPOLATION USING POLYHARMONIC SPLINES

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Polyharmonic splines solve the polyharmonic equation and have a lot of interesting properties. It is sometimes advantageous to solve various mathematical problems with the help of polyharmonic functions. In the contribution, we are concerned with the smooth interpolation of the measured data by polyharmonic functions.

Polyharmonic functions, when employed for interpolation, are radial basis functions. We show which conditions required in the general variational approach to smooth interpolation give polyharmonic functions as a result. To this end, we choose the space of functions $\exp(-ik \cdot x)$ for the space where we minimize functionals and measure the smoothness of the result. The general form of the interpolation formula is then the linear combination of the values of some radial basis functions and low-order polynomials (called the trend) at nodes. The dimension of the interpolated data considered in this contribution can be higher than 1.

We also mention the problem of smooth curve fitting (data smoothing) and present a numerical example.

ADAPTIVE WEAK GALERKIN METHOD FOR CONVECTION-DIFFUSION PROBLEMS

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The accuracy of numerical solutions to convection-diffusion problems is often marred by the presence of layers in a convection-dominated regime. A natural tool to overcome this difficulty is to adaptively refine the mesh in regions where these layers get formed. In this talk, we present an adaptive weak Galerkin (WG) method to serve this purpose. Since the WG method uses discontinuous approximating functions on polytopal meshes, it is very suitable for mesh adaptivity. Furthermore, in this formulation, there are no extra conditions on the convection coefficient and the formulation itself is simple with an upwind choice of the convection stabilization term. We prove that just like the a priori error analysis presented in [1], our a posteriori error analysis too, is simple, short and yields upper bounds for the error which are uniformly bounded with respect to the diffusion coefficient. Numerical results are presented to illustrate the performance of the estimator in the presence of boundary and interior layers.

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SPACE-TIME DISCONTINUOUS GALERKIN METHOD FOR THE WAVE EQUATION USING THE SYMMETRIC INTERIOR PENALTY FLUX

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In this presentation we will discuss the space time discontinuous Galerkin (dG) finite element discretisation for the scalar wave equation using the symmetric interior penalty flux. In this discretization no distinction is made between the space and time variables and discontinuous basis functions are used, both in space and time. This approach results in an accurate space- time-discretization, that is also suitable for hp-adaptation. We first write the space-time discretization as a first order system and then modify it further into a symmetric form, which is essential in obtaining a stability estimate for the space-time dG discretization of the scalar wave equation. This stability result then provides the necessary bounds to conduct the error analysis. Based on the error analysis we obtain a convergence rate for the space-time discretization in the dG-norm.

EQUIVALENCE OF LOCAL- AND GLOBAL-BEST APPROXIMATIONS IN $H(\mathrm{DIV})$ WITH RAVIART–THOMAS–NÉDÉLEC ELEMENTS

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We prove an equivalence between the local-best and global-best approximation errors of Raviart–Thomas–Nédélec finite element spaces in $H(\mathrm{div})$. More precisely, given an arbitrary function in $H(\mathrm{div})$, we show that the error attained by the global-best approximation by $H(\mathrm{div})$-conforming piecewise polynomial Raviart–Thomas–Nédélec elements under additional constraints on the divergence and normal flux on the boundary, is, up to a generic constant, equivalent to the sum of independent local-best approximation errors over individual mesh elements, without constraints on the divergence or normal fluxes. The generic constant only depends on the shape-regularity of the underlying simplicial mesh, the space dimension, and the polynomial degree of the approximations. We also present a variant of this result, where robustness of the constant with respect to the polynomial degree is attained for unbalanced polynomial degrees between local and global approximations. These results enable us to derive optimal rates of convergence in both the mesh size and polynomial degree for vector fields with finite elementwise Sobolev regularity, which can be readily applied to *a priori* error estimates for mixed finite element and least-squares methods. Our analysis also give rise to a simple, stable, commuting, local projector in $H(\mathrm{div})$ with an error equivalent to the local-best approximation, which is of independent interest.

SEMISMOOTH NEWTON METHODS FOR HJB EQUATIONS

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The numerical solution of fully nonlinear Hamilton–Jacobi–Bellman (HJB) partial differential equations (PDE) leads to the task of solving large systems of equations, with a nonlinearity that is often not differentiable in a classical sense. Nevertheless, a well-established iterative method, commonly called policy iteration or Howard's algorithm, often converges rapidly in practice, as well as constituting an essential ingredient for constructive proofs of the existence of discrete numerical solutions for monotone discretization schemes. More recently, it has become apparent that the notions of semismoothness and of semismooth Newton methods provide a suitable framework for establishing the superlinear convergence of the algorithm. In this talk, we present the proof of semismoothness of HJB differential operators posed on Sobolev spaces, with a possibly infinite control set that is merely assumed to be a compact metric space. In particular, we will show how the measurable selection theorem of Kuratowski and Ryll-Nardzewski plays a central role in guaranteeing the existence of a generalized differential for the HJB operator. We illustrate the theory with numerical experiments showing the performance of the semismooth Newton method in applications to high-order discretizations of HJB equations with Cordes coefficients.

A CONVERGENT LAGRANGIAN DISCRETIZATION FOR P-WASSERSTEIN AND FLUX-LIMITED DIFFUSION EQUATIONS

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A Lagrangian numerical scheme for solving a non-linear drift diffusion equation of the form

$$\partial_t u = \partial_x(u \cdot (c^*)'[\partial_x(h'(u) + V)])$$

on an interval with no-flux boundary conditions is presented. Here h is the internal energy density, V an external energy potential and c^* the Legendre-transform of a transport cost c from a family of L^p-like cost functions, but possibly with discontinuities. Examples include the Fokker-Planck equation, the Porous medium equation, the parabolic p-Laplace equation and the so-called relativistic heat equation.

Our numerical scheme is based on the equation's gradient flow formulation in a Wasserstein-like metric for the cost function c. Specifically, we use the representation in terms of the inverse distribution function and perform a spatio-temporal discretization in these coordinates.

The discretization inherits various properties from the continuous flow, like entropy monotonicity, mass preservation, a minimum/maximum principle and flux-limitation in the case of flux-limiting cost. Our main result is that of convergence in the spatio-temporal continuous limit.

FINITE VOLUME METHODS FOR THE FRACTIONAL KLEIN-KRAMERS EQUATION

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The fractional Klein-Kramers equation describes the process of subdiffusion in the presence of an external force field in phase space. We present a family of finite volume schemes for the fractional Klein-Kramers equation, that includes first or second order schemes in phase space, and implicit or explicit schemes in time. We prove, for the open domain, that the schemes satisfy the positivity preserving property. For a bounded domain in space we consider two types of boundary conditions, absorbing boundary conditions and reflecting boundary conditions. The inclusion of boundary conditions leads to some technical complications that require changes in the finite volume schemes near the boundary. Numerical tests are presented in the end.

GUARANTEED A POSTERIORI BOUNDS FOR EIGENVALUES AND EIGENVECTORS: MULTIPLICITIES AND CLUSTERS

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In this talk we present a posteriori error estimates for conforming numerical approximations of eigenvalue clusters of second-order self-adjoint elliptic linear operators with compact resolvent. Given a cluster of eigenvalues, we estimate the error in the sum of the eigenvalues, as well as the error in the eigenvectors given through the density matrix, i.e., the orthogonal projector on the associated eigenspace. This allows us to deal with degenerate (multiple) eigenvalues within the framework. All the bounds are valid under the only assumption that the cluster is separated from the surrounding smaller and larger eigenvalues; we show how this assumption can be numerically checked. Our bounds are guaranteed and converge with the same speed as the exact quantities. They can be turned into fully computable bounds as soon as an estimate on the dual norm of the residual is available, which is presented in two particular cases: the Laplace eigenvalue problem discretized with conforming finite elements, and a Schrödinger operator with periodic boundary conditions of the form $-\Delta + V$ discretized with planewaves. For these two cases, numerical illustrations are provided on a set of test problems.

MOMENTUM-CONSERVATIVE STRESS APPROXIMATION METHODS IN ELASTOPLASTICITY

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In many applications in computational solid mechanics, one is primarily interested in accurate approximations of the associated stresses. This is due to the fact that stresses are responsible for effects like plastic material behavior, damage or failure due to surface forces. In particular, $H(\mathrm{div})$-conforming stress finite element approximations with local momentum conservation properties possess some advantageous properties in this context.

Two approaches for the computation of such stress approximations in the $H(\mathrm{div})$-conforming Raviart-Thomas finite element space will be treated in this talk: Directly, via the dual variational formulation known as Hellinger-Reissner principle [BBF09] and indirectly, via a stress equilibration procedure based on some primal finite element approximation [BKMS18]. Both approaches lead to weakly symmetric stresses with local momentum conservation and crucially depend on the inf-sup stability of the underlying constraint minimization problem.

The extension to elastoplasticity will turn out to be more complicated than the purely elastic case due to the additional inequality constraint. The case of a von Mises flow rule with hardening as well as perfect plasticity will be discussed. For the latter, a weakly symmetric generalization of the nonconforming stress elements of [GG11] will prove to be useful.

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SPACE-TIME BEM FOR THE HEAT EQUATION

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In this talk we present a new framework for the numerical analysis of space-time boundary element methods for the heat equation. As for elliptic problems we first consider domain variational formulations in anisotropic Sobolev spaces of Galerkin-Petrov type, or equivalently of Galerkin-Bubnov type when using a Hilbert type transformation. From this we derive all mapping properties of boundary integral operators and we discuss unique solvability of related boundary integral equations.

For the space-time discretization we consider boundary element spaces which are defined with respect to either tensor product or rather general boundary element meshes of the space-time boundary. For the approximate solution we provide related a priori error estimates, and we discuss the iterative solution when using preconditioning by operators of opposite order.

This presentation is based on joint work with Stefan Dohr and Marco Zank.

ADAPTIVE STRATEGIES FOR TRANSPORT EQUATIONS

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We consider linear transport equations with a variable convection field. A discontinuous Petrov-Galerkin (DPG) discretization is presented that is uniformly inf-sup stable whilst applying a test search space with a dimension that is proportional to that of the trial space ('practical' DPG method). Applying the same test search space we show that the natural a posteriori error estimator is efficient and, modulo a data-oscillation term, reliable. Finally we discuss a bulk chasing adaptive scheme driven by this estimator. For the one-dimensional case we show a fixed error reduction in each step, where a corresponding result in multiple dimensions is currently partly based on a conjecture.

STABILIZED MIXED BOUNDARY ELEMENTS FOR THE WAVE EQUATION AND HYPERBOLIC VARIATIONAL INEQUALITIES

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We discuss the numerical analysis of mixed formulations for the wave equation using time-dependent boundary element methods. Stabilized mixed methods are used for the Signorini problem, a scalar model problem for dynamic contact in elasticity. In a first step, the wave equation with Signorini boundary conditions is reduced to a variational inequality for the Poincare-Steklov operator on the contact boundary, which is numerically realized in terms of retarded potentials.
We review the existence of solutions to the dynamic contact problem and, assuming existence, discuss the a priori error analysis of an equivalent mixed formulation, as well as its minimal stabilization based on local projections. Even for time independent problems our approach provides a simplified stabilization of boundary element discretizations. We further discuss extensions to boundary problems for the wave equation involving Tresca friction. Numerical results illustrate the efficiency of our methods for dynamic contact in three dimensions.

TENT PITCHING AND A TREFFTZ-DG METHOD FOR THE ACOUSTIC WAVE EQUATION

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We present a space-time Trefftz discontinuous Galerkin (DG) method for the approximation of the acoustic wave equation on space-time tent-pitched meshes. Tent-pitching is a front-advancing mesh technique that allows to completely localize the solution of the discrete system. Trefftz basis functions are local solutions to the wave equation, that allow to simply advance the solution from the bottom to the top of each tent-element. The method has been implemented in NGSolve, solving the space-time elements in parallel. Insights into the implementation details are given, including the case of propagation in heterogeneous media.

Compared to the classical approach, where one uses finite element methods to discretize space and then uses time stepping schemes to advance in time, we take a different approach, using finite element approximation simultaneously in space and time. This requires to mesh the full space-time domain and increases the dimension of the approximation space by the dimension of time. On the upside, *hp*-refinement is made possible in space-time. Furthermore, the space-time mesh is not forced to be a product mesh, as it is for time stepping schemes. This gives us the possibility to devise suitable mesh design strategies in order to circumvent the CFL-condition, which usually limits the global time-step size by the size of the smallest spatial element, instead allowing locally optimal time advances. The tent pitched space-time mesh, complies with the causality properties of the hyperbolic PDE, solve the PDE from local information only, allowing for a high degree of parallelism between independent mesh elements. Trefftz methods allow to enforce properties of the PDE in the test and trial spaces, resulting in smaller approximation spaces, but preserving approximation properties, reducing the cost of the increased dimension of the discretized space.

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FINITE ELEMENT APPROXIMATIONS FOR SEVERAL NON-SELFADJOINT EIGENVALUE PROBLEMS

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In this talk, we shall discuss the finite element approximations for several non-selfadjoint eigenvalue problems including a Steklov eigenvalue problem, a transmission eigenvalue problem, and a scattering resonance problem in a narrow metallic slit. A new eigenvalue solver for the non-Hermitian matrices resulting from the discretization of the above problems will be introduced. Numerical examples are presented as well.

PHYSICS-PRESERVING ALGORITHMS FOR MULTI-PHASE FLOW IN POROUS MEDIA

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Simulation of multiphase flow in porous media has wide applications, which includes in particular the management of existing petroleum fields and the development of new oil and gas reservoirs. In this talk we present a new efficient IMplicit Pressure Explicit Saturation (IMPES) scheme for multi-phase flow in porous media with capillary pressure. Compared with the conventional IMPES schemes, the new IMPES scheme is inherently physics-preserving, namely, the new algorithm is locally mass conservative for all phases and it also enjoys another merit that the total velocity is continuous in the normal direction. Moreover, the new scheme is unbiased with regard to the phases and the saturations of all phases are bounds-preserving if the time step size is smaller than a certain value. We also present some interesting examples to demonstrate the efficiency and robustness of the new algorithm.

SOLVING PARABOLIC PROBLEMS ON ADAPTIVE POLYGONAL MESHES WITH VIRTUAL ELEMENT METHODS

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We will discuss some recent advances in developing numerical schemes for solving parabolic problems using adaptive meshes consisting of general polygonal or polyhedral elements, based on the virtual element method. The adaptive algorithms we present are driven by rigorous a posteriori error estimates, developed by building on previous results for virtual element methods for elliptic problems through elliptic reconstruction techniques modified for the present setting. Numerical results will be shown to demonstrate the practical performance of these algorithms on certain benchmark problems including pattern forming mechanisms in a three-species cyclic competition system.

A HIGH-ORDER B-SPLINE MATERIAL POINT METHOD

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The Material Point Method (MPM) [1] has shown to be succesful in simulating problems that involve large deformations and history-dependent material behaviour. MPM can be considered as a hybrid Eulerian-Langranian method that combines the use of a set of particles, called material points, with a fixed background grid. The equations of motion are solved on this background grid within a variational framework, typically adopting piece-wise linear (Lagrangian) basis functions. Integrals resulting from the variational formulation are then approximated by using the material points as quadrature points.

The use of piecewise-linear basis functions leads however to unphysical oscillations (so called 'grid crossing errors') in the numerical solution, due to the discontinuity of the gradient of these basis functions. Furthermore, the use of material points as integration points leads to a quadrature rule of which the quality is uncertain.

Recently, different strategies have been proposed to overcome these shortcomings. The use of quadratic B-spline basis functions within MPM (i.e. B-spline MPM [2]) completely removes grid-crossing errors, due to the C^1-continuity of the basis functions. The application of a Taylor Least-Squares (TLS) reconstruction [3] has shown to lead to more accurate integration, while conserving the total mass and momentum within MPM.

In this talk, we present prelimenary results obtained with a novel implementation of B-spline MPM within the C++ library G+Smo [4]. In this implementation, a TLS reconstruction to approximate the integrals in the variational formulation is included. Furthermore, it enables the use of MPM within a high performance computing (HPC) framework. Numerical results, obtained for different two-dimensional benchmarks, show that this version of the MPM potentially shows $\mathcal{O}(h^{p+1})$ spatial convergence.

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SIMULATION OF LOCALIZED SURFACE PLASMON RESONANCES VIA DIRICHLET-NEUMANN OPERATORS AND IMPEDANCE-IMPEDANCE OPERATORS

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It is important to engineers and scientists alike to simulate scattering returns of electromagnetic radiation from bounded obstacles. In this talk we present High-Order Perturbation of Surfaces algorithms for the simulation of such configurations, implemented with Dirichlet-Neumann Operators and Impedance-Impedance Operators. With an implementation of these approaches we demonstrate the stable, robust, and highly accurate properties of our algorithms. We also demonstrate the validity and utility of our approaches with a sequence of numerical experiments. Moreover, we show how our formulation delivers a straightforward proof of existence, uniqueness, and analyticity of solutions to this problem.

SCATTERING PROBLEMS WITH OSCILLATING, NON-PERIODIC AND DISCONTINUOUS WAVE SPEED

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We study the Helmholtz equation in heterogeneous media in $\mathbb{R}^d$, $d = 1, 2, 3$ modelled in the frequency domain. For a class of oscillatory discontinuous coefficients with spherical symmetry, we present a new theoretical approach to bound the norm of the solution operator by a term which is exponential in the frequency and independent of the number of discontinuities. We present examples of coefficients showing that our estimates are sharp. In particular our examples in 3D differ from the wave localisation effects appearing at a single discontinuity in the geometry or the material ("whispering gallery" modes). Instead, the growth of the stability constant is caused by a highly varying wave speed.

A FINITE ELEMENT SCHEME FOR VISCOPLASTIC MODELS IN METAL FORMING PROBLEMS

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The mathematical modeling and the numerical simulation of rolling metal processes, i.e., the plastic deformation of a metal plate passing through a pair of rotating rolls, are subjects of investigation of many researchers. In this work we consider a rigid-viscoplastic model (Norotn-Hoff power law model) for describing a plane strain rolling process and develop a continuous finite element scheme for its discretization. The unilateral conditions are described by inequality constraints and the stick/slip motion along the interface between the roll and the plate is described by extending the usual Coulomb's law to viscoplastic frame. The associated conditions are incorporated in the finite element scheme by using Nitsche-type (penalty) terms. These terms involve tangential and normal component terms of the relative velocity, in order to impose weakly the relative frictional sliding motion and the non penetration constraints. The discontinuous nature of this approach gives several advantages for the case of having general non-matching interface meshes. Numerical results related to the variation of the important variables, e.g., velocity components, normal stress, etc, after long time integration will be discussed.

The results presented in this talk are based on [2], [3]. This work is supported by the project COMET K2 XTribology, No 849109, Project grantee: Excellence Center for Tribology. The first author is partially supported by the project "JKU-LIT-2017-4-SEE-004".

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BOUNDARY ELEMENT METHODS FOR ELECTROMAGNETIC RESONANCE PROBLEMS IN OPEN SYSTEMS

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We consider Galerkin boundary element methods for the approximation of different kinds of electromagnetic resonance problems in open systems. Examples are the scattering-resonance problem for dielectric and plasmonic scatterers. An analysis of the used boundary integral formulations and their numerical approximations is presented in the framework of eigenvalue problems for holomorphic Fredholm operator-valued functions. We employ recent abstract results [3] to show that the Galerkin approximation with Raviart-Thomas elements provides a so-called regular approximation of the underlying operators of the eigenvalue problems. This enables us to apply classical results of the numerical analysis of eigenvalue problems for holomorphic Fredholm operator-valued functions [1, 2] which implies convergence of the approximations and quasi-optimal error estimates [4].

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A NEW APPROACH TO SPACE-TIME BOUNDARY INTEGRAL EQUATIONS FOR THE WAVE EQUATION

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Space-time discretization methods are becoming increasingly popular, since they allow adaptivity in space and time simultaneously, and can use parallel iterative solution strategies for time-dependent problems. However, in order to exploit these advantages, one needs to have a complete numerical analysis of the corresponding Galerkin methods.

Different strategies have been used to derive variational methods for the time domain boundary integral equations for the wave equation. The more established and succesful ones include weak formulations based on the Laplace transform, and also time-space energetic variational formulations. However, their corresponding numerical analyses are still incomplete and present difficulties that are hard to overcome, if possible at all.

As an alternative, we pursue a new approach to formulate the boundary integral equations for the wave equation, which aims to provide the missing mathematical analysis for space-time boundary element methods. In this talk, we discuss some of our preliminary results.

THE STOKES COMPLEX FOR VIRTUAL ELEMENTS

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In [1] and [2] we introduced a Virtual Element velocities space $\boldsymbol{V}_h$ carefully designed to solve the Stokes and Navier–Stokes problem. In connection with a suitable pressure space Q_h, the proposed Virtual Element space leads to an exactly divergence-free discrete velocity solution.

In the present talk, we investigate the underlying Stokes complex structure of the Virtual Elements by exploiting the divergence-free nature of the discrete kernel. We provide a virtual element counterpart of the continuous Stokes complex:

$$0 \xrightarrow{\quad i \quad} H^2_0(\Omega) \xrightarrow{\quad \text{curl} \quad} [H^1_0(\Omega)]^2 \xrightarrow{\quad \text{div} \quad} L^2_0(\Omega) \xrightarrow{\quad 0 \quad} 0\,,$$

by introducing a virtual element space $\Phi_h \subset H^2(\Omega)$ such that

$$0 \xrightarrow{\quad i \quad} \Phi_h \xrightarrow{\quad \text{curl} \quad} \boldsymbol{V}_h \xrightarrow{\quad \text{div} \quad} Q_h \xrightarrow{\quad 0 \quad} 0$$

is an exact sequence.

As a byproduct of the above exact-sequence construction, we obtain a discrete curl formulation of the Stokes problem (set in the smaller space Φ_h) that yields the same velocity as the original velocity-pressure method. We compare both approach in terms condition number and size of the resulting linear system.

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NUMERICAL SOLUTION OF TRAFFIC FLOW MODELS

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Modelling of traffic flows will have an important role in the future. With a rising number of cars on the roads, we must optimize the traffic situation. That is the reason we started to study traffic flows. It is important to have working models which can help us to improve traffic flow. We can model real traffic situations and optimize e.g. the timing of traffic lights or local changes in the speed limit. The benefits of modelling and optimization of traffic flows are both ecological and economical.

Our work (Vacek, 2018) describes the numerical solution of traffic flows on networks. There are two fundamental approaches: microscopic and macroscopic. The microscopic approach follows every single car. The macroscopic approach consider the traffic to be a continuum which flows through the roads.

We solve especially the macroscopic models. Using these models, it is possible to make simulations on big networks with a lot of cars. These models are described by partial differential equations in the form of conservation laws:

$$\frac{\partial}{\partial t}\rho\left(x,t\right)+\frac{\partial}{\partial x}\left(\rho\left(x,t\right)V\left(x,t\right)\right)=0, \tag{1}$$

where $\rho\left(x,t\right)$ and $V\left(x,t\right)$ are the unknown traffic density and mean traffic flow velocity, respectively. We have only one equation (1) for two unknowns. Thus, we need an equation for the mean traffic flow velocity $V\left(x,t\right)$, for which there are many approaches, cf. (Vacek, 2018).

Due to the character of equation (1), we can expect discontinuity of the traffic density $\rho\left(x,t\right)$. Therefore, for the numerical solution of our models, we use the discontinuous Galerkin method in space and a multistep method in time. We introduced limiters which prevent spurious oscillations in the numerical solution and keep density in an admissible interval. All the above was performed on networks. Thus, we had to deal with the problem of boundary conditions at the junctions.

We introduce our own approach for boundary conditions at junction, which uses special numerical flow choices. This approach is new and the behaviour of the resulting model can be understood as the introduction of branching lanes in front of the junction. This is a different approach to models in (Garavello, Piccoli, 2006) and (Čanić et al, 2014), which do not have branching lanes and overtaking is prohibited. The using of the discontinuous Galerkin method on networks is not standard, we can compare our approach with the paper (Čanić et al, 2014).

We present several numerical results. We compare different traffic flow approaches such as Greenshields model, Greenberg model and Underwood model. We present the behaviour at junctions. Finally, we can compare our result with real data on highways.

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THE MHM METHOD ON NON-CONFORMING POLYGONAL MESHES

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This work revisits the general form of the Multiscale Hybrid-Mixed (MHM) method [1, 2] for the second-order Laplace (Darcy) equation under the perspective of non-convex non-conforming polyhedral meshes. In this context, we propose new stable multiscale finite elements [3] such that they preserve the well-posedness, super-convergence and local conservation properties of the original MHM method under mild regularity conditions. Precisely, we show that piecewise polynomial of degree $k+1$ and k, $k \geq 0$, for the Lagrange multipliers (flux) along with continuous piecewise polynomial interpolations of degree $k+1$ posed on second-level sub-meshes are stable if the latter is refined enough. Such one- and two-level discretization impact the error in a way that the discrete primal (pressure) and dual (velocity) variables achieve super-convergence in the natural norms under extra local regularity only. Numerical tests assess theoretical results.

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POSITIVITY PRESERVING LIMITERS FOR TIME-IMPLICIT HIGHER ORDER DISCONTINUOUS GALERKIN DISCRETIZATIONS

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In the numerical solution of partial differential equations it is frequently necessary to ensure that certain variables, e.g. density, pressure, or probability density distribution, remain within strict bounds. Strict observation of these bounds is crucial otherwise unphysical or unrealistic solutions will be obtained that might result in the failure of the numerical algorithm. Bounds on certain variables are generally ensured using positivity preserving limiters, which locally modify the solution to ensure that the constraints are satisfied. For discontinuous Galerkin methods, in combination with explicit time integration methods, this approach works well and many accurate positivity preserving limiters are available, see e.g. [1]. The combination of (positivity preserving) limiters and implicit time integration methods results, however, in serious problems. Many limiters have a complicated, non-smooth formulation, which hampers the use of standard Newton methods to solve the nonlinear algebraic equations of the implicit time discretization.

In this presentation, we will discuss a different approach to ensure that a higher order accurate numerical solution satisfies the positivity constraints [2]. Instead of using a limiter, we impose the positivity constraints directly on the algebraic equations resulting from a higher order accurate time implicit discontinuous Galerkin discretization by reformulating the DG equations with constraints using techniques from mathematical optimization theory [3]. The resulting algebraic equations are then solved using a semi-smooth Newton method that is well suited to deal with the resulting nonlinear complementarity problem [3]. This approach allows the direct imposition of constraints in higher order accurate discontinuous Galerkin discretizations combined with Diagonally Implicit Runge-Kutta methods and results in more efficient solvers for time-implicit discretizations. We will demonstrate the novel algorithm on a number of model problems, namely the advection, Burgers, Allen-Cahn, Barenblatt, and Buckley-Leverett equations, both in 1D and 2D, using time-implicit DG-DIRK discretizations with order of accuracy ranging between 2 and 5.

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QUASI-OPTIMAL RESIDUAL MINIMIZATION FOR WEAK ADVECTION–REACTION IN BANACH SPACES

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In this contribution I consider a minimal-residual method in discrete dual norms for approximating the solution of the advection-reaction equation in a weak Banach-space setting. The weak formulation allows for the direct approximation of solutions in the Lebesgue L^p-space, $1 < p < \infty$, hence suitable for rough data and highly irregular solutions.

I will first recall the nonlinear Petrov-Galerkin (NPG) method that arises from residual minimization in non-Hilbert settings. When measuring the residual in negative (dual) norms, an inexact (discrete) inversion of the duality map (the Banach-space extension of the Riesz map) is required, so that the method is equivalent to a mixed method with monotone nonlinearity. I will then discuss several compatible finite element pairs guaranteeing the stability and quasi-optimality of the method within the weak Banach-space setting.

APPLICATION OF BOUNDARY CONDITIONS IN MPM

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The material point method (MPM) typically has two discretisations; one for the simulated bodies (into material points or material point clusters) and the second for a (background) mesh where the analysis is undertaken. Moreover, both fluid and solid mechanics (and coupled problems) are able to be simulated via MPM. Boundary conditions have, in general, been applied to background mesh locations, where the calculation takes place, although sometimes they are applied to individual material points. However, this is only for ease of the computation. In this work, the general conditions required for a complete description of the boundary conditions have been outlined. In addition, special treatment required when boundary conditions are applied to the material discretisation is outlined.

TOWARDS AN OSCILLATION FREE (IMPLICIT) MATERIAL POINT METHOD

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The material point method (MPM) suffers from a series of numerical inaccuracies which are often termed oscillations. These oscillations were addressed in the finite element method via the use of Gauss locations for the integration points; however these are typically abandoned for MPM. A number of proposed changes have been made and presented in literature, and mainly tested using 1D problems, e.g. compacting columns. Moreover, generally explicit formulations have been used, which eliminate the stiffness matrix, but utilise very small timesteps, resulting in long computation times. A detailed investigation of the causes of numerical inaccuracies and proposed improvement methods (both novel and proposed in literature) has been carried out. As a result, a proposed method to virtually eliminate the observed inaccuracies is presented.

LOCKING AND COUPLING IN FINITE ELEMENT APPROXIMATION

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Motivated by finite element methods for models with extreme parameter values, we consider the approximation in a parameter-dependent norm. We analyze whether and how locking occurs, i.e., whether and how the approximation capability of a finite element space deteriorates as the parameter approaches a critical value.

To this end, we first observe that locking may be caused only by inappropriate choices of the element shape functions or their coupling between adjacent elements. Second, in the case that the error norm is a parameter-dependent combination of two norms, we ensure an instantly locking-free coupling irrespective of regularity by suitable conditions on the two involved norms.

This approach can be applied to approximation problems suggested, e.g., by nearly incompressible elasticity, anisotropic and reaction-dominated diffusion. These examples, as well as an application to adaptive tree approximation, underline the crucial role of the coupling.

ON QUASI-OPTIMALITY OF FINITE ELEMENT METHODS FOR THE OBSTACLE PROBLEM

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A finite element method is quasi-optimal if the error of its approximate solution is bounded in terms of the best error in the trial space and a multiplicative constant for any exact solution. Quasi-optimality is a very useful property, in particular in an adaptive context. In fact, adaptive decision are usually based upon the approximate solution and affect the approximation properties of the underlying trial space.

The elliptic obstacle problem may be viewed as a model case for variational inequalities. In this talk, we shall discuss the quasi-optimality of selected finite element methods for this model case.

RIGOROUS AND FULLY COMPUTABLE A POSTERIORI ERROR BOUNDS FOR EIGENFUNCTIONS

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Using Laplace eigenvalue problem

$$-\Delta u_i = \lambda_i u_i \quad \text{in } \Omega, \qquad u_i = 0 \quad \text{on } \partial\Omega,$$

as a model problem, a generalization of error bounds from [1] to the case of tight clusters and multiple eigenvalues is presented. Individual eigenfunctions do not depend continuously on problem data, in general, and they are sensitive to small perturbation of the problem in the case of tight clusters and multiple eigenvalues. Therefore, we propose to estimate entire spaces of eigenfunctions corresponding to clusters and multiple eigenvalues.

We derive a guaranteed and fully computable upper bound on a distance between the space of exact and the space of approximate eigenfunctions. The derived bound depends on the width of the cluster, spectral gap between the last cluster and the following eigenvalues, and on the possible non-orthogonality of approximate spaces corresponding to the preceding clusters. The derived bound can be easily computed from two-sided bounds on eigenvalues and the approximate eigenfunctions. No flux reconstructions are needed. It is naturally evaluated recursively, starting from the lowest cluster. Numerical experiments compare several versions of the bound both in the energy and $L^2(\Omega)$-norms. Optimal rates of convergence are observed. More details are presented in [5].

An alternative approach [4] is a generalization of concepts from [2, 3] to the case of clusters and multiple eigenvalues.

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AN ADAPTIVE HP-DG-FE METHOD FOR ELLIPTIC PROBLEMS. CONVERGENCE AND OPTIMALITY IN THE 1D CASE

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We propose and analyze an hp-adaptive **DG-FEM** algorithm, termed hp-**ADFEM**, and a realization of it in one space dimension which is convergent, instance optimal, and h- and p-robust. The procedure consists of iterating two routines: one hinges on Binev s algorithm for the adaptive hp-approximation of a given function, and finds a near-best hp-approximation of the current discrete solution and data to a desired accuracy; the other one improves the discrete solution to a finer but comparable accuracy, by iteratively applying Dörfler marking and h-refinement.

THE CONFORMING VIRTUAL ELEMENT METHOD FOR POLYHARMONIC PROBLEMS

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In this talk, we exploit the capability of virtual element methods in accommodating approximation spaces featuring high-order continuity to numerically approximate differential problems of the form $(-\Delta)^p u = f$, $p \geq 1$. More specifically, we develop and analyze the conforming virtual element method for the numerical approximation of polyharmonic boundary value problems, and prove a priori error estimates in different norms.

COMPUTATIONAL HIGH-FREQUENCY WAVE PROPAGATION IN HETEROGENEOUS HIGH-CONTRAST MEDIA

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(Wave) scattering and propagation in heterogeneous high-contrast media experiences a rising interest because such materials can develop unusual optical or acoustic properties, such as a negative refractive index or wave guiding, which are important in practical applications. From the numerical side, the solution of such problems exhibits several challenges: (i) spatially rough PDE coefficients and (ii) the high-frequency regime of wave propagation. Through the high contrast in the coefficients even moderate wave numbers can suddenly imply a high-frequency regime in certain parts of the computational domain, thereby even amplifying the aforementioned numerical challenges.

In this talk, we discuss a computational multiscale method in the spirit of the Localized Orthogonal Decomposition to deal with the combination of rough high-contrast coefficients and high-frequency regime. The method does not require additional structures in the coefficients, such as periodicity or scale separation. In the spirit of a generalized finite element method, special multiscale and problem-adapted basis functions are constructed based on the solution of local fine-scale problems. For the global computation, however, only coarse meshes are used, which do not need to resolve the oscillations and discontinuities of the coefficients. Rigorous numerical analysis allows to estimate the discretization error a priori and is confirmed by numerical examples. Furthermore, the numerical experiments also illustrate some astonishing effects of wave scattering in heterogeneous high-contrast media, such as band gaps, flat lenses, or wave guides.

ISOGEOMETRIC ANALYSIS OF A REACTION-DIFFUSION MODEL FOR HUMAN BRAIN DEVELOPMENT

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Neural development has become a topic of growing interest in the past decades. On the one hand healthy adult individuals exhibit qualitatively similar neural structures, on the other hand neural development exhibits a substantial degree of randomness, which is largely confirmed by the observation that even monozygotic twins exhibit significant anatomical differences. Among other factors, this neural 'fingerprint' manifests itself mainly through the patterns formed in the neural folding and buckling process occurring naturally after the twentieth week of fetal development.

This suggests that environmental factors can have a profound influence on the course of neural development, which in turn suggests that the underlying biological process, mathematically, exhibits a high degree of sensitivity toward perturbations in the initial condition. On the other hand, a proficient model for human brain development should be capable of producing qualitatively similar outcomes for similar setups and explain neural pathologies like lissencephaly and polymicrogyria by quantitatively different starting conditions. The derivation of proficient models for human brain development is greatly hindered by the unethicalness of experimentation on human fetuses.

We propose a numerical scheme based on Isogeometric Analysis (IgA) for the development of the geometry of a brain. The development is modelled by the use of the Gray-Scott equations for pattern formation in combination with an equation for the displacement of the brain surface. The method forms an alternative to the classical finite-element method. Our method is based on a partitioning of a sphere into six patches, which are mapped onto the six faces of a cube. Major advantages of the new formalism are the use of a smooth reconstruction of the surface based on the third-order basis functions used for the computation of the concentrations. These features give a smooth representation of the brain surface. Though the third order basis functions outperform lower order basis functions in terms of accuracy, a drawback remains its higher cost of assembly. This drawback is compensated by the need of a lower resolution in case of higher order basis functions.

A DISCONTINUOUS GALERKIN MODEL FOR THE SIMULATION OF CHEMOTAXIS PROCESS: APPLICATION TO STEM CELL INJECTION AFTER A MYOCARDIAL INFARCTION

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In many biological processes cells migrate in the direction to the gradient of a concentration. This process is commonly referred to as chemotaxis or haptotaxis in fluidic or solid environments, respectively. Chemotaxis of cells occurs in many important biological processes, such as wound healing, but also in tumour growth and metastasis. Healing processes typically involve the repair of tissues and to this end it is necessary that certain cells migrate and regenerate the appropriate tissues such as bone or skin. Cells secrete signalling agents by which either cells of the same or different phenotypes are attracted towards them so that certain biological processes like the repair of extracellular matrix can occur. Furthermore, the immune response system operates on the basis of chemotactic migration of white blood cells towards pathogens as a result of biotic lactates that are effectively transported away from pathogens as a result of the acidification of the environment. In various treatments, it is aimed at trying to make certain cells migrate to desired locations. In this chapter, we consider the application of stem cell therapy to improve the structure and efficacy of the heart muscle, where stem cells activate migration of endothelial cells to damaged regions of the heart. An experimental study on stem cell migration induced by chemokines was presented in, among many other studies, Baek et al. (2011).

We present a mathematical formalism for the simulation of angiogenesis treatment in the heart after a myocardial infarction. The formalism treats the injection of stem cells at the surface of the heart, which then, release growth factor TG-β. This growth factor attracts the endothelial cells that migrate towards the stem cells as a result of chemotaxis. The description of the formation of a vascular network is characterised by taking into account the vessel tips as well as their sprouts. The method is based on a Keller-Segel formalism for chemotaxis for the vessel tips, combined with a 'snail trail' mechanism to simulate the migration of the sprouts. The paper presents a Discontinuous Galerkin method on quadrilateral meshes to solve the system of partial differential equations in two spatial dimensions.

The current contribution is merely an application of discontinuous Galerkin, rather than a solid theoretical evaluation of the used methodology.

A POSTERIORI ERROR ESTIMATION FOR THE STOCHASTIC COLLOCATION FINITE ELEMENT APPROXIMATION OF A HEAT EQUATION

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In this talk we present a residual based a posteriori error estimation for a heat equation with a random forcing term and a random diffusion coefficient which is assumed to depend affinely on a finite number of independent random variables. The problem is discretized by a stochastic collocation finite element method and advanced in time by the theta-scheme. The a posteriori error estimate consists of three parts controlling the finite element error, the time discretization error and the stochastic collocation error, respectively. These estimators are then used to drive an adaptive choice of FE mesh, collocation points and time steps. We study the effectiveness of the estimate and the performance of the adaptive algorithm on a numerical example.

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LOCALIZATION OF GLOBAL NORMS AND ROBUST A POSTERIORI ERROR CONTROL FOR TRANSMISSION PROBLEMS WITH SIGN-CHANGING COEFFICIENTS

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We present a posteriori error analysis of diffusion problems where the diffusion tensor is not necessarily symmetric and positive definite and can in particular change its sign. We first identify the correct intrinsic error norm for such problems, covering both conforming and nonconforming approximations. It combines a dual (residual) norm together with the distance to the correct functional space. Importantly, we show the equivalence of both these quantities defined globally over the entire computational domain with the Hilbertian sums of their localizations over patches of elements. In this framework, we then design a posteriori estimators which deliver simultaneously guaranteed error upper bound, global and local error lower bounds, and robustness with respect to the (sign-changing) diffusion tensor. Robustness with respect to the approximation polynomial degree is achieved as well. The estimators are given in a unified setting covering at once conforming, nonconforming, mixed, and discontinuous Galerkin finite element discretizations in two or three space dimensions. Numerical results illustrate the theoretical developments.

ON THE INF-SUP STABILITY OF THE LOWEST ORDER TAYLOR-HOOD PAIR ON AFFINE ANISOTROPIC MESHES

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Uniform LBB conditions are desireable to approximate the solution of Navier-Stokes, Oseen, and Stokes equations on anisotropic meshes and to enable anisotropic refinements. In this talk, we present such conditions for the second order Taylor–Hood pairs Q2 x Q1 and P2 x P1 on a class of affine anisotropic meshes. These meshes may contain refined edge and corner patches. To prove this, we generalised Verfürth's trick and recent results by the authors.

Previous results were mainly negative, in the sense that there were meshes on which the inf-sup constants degenerate with the aspect-ratio. We have then proposed minimal conditions for the lowest order TH pair to be stable with a constant independent of the aspect ratio.

The main ideas of the proof are presented, and also we show some possible extensions and numerical evidence.

RESIDUAL-TYPE A POSTERIORI ESTIMATORS FOR THE SINGULARLY PERTURBED VARIATIONAL INEQUALITY IN QUASI-STATIC FRACTURE PHASE-FIELD MODELS

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We consider a quasi-static fracture phase-field model which is given by a coupled system of an equation and a singularly perturbed variational inequality. The unknowns of the system are the displacements $\boldsymbol{u}$ of a linear elastic body and the phase-field variable φ which describes a diffusive transition zone between the broken ($\varphi = 0$) and the unbroken material ($\varphi = 1$). This zone has a half bandwidth ϵ, which is a model regularization parameter. The phase-field variable is constrained by the irreversibility condition, i.e. $\varphi^{n+1} \leq \varphi^n$ where n denotes the time step.

In the numerical simulation we are especially interested in a good approximation of the fracture growth. Therefore we use adaptive finite element methods which are based on a residual-type a posteriori estimator which we present here. Due to the irreversibility constraint standard residual a posteriori estimators are inappropriate. They would cause an overestimation where the constraints are active which is for example in the unbroken area. Thus, in order to derive a residual-type a posteriori estimator under the aspects of reliability, efficiency and robustness we follow a new approach [A. Veeser, Efficient and reliable a posteriori error estimators for elliptic obstacle problems. SIAM J. Numer. Anal. 39, 2001. pp. 146–167] for variational inequalities. We use an ϵ-dependent energy norm to measure the error in the phase-field variable and the corresponding dual norm to measure the error in the constraining forces. The resulting estimator [M. Walloth, Residual-type A Posteriori Estimators for a Singularly Perturbed Reaction-Diffusion Variational Inequality – Reliability, Efficiency and Robustness. Preprint 2018, arXiv:1812.01957] generalizes well-known and approved estimators such as standard residual estimators for linear elliptic problems, residual-type a posteriori estimators for obstacle problems and robust a posteriori estimators for singularly perturbed reaction-diffusion equations [R. Verfürth, Robust a posteriori error estimators for a singularly perturbed reaction-diffusion equation. Numer. Math. 78, 1998, pp. 479–493]. Numerical results complement the theoretical analysis.

UNCONDITIONALLY CONVERGENT $L1$-GALERKIN FEMS FOR NONLINEAR TIME-FRACTIONAL SCHRÖDINGER EQUATIONS

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In this work, a linearized $L1$-Galerkin finite element method is proposed to solve the multi-dimensional nonlinear time-fractional Schrödinger equation. In terms of a temporal-spatial error splitting argument, we prove that the finite element approximations in L^2-norm and L^∞-norm are bounded without any time stepsize conditions. More importantly, by using a discrete fractional Gronwall type inequality, optimal error estimates of the numerical schemes are obtained unconditionally, while the classical analysis for multi-dimensional nonlinear fractional problems always required certain time-step restrictions dependent on the spatial mesh size. Numerical examples are given to illustrate our theoretical results.

DEVELOPMENT OF CONSTITUTIVE MODEL FOR FIBRE REINFORCED COMPOSITE DAMAGE

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Predictive modelling and experimental characterisation of carbon fibre reinforced polymers (CFRP), even in basic quasi-static mechanical tests, is challenging due to their anisotropy resulting from the material microstructure. This paper presents a new constitutive model developed within the framework of irreversible thermodynamics with internal state variables. The model is based on spectral decomposition of the elasticity and damage characteristic tensors, where the damage evolution is controlled with associative damage model. Two damage potential formulations were investigated: model 1, with decoupled damage modes (without the interaction between the damage modes); and model 2, with the damage modes interaction. Model calibration is based in extensive mesoscale modelling, while verification and validation have been based on the modelling physical damage effects defined at the mesoscale level.

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AUTOMATED SHAPE DIFFERENTIATION IN FENICS AND FIREDRAKE

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While only relying on basic transformation rules, the calculation of shape derivatives is often a lengthy and error prone exercise. The reason for this is that even simple, linear PDEs or objectives are usually non-linear with respect to the domain under consideration.

We present a reformulation of shape derivatives in the context of finite elements as a classical Gâteaux derivative on the reference element. Based on this new approach, we show that the Unified Form Language (UFL), which underlies the popular finite element libraries Firedrake and FEniCS, can be extended to calculate first and higher order shape derivatives in an automated fashion.

CROSSBREADS—IDEAS BEHIND ALMOST MATRIX-FREE, ALGEBRAIC-GEOMETRIC MULTIGRID SOLVERS

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Geometric multigrid solvers with operator rediscretisation are the method of choice to solve large-scale elliptic problems. They have a small memory footprint, we can implement them in a streaming fashion, there is not much administrative overhead if we combine them with tree-based adaptive meshes, and so forth. There's only one problem: they tend not to work as soon as we tackle non-trivial problems with anisotropic operators, jumping material parameters or convection terms. We present a merger of geometric multigrid relying on spacetrees with the algebraic BoxMG technique. A combination with FAC/HTMG allows us to support arbitrary dynamic adaptivity straightforwardly, while pipelining allows us to write single-touch implementations. On-the-fly compression of the data finally yields an algebraic solver with a memory footprint close to its geometric counterpart.

EMBEDDED/HYBRIDIZED DISCONTINUOUS GALERKIN METHOD FOR INCOMPRESSIBLE FLOWS

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We present an embedded/hybridized discontinuous Galerkin method for velocity-pressure formulations of incompressible flows. The method maintains the attractive features of hybridized methods, namely a H(div)-conforming velocity field, pointwise solenoidal velocity field (without post-processing), local momentum conservation, and energy stability when applied to the Navier-Stokes equations. By using an 'embedded' approach for the velocity field with the facet fields being continuous, the method is significantly faster than a full hybridized method to reach a specified error tolerance. Moreover, the embedded/hybridized method is suited to preconditioners that are known to be effective for continuous problems. We present analysis results, including a result showing that error estimates for the velocity are independent of the pressure. Analysis results are supported by a range of numerical examples.

INFINITE ELEMENTS FOR EXTERIOR HELMHOLTZ RESONANCE PROBLEMS BASED ON A FREQUENCY DEPENDENT COMPLEX SCALING

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Complex scaling is a popular method to treat scattering and resonance problems in open domains. Thereby the unbounded domain is decomposed into a bounded interior and an unbounded exterior part. Subsequently the technique of complex scaling is applied to the exterior domain to obtain exponentially decreasing solutions. Finally the complex scaled exterior is usually truncated and discretized using finite elements.

In our work we suggest a number of improvements to the method described above. To resonance problems usually frequency independent scalings are applied, to conserve the linearity of the resulting eigenvalue problem. Unfortunately, a frequency independent complex scaling works well only for a very narrow range of frequencies and the quality of the approximation depends heavily on the specific choice of the scaling function. To overcome this problem we use frequency dependent scaling functions, as it is common when treating scattering problems, for resonance problems as well. This approach leads to polynomial or rational eigenvalue problems instead of linear ones (cf. [2]).

For discretizing the exterior complex scaled problems we use a tensor product method, describing the exterior by a normal and an interface coordinate. Due to this ansatz we evade having to explicitly mesh the exterior domain. To avoid truncation and obtain super-algebraic approximation properties we make use of infinite elements in normal direction, which are based on Hardy space infinite Elements (cf. [1]).

We solve the resulting discrete eigenvalue problems by making use of an adapted version of the shift-and-invert Arnoldi algorithm. Applying this method requires no significant extra computational effort compared to solving linear eigenvalue problems.

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DUAL-WEIGHTED RESIDUAL A POSTERIORI ERROR ESTIMATION FOR MULTIPLE GOAL FUNCTIONALS

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In this presentation, we further develop multigoal-oriented a posteriori error estimation with two objectives in mind. First, we formulate goal-oriented mesh adaptivity for multiple functionals of interest for nonlinear problems in which both the Partial Differential Equation (PDE) and the goal functionals may be nonlinear. Our method is based on a posteriori error estimates in which the adjoint problem is used and a partition-of-unity is employed for the error localization that allows us to formulate the error estimator in the weak form. We provide a careful derivation of the primal and adjoint parts of the error estimator. The second objective is concerned with balancing the nonlinear iteration error with the discretization error yielding adaptive stopping rules for Newton's method. Our techniques are substantiated with several numerical examples including scalar PDEs, PDE systems, and an optimal control setting.

A SPACE-TIME DPG METHOD FOR ACOUSTIC WAVES IN HETEROGENEOUS MEDIA

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We apply the discontinuous Petrov-Galerkin method (DPG) to linear acoustic waves in space and time using the framework of first-order Friedrichs systems. Based on results for operators and semigroups of hyperbolic systems, we show that the ideal DPG method is well-posed on a suitable subset of the space-time cylinder. Therefore, we use the graph norm of the space-time differential operator, and traces are implicitly defined as distributions. Then, the practical DPG method is analyzed by constructing a Fortin operator numerically, and nonconforming traces are considered by comparison with an equivalent conforming scheme.

For our numerical experiments we introduce a simplified DPG method with discontinuous ansatz functions on the faces of the space-time skeleton, where the error is bounded by an equivalent conforming DPG method. Examples for a plane wave configuration confirms the numerical analysis, and the computation of a diffraction pattern illustrates a first step to applications. Finally, we present results for a benchmark configuration in seismic imaging with a point source and a small region with measurement points, where we show that the computation on a truncated space-time cylinder allows for a substantial reduction of degrees of freedom.

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ADAPTIVE ITERATIVE LINEARIZATION GALERKIN METHODS FOR NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS

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A wide variety of (fixed-point) iterative methods for the solution of nonlinear equations (in Hilbert spaces) exists. In many cases, such schemes can be interpreted as iterative local linearization methods, which can be obtained by applying a suitable linear preconditioning operator to the original (nonlinear) equation. Based on this observation, we will derive a unified abstract framework which recovers some prominent iterative schemes. Furthermore, in the context of numerical solutions methods for nonlinear partial differential equations, we propose a combination of the iterative linearization approach and the classical Galerkin discretization method, thereby giving rise to the so-called *iterative linearization Galerkin (ILG)* methodology. Moreover, still on an abstract level, based on elliptic reconstruction techniques, we derive a posteriori error estimates which separately take into account the discretization and linearization errors. Furthermore, we propose an adaptive algorithm, which provides an efficient interplay between these two effects. In addition, some iterative methods and numerical computations in the specific context of finite element discretizations of quasilinear stationary conservation laws will be presented.

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THE HP-VERSION DISCONTINUOUS GALERKIN TIME STEPPING SCHEME IS UNIFORMLY L^∞-STABLE

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We investigate the L^∞-stability of fully discrete approximations of (abstract) linear parabolic partial differential equations (PDE). The method under consideration is based on an *hp*-type discontinuous Galerkin (dG) time stepping scheme in combination with general conforming Galerkin discretizations in space. Our main result shows that the global-in-time maximum norm of the discrete solution is bounded by the data of the PDE, with a constant that is robust with respect to the discretization parameters (in particular, it is uniformly bounded with respect to the local time steps and approximation orders). Our theory is based on a discrete Duhamel principle, which mimics closely the semigroup structure of the underlying PDE, and on the p-independent stability of the inverse of the fully discrete parabolic dG operator.

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AFEM FOR ELLIPTIC-H(CURL) VARIATIONAL INEQUALITIES OF THE SECOND KIND

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In this talk we discuss the analysis of an adaptive mesh refinement strategy for elliptic **curl-curl** variational inequalities of the second kind. We present a posteriori error estimators based on a careful combination between the Moreau-Yosida regularization approach and Nédélec's first family of edge elements. The reliability and efficiency of the estimators are proved through the use of a specific linear auxiliary problem involving the discrete Moreau-Yosida-regularized dual variable in combination with a local regular decomposition for $\mathbf{H}(\mathbf{curl})$-functions and the well-known bubble functions. Hereafter, we propose an AFEM algorithm and discuss the convergence analysis thereof by using a limiting-space approach. Under a certain condition on the regularization parameter depending on the adaptive mesh size, we derive convergence results for the maximal error indicator and the corresponding residual. Finally, the strong convergence of the sequence of the adaptive solutions generated by the AFEM algorithm follows by combining all these mathematical findings. In the last part of the talk, the implementation of the algorithm is presented and applied to a problem stemming from the type-II (high-temperature) superconductivity.

ERROR ESTIMATES FOR NORMAL DERIVATIVES AND DIRICHLET CONTROL PROBLEMS ON BOUNDARY CONCENTRATED MESHES

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The aim of this talk is to investigate the convergence behaviour of finite element approximations for the normal derivatives of the solution of the Poisson equation. In order to improve the convergence rates we use boundary concentrated meshes, i. e., meshes that are refined towards the boundary such that the diameters of elements touching the boundary are of order h^2, where h denotes the global mesh size. These meshes allow for a second-order approximation of normal derivatives in the $L^2(\Gamma)$-norm, provided that the solutions are sufficiently smooth. In the case that the computational domain is polygonal, corner singularities may reduce the regularity of solutions and thus also the convergence rates. We will observe that this is the case when an opening angle of a corner of the domain is larger than 120°.

As an application of these results, we also investigate boundary control problems governed by elliptic equations for the case that the control is the Dirichlet datum. For these kind of problems, error estimates for the normal derivative of an adjoint state variable has to be proved. In general, solutions of these kind of problems are very irregular and hence, local mesh refinement is absolutely necessary to obtain reasonable solutions. Finally, we present numerical experiments which confirm that the predicted convergence results are sharp.

AN EXPLICIT MAPPED TENT PITCHING SCHEME FOR HYPERBOLIC SYSTEMS

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The presented Mapped Tent Pitching (MTP) method is based on a tent pitching algorithm (see [1, 2]). These tent pitching algorithms use an unstructured spatial mesh and advance in time by consecutively incrementing the time coordinates of the mesh vertices, while respecting causality. By generating these advancing fronts, the algorithm partitions the spacetime domain into tent-shaped regions that respect causality. Such meshes can be combined with spacetime discontinuous Galerkin methods as presented in [3]. Instead of constructing $(d+1)$-dimensional finite elements, we introduce a transformation which maps each tent to a domain with tensor product structure of the spatial domain with a time interval. This allows to discretize space and time independently, as presented in [1]. After discretizing space with a discontinuous Galerkin method, we obtain a system of ordinary differential equations in time. Using standard explicit Runge-Kutta methods to solve these local systems in time leads a reduction of the spatial convergence order. To regain the desired high order convergence for smooth solutions, we construct a Runge-Kutta type time-stepping which takes the special structure of our semidiscrete problems into account. Numerical results for non-liner hyperbolic systems will be presented to validate the expected high order convergence of the MTP method.

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PHASE-FIELD SIMULATIONS OF LUNG BRANCHING MORPHOGENESIS

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A Turing Pattern-based framework can predict the experimentally determined growth field and thus locations of the emerging branches in lung morphogenesis. We developed a phase-field model to describe the lung geometry and model the non-linear interaction of the involved proteins in the bulk and on the surface of the growing lung. This way we can circumvent meshing problems due to the complex deformations during morphogenesis. In this talk, we show the modelling aspect as well as simulation results and compare to biological data.

COMPARISON AND UNIFICATION OF MATERIAL POINT AND OPTIMAL TRANSPORTATION MESHFREE METHODS

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Both the Material Point Method (MPM) [1] and Optimal Transportation Meshfree (OTM) method [2] have been developed for efficient and robust integration of the weak form equations that originate from applications in computational mechanics. However, the methods are derived in a different fashion and have been studied independently of one another. In this study, we provide a direct step-by-step comparison of the MPM and OTM algorithms. Based on this comparison, we derive the conditions, under which the two approaches can be related to each other, thereby bridging the gap between the MPM and OTM communities. In addition, we introduce a novel unified approach that combines the design principles from B-spline MPM (BSMPM) and OTM methods. The proposed approach is significantly cheaper than the standard OTM method and allows for the use of a consistent mass matrix without stability issues that are typically encountered in MPM computations.

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FINITE ELEMENT ERROR IN THE CONTROL OF DAMAGE PROCESSES

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Within this talk, we will discuss the finite element approximation of optimization problems subject to phase-field damage processes as constraints. To utilize standard (smooth) optimization algorithms, the irreversibility of the damage is relaxed by a penalty. We will discuss regularity of solutions to these regularized damage-models, and show that the regularity carries over to the limit in the regularization. Based on these new regularity results, we will discuss the approximability of the problem by finite elements.

NEW ANALYSIS OF GALERKIN FEMS FOR MISCIBLE DISPLACEMENT IN POROUS MEDIA

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The paper is concerned with optimal error estimates of classical Galerkin FEMs for the equations of incompressible miscible flows in porous media. The analysis done in the last several decades shows that classical Galerkin FEMs provide the numerical concentration of the accuracy $O(\tau^k + h^{r+1} + h^s)$ in L^2-norm. This analysis leads to the use of higher order finite element approximation to the pressure than that to the concentration in various numerical simulations to achieve the best rate of convergence. However, this error estimate is not optimal. The purpose of this paper is to establish the optimal L^2 error estimate $O(\tau^k + h^{r+1} + h^{s+1})$, from which one can see that the best convergence rate can be achieved by taking the same order ($r = s$) approximation to the concentration and pressure. Clearly Galerkin FEMs with $r = s$ are less expensive in computation and easier for implementation. Numerical results for both two and three-dimensional models are presented to confirm our theoretical analysis.

CONVERGENCE ANALYSIS OF A PETROV-GALERKIN METHOD FOR FRACTIONAL WAVE PROBLEMS WITH NONSMOOTH DATA

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A Petrov-Galerkin method is analyzed for time fractional wave problems with nonsmooth data. Well-posedness and regularity of the weak solution to the time fractional wave problem are established, and optimal convergence with nonsmooth data is derived. Several numerical experiments are provided to validate the theoretical results. This is joint work with Binjie Li and Hao Luo.

A POSTERIORI ERROR ESTIMATION AND ADAPTIVITY IN STOCHASTIC GALERKIN FEM FOR PARAMETRIC ELLIPTIC PDES: BEYOND THE AFFINE CASE

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We consider a linear elliptic partial differential equation (PDE) with a generic uniformly bounded parametric coefficient. The solution to this PDE problem is approximated in the framework of stochastic Galerkin finite element methods. We present a reliable and efficient a posteriori estimate of the energy error in Galerkin approximations generalising the results of [1, 2]. Practical versions of this error estimate are discussed and tested numerically for a model problem with non-affine parametric representation of the coefficient. Furthermore, we use the error reduction indicators derived from spatial and parametric error estimators to guide an adaptive solution algorithm for the given parametric PDE problem. The performance of the adaptive algorithm is tested numerically for a model problem with non-affine parametric representation of the coefficient.

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POSITIVITY PRESERVING HIGHER ORDER TIME-IMPLICIT LOCAL DISCONTINUOUS GALERKIN METHODS FOR NONLINEAR PARABOLIC PROBLEMS

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In this presentation, we will discuss positivity preserving higher order accurate local discontinuous Galerkin (LDG) discretizations coupled with Diagonally Implicit Runge-Kutta (DIRK) methods for nonlinear parabolic equations with gradient flow [1, 2]. By giving some assumptions corresponding to the entropy, the efficient DIRK-LDG structure are constructed. Further, we prove that the semi-discrete and backward Euler fully-discrete schemes are unconditionally energy stable with the appropriate choice of the numerical flux. Since the solution of the nonlinear and possibly degenerate parabolic equations represents in many cases a density, it is essential to ensure the positivity of the corresponding numerical solution.

In this presentation we will discuss a novel positivity preserving LDG discretization for nonlinear parabolic equations using the Karush-Kuhn-Tucker (KKT) limiter, see [3, 4]. This discretization is obtained by coupling positivity constraints with higher order time-implicit DIRK-LDG methods using Lagrange multipliers. The main difficulty in solving the KKT limiter equations is that the resulting equations are only locally Lipschitz continuous and have a quite different structure compared to many related constrained optimization problems. We therefore use an active set semi-smooth Newton method, and the Jacobian matrix is derived by calculating a quasi-directional derivative. Since the positivity constraint works only in areas where positivity must be imposed, it will not affect the higher order time-implicit LDG scheme elsewhere. The accuracy and stability of the DIRK-LDG discretization will be demonstrated by numerical tests for different kinds of nonlinear parabolic equations.

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LAPLACE TRANSFORM METHOD FOR SOLVING FRACTIONAL CABLE EQUATION WITH NONSMOOTH DATA

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We introduce two time discretization schemes for solving time fractional cable equation. The time derivative is approximated by using the backward Euler method and the second order backward difference formula, respectively. The Riemann-Liouville fractional derivatives are approximated by using the backward Euler convolution quadrature method and the second order backward difference convolution quadrature method, respectively. The nonsmooth data error estimates with the convergence orders $O(k)$ and $O(k^2)$ are proved in detail. Instead of using the discretized operational calculus approach to prove the nonsmooth data error estimates of the time discretization schemes for solving time fractional cable equation as used in literature, we directly bound the kernel function in the resolvent and obtain the nonsmooth data error estimates. To the best of our knowledge, this is the first work to consider the nonsmooth data error estimates for solving time fractional cable equation by directly bound the kernel function in the resolvent. This argument may be applied to consider the nonsmooth data error estimates for solving time fractional cable equation where the Riemann-Liouville fractional derivatives are approximated by using other schemes, for example, L1 scheme.

A MIXED ELASTICITY FORMULATION FOR FLUID POROELASTIC STRUCTURE INTERACTION

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We study a mathematical model and its finite element approximation for solving the coupled problem arising in the interaction between a free fluid and a fluid in a poroelastic material. The free fluid flow is governed by the Stokes equations, while the poroelastic material is modeled using the Biot system of poroelasticity. The model is based on a mixed stress-displacement-rotation elasticity formulation and mixed velocity-pressure Darcy and Stokes formulations. The mixed finite element approximation provides local mass and momentum conservation in the poroelastic media. We discuss well posedness of the mathematical model as well as stability, accuracy, and robustness of the numerical method. Applications to flows in fractured poroelastic media and arterial flows are presented.

A MULTIPOINT STRESS-FLUX MIXED FINITE ELEMENT METHOD FOR THE STOKES-BIOT MODEL

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We study a fully mixed formulation of the Stokes-Biot model for fluid poroelastic structure interaction and its mixed finite element approximation. The Stokes formulation is based on weakly symmetric deviatoric stress, velocity, and vorticity. The elasticity formulation is based on weakly symmetric stress, displacement, and rotation. The porous media flow formulation is based on Darcy velocity and pressure. Well posedness of the variational formulation is established. The multipoint stress mixed finite element method is employed for the discretization of the Stokes and elasticity equations. The multipoint flux mixed finite element method is utilized for the Darcy flow. The methods are based on the lowest order BDM spaces for the stresses and the Darcy velocity. A vertex quadrature rule is employed for the bilinear forms involving these variables, which allows for their local elimination, as well as the local elimination of vorticity and rotation. This results in a symmetric and positive definite cell centered system involving only Stokes velocity, displacement, and pressure. We study the stability and accuracy of the method and present numerical experiments.

GUARANTEED AND ROBUST L^2 A POSTERIORI ERROR ESTIMATES FOR 1D LINEAR ADVECTION PROBLEMS

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We propose a reconstruction-based a posteriori error estimate for linear advection problems in one space dimension. In our framework [1], a stable variational ultra-weak formulation is adopted, and the equivalence of the L_2-norm of the error with the dual graph norm of the residual is established. This dual norm is showed to be localizable over patch subdomains of the computational domain under the condition of the orthogonality of the residual to the piecewise affine hat functions. We show that this condition is valid for some well-known numerical methods including continuous/discontinuous Petrov–Galerkin and discontinuous Galerkin methods. Consequently, a well-posed local problem on each patch is identified, which leads to a global reconstruction of the solution belonging to the graph space. We prove that this reconstruction provides a guaranteed upper bound on the L_2 error. Moreover, up to a constant, it also gives local lower bounds on the L_2 error, where the generic constant is proven to be independent of mesh-refinement, polynomial degree of the approximation, and the advective velocity. This leads to robustness of our estimates with respect to the advection as well as the approximation polynomial degree. All the above properties are verified in a series of numerical experiments, additionally yielding asymptotic exactness.

Motivated by these results, we finally propose a heuristic extension of our methodology to any space dimension, achieved by solving local least squares problems on the patches. Though not anymore guaranteed, the resulting error indicator is numerically still robust with respect to both advection and polynomial degree, for a collection of two-dimensional test cases including discontinuous solutions.

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TOWARD POSITIVITY, MONOTONICITY AND BOUNDEDNESS PRESERVATION CHARACTERISTICS OF POLYNOMIAL PROJECTIONS USING CONSTRAINED OPTIMIZATION APPROACH

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Finite element simulations have been used to solve a variety of Partial Differential Equations (PDEs) that model many physical, chemical and biological phenomena. Discretized solutions to PDEs often do not satisfy desired physical properties, such as positivity or monotonicity. Such invalidity in solutions as negative values or a non-monotonic pattern of values pose a challenge to model the real-world properties accurately. We consider the problem of finding a solution to these PDEs that preserves the desired properties as additional constraints on the solution. Such constraints can be cast as convex constraints. We can therefore consider a convex optimization problem that computes a solution that does satisfy the desired properties.

In this talk we propose a filtering approach applied to the standard Galerkin projections in one dimension to prevent the solutions from becoming negative or losing monotonicity at the points of interest in the domain. We investigate this approach by applying an optimization procedure as a post-processing step in our experiments. We can view this approach as a type of filter: an operation that corrects "undesired" behavior in a solution. With this relatively ad-hoc procedure, we show that we can obtain accurate solutions, both for function approximation and for solutions to differential equations. This can be particularly useful in discontinuous Galerkin (DG) projections where the solution invalidity is usually observed at the element boundaries. This, in turn, leads to incorrect simulations and may even cause the simulation to fail. The algorithm proposed is efficient for DG solutions since it is an element-by-element procedure, and hence easily lends itself to parallelism. This work is not directly concerned with establishing approximation theory for this problem, and we largely provide empirical tests. In particular, we focus on the one dimensional case, although all the mathematics carry over to the multidimensional case without essential change.

This approach of enforcing constraints, requiring optimization, can be computationally intensive. The task of developing efficient algorithms to accomplish this proposed algorithm is the subject of ongoing work. We report empirical tests showing that, for the problems we have tried, polynomial rates of the convergence of functions of varying degrees of smoothness are unchanged by using this procedure. We performed numerical tests to verify the positivity and monotonicity preserving property, high and low order accuracy, and good resolution for smooth and discontinuous solutions.

SPACE-TIME FEM WITH LOCAL MESH REFINEMENT FOR THE SECOND-ORDER WAVE EQUATION

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For the discretisation 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 discretised and the resulting global linear system is solved at once. In any case, CFL conditions play a decisive role for stability. For hyperbolic problems, usually space-time discontinuous Galerkin finite element methods are used, which increase the number of degrees of freedom, and which involve certain parameters to be chosen to ensure stability. Another possibility is the usage of space-time continuous Galerkin finite element methods in connection with a stabilisation. In this talk, the latter is applied as discretisation for the model problem of the scalar second-order wave equation with Dirichlet boundary conditions, which leads to an unconditionally stable method for the tensor-product case, see [1, 2] for details. First, a space-time variational formulation of the wave equation and its discretisation via a tensor-product approach including a stabilisation are motivated and discussed. Second, possibilities for a local mesh refinement are given. In the last part of the talk, numerical examples are shown.

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A QUASI-OPTIMAL AND PRESSURE ROBUST NONCONFORMING DISCRETIZATION OF THE STOKES EQUATIONS

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We present a modification of the lowest-order nonconforming Crouzeix-Raviart discretization of the Stokes equations in arbitrary dimension. Our discretization is quasi-optimal, in the sense that the error of the discrete velocity field in the broken H^1-norm is proportional to the error of the best approximation to the analytical velocity field. This readily implies pressure robustness, in that the velocity error is independent of the pressure. We prove also that the sum of the velocity error times the viscosity plus the pressure L^2-error is proportional to the sum of the respective best errors. None of these properties could be achieved with the standard Crouzeix-Raviart discretization. All proportionality constants involved in our analysis are bounded in terms of shape regularity and do not depend on the viscosity. Our modification only affects the right-hand side. Moreover, the cost for building the modified load vector is proportional to the cost for building the load vector in the standard discretization.

PARALLEL ADAPTIVE CROSS APPROXIMATION FOR DISTRIBUTED MEMORY SYSTEMS

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We present a parallel version of the boundary element method accelerated by the adaptive cross approximation (ACA). The boundary of the computational domain is decomposed into patches defining a block structure of boundary element matrices. The blocks are then distributed across computational nodes by a graph algorithm providing a load balancing strategy. Each block is compressed individually by a slightly modified ACA algorithm able to recognize zero blocks generated e.g. by double-layer kernels. The intra-node implementation further utilizes threading in shared memory and in-core SIMD vectorization to make use of all features of modern processors. The suggested approach is validated on a series of numerical experiments presented in the paper.

Furthermore, we present preliminary results of the application of the algorithm for scattering problems with composite scatterers. The problem is modeled by the local version of the multi-trace formulation which allows for operator preconditioning even for skeletons with junction points. Individual Caldern projectors are treated independently, i.e. the boundary of every homogeneous subdomain is decomposed into clusters of elements. The algorithm then proceeds as in the case of single domain problems.

A RATE OF CONVERGENCE OF NUMERICAL OPTIMAL TRANSPORT PROBLEM WITH QUADRATIC COST

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In recent years, optimal transport has many applications in evolutionary dynamics, statistics, and machine learning. The goal in optimal transportation is to transport a measure $\mu(x)$ into a measure $\nu(y)$ with minimal total effort with respect to a given cost function $c(x, y)$. On way to approximate the optimal transport solution is to approximate the measure μ by the convex combination of Dirac measure μ_h on equally spaced nodal set and solve the discrete optimal transport between μ_h and ν. If the cost function is quadratic, i.e. $c(x, y) = |x - y|^2$, the optimal transport mapping is related to an important concept from computational geometry, namely Laguerre cells. In this talk, we study the rate of convergence of the discrete optimal mapping by introducing tools in computational geometry, such as Brun-Minkowski inequality. We show that the rate of convergence of the discrete mapping measured in W_1^1 norm is of order $O(h^2)$ under suitable assumptions on the regularity of the optimal mapping.

STABILITY ANALYSIS AND ERROR ESTIMATES IN L^2-NORM OF RUNGE-KUTTA DISCONTINUOUS GALERKIN METHOD FOR LINEAR HYPERBOLIC EQUATION

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In this talk we propose a simple and unified framework to investigate the L^2-norm stability of the explicit Runge-Kutta discontinuous Galerkin (RKDG) methods with the upwind-biased numerical fluxes, when solving the linear constant-coefficient hyperbolic equations. Two key ingredients in the energy analysis are the temporal differences of numerical solutions in different Runge-Kutta stages, and a matrix transferring process. Many popular RKDG(s, r, k) schemes are discussed to show that the presented technique is flexible and useful. Here $s \geq r$ and $r \leq 12$ are respectively the numbers of stages and order of the used time-marching, and $k \geq 0$ is the degree of piecewise polynomials. Different performances in the L^2-norm stability of different RKDG schemes are carefully investigated. For some lower-degree piecewise polynomials, the monotonicity stability under the usual CFL condition is always achieved as long as the stability mechanism can be provided in the semi-discrete scheme. Based on the above discussions, the optimal error estimates in space and time are easily obtained for many schemes, including the fourth order ($r = 4$) RKDG schemes with arbitrary degree $k \geq 0$. Some numerical examples are also given.

FORMULATION OF NONLOCAL BOUNDARY VALUE PROBLEM AND ITS ASYMPTOTIC ANALYSIS

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Nonlocal-type models are a class of emerging mathematical physics equations. A common feature of these equations is the involving of nonlocal integral operators. This feature presents some troubles to formulate boundary value problems of nonlocal type. Besides, conceptually, nonlocal models should be considered some kind of relaxation for the classical local differential models. In this talk, we propose the formulation of nonlocal boundary value problems of elliptic type, and study the asymptotic convergence rate between the nonlocal boundary value problems and their local counterparts.

CORRECTION OF HIGH-ORDER BDF CONVOLUTION QUADRATURE FOR FRACTIONAL EVOLUTION EQUATIONS

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We develop proper correction formulas at the starting $k-1$ steps to restore the desired k^{th}-order convergence rate of the k-step BDF convolution quadrature for discretizing evolution equations involving a fractional-order derivative in time. The desired k^{th}-order convergence rate can be achieved even if the source term is not compatible with the initial data, which is allowed to be nonsmooth. We provide complete error estimates for the subdiffusion case $\alpha \in (0,1)$, and sketch the proof for the diffusion-wave case $\alpha \in (1,2)$. Extensive numerical examples are provided to illustrate the effectiveness of the proposed scheme.

PARALLEL ADAPTIVE DISCONTINUOUS GALERKIN DISCRETIZATIONS IN SPACE AND TIME FOR VISCO–ELASTIC AND VISCO–ACOUSTIC WAVES

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We consider space-time Petrov-Galerkin methods for linear wave equations. Based on our results for Maxwells equations [1, 3] and acoustic and elastic waves in [2], our main focus lies now on the system for visco–elastic waves is heterogeneous media

$$\begin{aligned}
\rho\,\partial_t \boldsymbol{v} &= \operatorname{div}\boldsymbol{\sigma} + \boldsymbol{f}\,,\\
\partial_t \boldsymbol{\sigma} &= 2\mu(1+L\tau_{\mathrm{S}})\operatorname{dev}\boldsymbol{\varepsilon}(\boldsymbol{v}) + \kappa(1+L\tau_{\mathrm{P}})\operatorname{div}\boldsymbol{v}\,\mathbf{I} + \sum_{l=1}^{L}\boldsymbol{\eta}_l\,,\\
\tau_{\sigma,l}\,\partial_t \boldsymbol{\eta}_l &= -2\mu\tau_{\mathrm{S}}\operatorname{dev}\boldsymbol{\varepsilon}(\boldsymbol{v}) - \kappa\tau_{\mathrm{P}}\operatorname{div}\boldsymbol{v}\,\mathbf{I} - \boldsymbol{\eta}_l\,, \qquad l=1,\dots,L
\end{aligned}$$

in $Q = (0,T)\times\Omega \subset \mathbb{R}^{1+d}$. Based on the framework of generalized standard materials this extends the system for velocity $\boldsymbol{v}$ and stress $\boldsymbol{\sigma}$ by memory tensors $\boldsymbol{\eta}_l$ describing the attenuation of elastic waves in geophysical applications. The visco–acoustic case corresponds to the case $\mu \to 0$ and $\boldsymbol{\sigma} = p\mathbf{I}$, where p is the the hydrostatic pressure.

We use a tensor product space-time mesh with a discontinuous Galerkin finite element method with full upwind flux for the spatial discretization and a Petrov–Galerkin discretization in time. For this setting we establish convergence by verifying discrete inf-sup stability with a constant independent of the polynomial degree of the finite element space. The full space-time linear system is solved by a parallel multilevel preconditioner.

The method is adaptive with variable polynomial degrees in the space-time cells with a refinement strategy based on a goal-oriented dual-weighted error estimator. This reduces the error with respect to a given goal functional within several adaptive iterations. In our numerical examples we choose a linear goal functional corresponding to a space-time region of interest and we show that the adaptive procedure clearly identifies the subset of the space-time cylinder which is required for the accurate evaluation of the goal functional.

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A UNIFIED APPROACH FOR MIXED FORMULATIONS OF ELLIPTIC PROBLEMS WITH APPLICATIONS IN STRUCTURAL MECHANICS

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A general and flexible approach will be presented how to derive mixed variational formulations of elliptic problems. The approach is based on the concept of densely defined linear operators and their adjoints, rather than on the well-known technique of integration by parts, which is typically used for the construction of mixed variational formulations otherwise. The construction of the mixed formulation starts with the primal variational formulation rather than the strong (or classical) form of the problem. This allows to address the relation between the primal and the mixed problem quite thoroughly and typically ensures the equivalence of the two problems without additional regularity assumptions.

As applications of the approach we will discuss known and new mixed formulations of Hellinger-Reissner type. As a particular application the Reissner-Mindlin plate bending model is discussed, for which a decomposition of the problem into three simpler second-order problems is shown.

A POSTERIORI ERROR ANALYSIS OF A CONFORMING FOUR-FIELD FORMULATION FOR BIOT'S CONSOLIDATION MODEL IN POROELASTICITY

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In this talk we present the *a priori* and *a posteriori* error analyses for the conforming approximation of the four-field formulation recently proposed in [2] for Biot's consolidation in poroelasticity, in which the solid displacement, the fluid pressure, the fluid flux and the total pressure, are the primal variables. For the *a priori* error analysis we provide suitable hypotheses on the corresponding finite dimensional subspaces ensuring that the associated Galerkin scheme becomes well posed. A feasible choice of subspaces is given by Raviart–Thomas elements of order $k \geq 0$ for the fluid flux, discontinuous polynomials of degree k for fluid pressure, and any stable pair of Stokes elements, such as Hood–Taylor elements, for the solid displacements and total pressure. In turn, we develop a reliable and efficient residual-based *a posteriori* error estimator. The proof of the realibilty is based on a stability result providing global inf-sup conditions on each one of the spaces involved, and stable Helmholtz decompositions. On the other hand, the usual localization technique of bubble functions and inverse inequalities, are the main tools behind the efficiency estimate. Both estimates are shown to be independent of the moludi of dilatation. Numerical examples in 2D and 3D illustrate the performance of the conforming scheme and show the good behaviour of the adaptive algorithm associated to the proposed *a posteriori* error indicator.

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