Coupling bulk and surface PDEs: Numerical approximation of dynamic biomembranes

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A parametric finite element approximation of a fluidic membrane, whose evolution is governed by a surface Navier–Stokes equation coupled to bulk Navier–Stokes equations, is presented. The elastic properties of the membrane are modelled with the help of curvature energies of Willmore and Helfrich type. Forces stemming from these energies act on the surface fluid, together with a forcing from the bulk fluid.

We introduce a stable parametric finite element method to solve this complex free boundary problem. Local inextensibility of the membrane is ensured by solving a tangential Navier–Stokes equations, taking surface viscosity effects of Boussinesq–Scriven type into account. In our approach the bulk and surface degrees of freedom are discretized independently, which leads to an unfitted finite element approximation of the underlying free boundary problem. Bending elastic forces resulting from an elastic membrane energy are discretized using an approximation introduced by Dziuk. The obtained numerical scheme can be shown to be stable and to have good mesh properties.

Joint work with John W. Barrett (Imperial College London, UK) and Harald Garcke (Regensburg University, Germany).

Dynamical low rank approximation of random time dependent PDEs.

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We investigate dynamical low rank approximations of time dependent PDEs with random data where at each time instant, the approximate solution is sought in the manifold of functions in separable form (separating space and stochastic variables) of fixed rank, and is obtained by Galerkin projection of the governing equations onto the tangent space to the manifold. Suitable equations are then derived for the evolution of the deterministic and stochastic modes. We discuss error estimates and implementation issues. In particular, we investigate and present numerical results on parabolic equations, Navier-Stokes equations for incompressible fluids at low Reynolds number, with emphasis on the case of stochastic boundary conditions, as well as second order wave equations.

[1] E. Musharbash and F. Nobile. Dual Dynamically Orthogonal approximation of incompressible Navier Stokes equations with random boundary conditions, MATHICSE REPORT n. 03-2017, EPFL, 2017.

[2] E. Musharbash, F. Nobile and T. Zhou. Error Analysis of the Dynamically Orthogonal Approximation of Time Dependent Random PDEs, in Siam Journal on Scientific Computing, vol. 37, num. 2, p. A776-A810, 2015.

Joint work with Eleonora Musharbash (Ecole Polytechnique Fédérale de Lausanne, Switzerland).

Causal discretizations of anisotropic eikonal equations.

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Motivated by applications to path planning and image segmentation, we develop numerical methods for finding globally optimal paths subject to non-holonomic constraints. This encompasses various forms of path curvature penalization, such as the Reeds-Shepp car, Euler elastica, or Dubins car models. For that purpose we discretize eikonal equations, or first order static Hamilton-Jacobi-Bellman PDEs, with respect to strongly anisotropic riemannian or finslerian metrics. Our approach relies on tools from discrete geometry, such as Voronoi's reductions of quadratic forms, to design numerical schemes obeying a property of causality, which are then efficiently solved via the single pass fast marching algorithm.

Convergence of adaptive discontinuous Galerkin methods

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Consulting the unprecedented developments of convergence and optimality theory of conforming adaptive finite element methods during the last two decades, the strict D"orfler marking and the resulting reduction of some error quantity appears to be fundamental for most of the results. A straight forward generalisation to discontinuous Galerkin (dG) methods is difficult due to the fact that the penalty term is not necessarily monotone. However, for large enough penalty parameters Karakashian and Pascal (2007) proved error reduction and Bonito and Nochetto (2010) proved optimality for the adaptive symmetric interior penalty method with D"orfler marking.

In contrast to these results, in this talk, we generalise the basic convergence analysis by Morin, Siebert, and Veeser (2008) for adaptive discontinuous Galerkin methods. On the one hand, this provides convergence without rates. On the other hand the theory covers different dG schemes as well as all practically relevant marking strategies. Another key feature of the presented result is, that it does not require an extra enlargement of the penalty parameter. The analysis is based on a quasi interpolation into a newly developed limit space of the adaptively created non-conforming discrete spaces.

Joint work with Emmanuil Gourgoulis, University of Leicester, UK and National Technical University, GR.

Numerical solution of nonsmooth problems and application to damage evolution and optimal insulation

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Nonsmooth minimization problems and singular partial differential equations arise in the description of inelastic material behavior, image processing, and modeling of non-Newtonian fluids. The numerical discretization and iterative solution is often based on regularizing or stabilizing terms. In this talk we address the influence of such modifications on error estimates and the robustness of iterative solution methods. In particular, we present an unconditional stability result for semi-implicit discretizations of a class of singular flows and devise a variant of the alternating direction of multipliers method with variable step sizes. The results and methods are illustrated by numerical experiments for a damage evolution model and a problem of optimal insulation leading to a break of symmetry.

Concurrent versus Sequential Multi-scale Methods for Atomistic Materials Modelling

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A common atomic-scale materials modelling task is to characterise the lattice defects that control material response. Due to their multi-scale nature (complex defect cores coupled to long-range elastic far-fields) **concurrent** multi-scale methods, including e.g. the popular Quasicontinuum and QM/MM methods, are a popular tool for their computational investigation.

A difficult challenge in the development of concurrent multi-scale schemes is the interface condition coupling models valid at different scales (e.g. quantum, atomistic and continuum). The emerging mathematical theory of concurrent multi-scale methods precisely quantifies the effect of the coupling and coarse-graining mechanisms on the numerical error, leading to optimised schemes with rigorous convergence rates.

A new realisation that has come out of this mathematical theory is that - with some care - **sequential** multi-scale methods, providing a static boundary condition to the atomistic simulation rather than a concurrent coupling, may provide comparable accuracy at significantly reduced model complexity. Indeed, as I will show in this talk, one can even surpass the accuracy of concurrent schemes.

Joint work with Julian Braun (Warwick), Huajie Chen (Peking Normal), Maciej Buze (Warwick) and Tom Hudson (Warwick).

A PDE approach to regularization in Deep Learning

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Deep neural networks have achieved significant success in a number of challenging engineering problems. There is consensus in the community that some form of smoothing of the loss function is needed, and there have been hundreds of papers and many conferences in the past three years on this topic. However, so far there has been little analysis by mathematicians.

The fundamental tool in training deep neural networks is Stochastic Gradient Descent (SGD) applied to the loss function, $f(x)$, which is high dimensional and nonconvex.

$$dx\_t = -\nabla f(x\_t)dt + dW\_t \tag{SDG}$$

There is a consensus in the field that some for of regularization of the loss function is needed, but so far there has been little progress. This may be in part because smoothing techniques, such a convolution, which are useful in low dimensions, are computationally intractable in the high dimensional setting.

Two recent algorithms have shown promise in this direction. The first uses a mean field approach to perform SGD in parallel. The second replaced f in (**??**) with $f_\gamma(x)$, the *local entropy* of f, which is defined using notions from statistical physics.

We interpret both algorithms as replacing f with f_γ, where $f_\gamma = u(x, \gamma)$ and u is the solution of the viscous Hamilton-Jacobi PDE

$$u_t(x,t) = -\frac{1}{2}|\nabla u(x,t)|^2 + \beta^{-1}\Delta u(x,t)$$

along with $u(x, 0) = f(x)$. This interpretation leads to theoretical validation for empirical results.

However, what is needed for (**??**) is $\nabla f_\gamma(x)$. Remarkably, for short times, this vector can be computed efficiently by solving an auxiliary convex optimization problem, which has much better convergence properties than the original non-convex problem. Tools from optimal transportation are used to justify the fast convergence of the solution of the auxiliary problem.

In practice, this algorithm has significantly improved the training time (speed of convergence) for Deep Networks in high dimensions. The algorithm can also be applied to nonconvex minimization problems where (**??**) is used.

Joint work with Pratik Chaudhari (UCLA), Stanley Osher (UCLA), Stefano Soatto (UCLA) and Guillaume Carlier (UCLA).

What are we computing with numerical methods for hyperbolic systems of conservation laws ?

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Efficient numerical methods for approximating hyperbolic systems of conservation laws have been in existence for the past three decades. However, rigorous convergence results to entropy solutions are only available in the case of scalar conservation laws. We present numerical evidence that demonstrates the lack of convergence of state of art numerical methods to entropy solutions of multi-dimensional systems. On the other hand, an ensemble averaged version of these numerical methods is shown to converge to entropy measure-valued solutions. However, these solutions are not unique. We impose additional admissibility criteria by requiring propagation of information on all multi-point correlations. This results in the concept of statistical solutions or time-parametrized probability measures on integrable functions, as a solution framework. We derive sufficient conditions for convergence of ensemble-averaged numerical methods to statistical solutions and present numerical experiments illustrating these solutions.

A first approach to Virtual Elements for magnetostatic problems

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The Virtual Element Method (VEM) is a recent technology for the discretization of partial differential equations that follows a similar paradigm to standard Finite Elements, but allows to make use of general polytopal meshes, including non-convex elements and hanging nodes. In addition, the flexibility of the VEM construction allows in many problems to develop new appealing schemes also for simplex and quad/hexa-type meshes.

In the present talk we investigate the development of some Virtual Element families for a simple (classical) magnetostatic problem. We start by introducing a first set of Virtual Spaces that constitute a complex and detail its application for the discretization of the problem. Afterwards, we present a modified set of spaces that are more efficient in terms of degrees of freedom (in particular in three dimensions) and still constitute a complex. We support the theoretical analysis of the scheme with a set of numerical tests.

Joint work with Franco Brezzi (IMATI-CNR, Pavia, Italy), Franco Dassi (Università di Milano-Bicocca, Italy), Donatella Marini (Università di Pavia, Italy) and Alessandro Russo (Università di Milano-Bicocca, Italy).

Adaptive wavelet methods for space-time variational formulations of evolutionary PDEs

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Space-time discretization methods require a well-posed space-time variational formulation. Such formulations are well-known for parabolic problems. The (Navier)-Stokes equations can be viewed as a parabolic problem for the divergence-free velocities. Yet to avoid the cumbersome construction of divergence-free trial spaces, we present well-posed variational formulations for the saddle-point problem involving the pair of velocities and pressure.

We discuss adaptive wavelet methods for the optimal adaptive solution of simultaneous space-time variational formulations of evolutionary PDEs. Thanks to use of tensor products of temporal and spatial wavelets, the whole time evolution problem can be solved at a complexity of solving one instance of the corresponding stationary problem.

Joint work with Christoph Schwab (ETH, Zürich).

Discrete theories for elliptic problems in non–divergence form

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In this talk, two discrete theories for elliptic problems in non-divergence form are presented. The first, which is applicable to problems with continuous coefficients and is motivated by the strong solution concept, is based on discrete Calderon-Zygmund-type estimates. The second theory relies on discrete Miranda-Talenti estimates for elliptic problems with discontinuous coefficients satisfying the Cordes condition. Both theories lead to simple, efficient, and convergent finite element methods. We provide numerical experiments which confirm the theoretical results, and we discuss possible extensions to fully nonlinear second order PDEs.

Joint work with Xiaobing Feng (The University of Tennessee) and Mohan Wu (University of Pittsburgh).

Weights and applications in numerics

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The use of weights and weighted norm inequalities has a rich history in harmonic analysis and the study of regularity properties to solutions of partial differential equations (PDE). Starting from classical results, we will present an overview of the application of some of these ideas to the numerical analysis of PDEs. Our main attention will be on some recent results concerning the use of weights in fractional diffusion, problems with singular data and PDE constrained optimization problems. Although these seem as disparate and unrelated applications, it is remarkable that the only structural assumption on the weight is that it belongs to a so-called Muckenhoupt A_p class, which has been thorougly studied in harmonic analysis since the 1970's.

Discrete maximal parabolic regularity for Galerkin finite element solutions and their applications

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Maximal parabolic regularity is an important analytical tool and has a number of applications, especially to nonlinear problems and/or optimal control problems when sharp regularity results are required. Recently, there have been a lot of interest in establishing similar results for various time discretization methods. In my talk, I will describe our results for discontinuous Galerkin time schemes and show how such results can be used, for example, in establishing pointwise best approximation estimates for fully discrete Galerkin solutions without any coupling between the spatial mesh size h and the time steps k.

Joint work with Boris Vexler, (TU Munich, Germany).

The Kuratowski–Ryll-Nardzewski Theorem and semismooth Newton methods for Hamilton–Jacobi–Bellman 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.

Joint work with Endre Süli (Oxford, UK).

C^1 ISOGEOMETRIC SPACES ON MULTIPATCH DOMAINS

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One key feature of isogeometric analysis is that it allows smooth shape functions. Indeed, when isogeometric spaces are constructed from p-degree splines (and extensions, such as NURBS), they enjoy up to C^{p-1} continuity within each patch. However, global continuity beyond C^0 on so-called multi-patch geometries poses some significant difficulties. We consider planar multi-patch domains that have a parametrization which is only C^0 at the patch interface. On such domains we study the h-refinement of C^1-continuous isogeometric spaces. These spaces in general do not have optimal approximation properties. The reason is that the C^1-continuity condition easily over-constrains the solution which is, in the worst cases, fully locked to linears at the patch interface. However, recent studies have given numerical evidence that optimal convergence occurs for bilinear two-patch geometries and cubic (or higher degree) C^1 splines. This is the starting point of our study. We introduce the class of analysis-suitable G^1 geometry parametrizations, which includes piecewise bilinear parametrizations. We then analyze the structure of C^1 isogeometric spaces over analysis-suitable G^1 parametrizations and, by theoretical results and numerical testing, discuss their approximation properties. We also consider examples of geometry parametrizations that are not analysis-suitable, showing that in this case optimal convergence of C^1 isogeometric spaces is prevented.

Joint work with Pablo Antolin (EPFL), Annabelle Collin (Institut Polytechnique de Bordeaux), Mario Kapl (RICAM Linz), and Thomas Takacs (JKU Linz),.