Book of Abstracts

ENUMATH 2017

European Conference on Numerical Mathematics and Advanced Applications

September 25 – 29, 2017, Voss, Norway

Preface

The European Conference on Numerical Mathematics and Advanced Applications (ENUMATH) is a series of conferences held every two years. Starting with the first ENUMATH conference in Paris (1995), successive conferences have been held at various locations across Europe, Heidelberg (1997), Jyvaskyla (1999), Ischia Porto (2001), Prague (2003), Santiago de Compostela (2005), Graz (2007), Uppsala (2009), Leicester (2011), Lausanne (2013), and Ankara (2015). This is the first time that this conference is being held in Norway and is being organized by the University of Bergen (UiB) as the local organizers.

ENUMATH has attracted top numerical and computational mathematicians with majority of participants from Europe but also across the globe. This conference carries forward this tradition. To ensure the highest scientific level, 11 keynote speakers were invited: A. Zanna (Bergen, Norway), R. Scheichl (Bath, UK), R. Nochetto (Maryland, US), V. Girault (Paris, France), S. Mishra (Zuerich, Switzerland), F. Nobile (Austin, US), B. Kaltenbacher (Klagenfuert, Austria), L. da Veiga (Milan, Italy), M. Rognes (Oslo, Norway), A. Patera (MIT, US), K-A. Mardal (Oslo, Norway). There are 325 registered participants (250 men and 75 female participants representing 128 institutions, 91 are PhD students). There are 29 minisymposia sessions and more than 300 talks (230 minisymposia talks and 73 contributed talks) spread over 5 days.

The scientific program has quite a variety and is likely to keep you busy! Besides the conference, the location at Voss is also ideal for wonderful trips in the surroundings to enjoy the beauty of Norway, its fjords and its hospitality.

The local organizing committee of ENUMATH 2017

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Mathematics & Medicine - how mathematics, modelling and simulation can lead to better diagnosis and treatment

Antonella Zanna[1]

[1] *University of Bergen, Norway* Antonella.Zanna@uib.no

The advance of technology and imaging has given rise to an incredible development in Medicine and Biology. This development has also made doctors and biologist understand that they need more mathematical tools (than just statistics) to solve more advanced problems and get better diagnosis and a personalized treatment. In this talk, I will present some of the medical projects I and my collaborators have been working on, involving image analysis, modelling and quantification of physiological parameters.

Numerical methods for porous media flows

Sorin Pop[1,2]

[1] *Hasselt University, Belgium* sorin.pop@uhasselt.be
[2] *University of Bergen, Norway*

Porous media flows are encountered in numerous applications of utmost societal and technological relevance. Examples in this sense are in water resource management, geological CO_2 sequestration, oil recovery, or geothermal energy. Mathematical modelling and numerical simulation are key approaches for understanding such processes in their entire complexity, and further for providing reliable predictive information.

In this presentation we start by addressing different aspects related to the modelling of porous media flows, including equilibrium and non-equilibrium cases. Next, after summarizing some existence and uniqueness results, we focus on the numerical methods. The discussion includes rigorous convergence of the discretization schemes, as well as linear iterative methods for approximating the solutions of the nonlinear, time discrete or fully discrete problems.

Finally, we consider heterogeneous media, and discuss some numerical results and relate these with experimental ones.

Some numerical simulation of hydraulic fractures in poro-elastic media

Vivette Girault[1]

[1] *UPMC, Paris, France* girault@ann.jussieu.fr

There are several models of hydraulic fracturing in poro-elastic media. Complete models are very complex and therefore I shall discuss mainly the numerical simulation (numerical analysis and algorithms) of two simplified models: a Reynolds lubrication model and a phase field model. The first one describes the opening of an existing fracture, without width, the width being included in the fracture flow equation. Its disadvantage is that the fracture cannot propagate, but its advantage is it treats the location of the fracture with precision, and avoids meshing the interior of the fracture. The phase field model locates a region surrounding the fracture, and thus does not describe precisely the position of the fracture, but it has the advantage of being able to describe the propagation of the fracture.

Model Order Reduction for Component-to-System Analysis of Parametrized Partial Differential Equations

Anthony T. Patera[1]

[1] *Massachusetts Institute of Technology, USA* patera@mit.edu

In this talk we describe and demonstrate a model order reduction methodology for efficient solution of partial differential equations characterized by many spatially distributed parameters. The approach is relevant in many-query and real-time contexts such as design, shape and topology optimization, parameter estimation, classification and monitoring, and reconditioning.

The numerical approach comprises four principal ingredients: component-to-system synthesis, formulated as a static condensation procedure; model order reduction, informed by evanescence arguments at component interfaces (port reduction) and low-dimensional parametric manifolds in component interiors (reduced basis techniques); offline-online computational decomposition strategies; and a posteriori error estimators for adaptivity and verification. The method is also well-suited for parallel calculation in both the offline and online stages.

We provide examples in acoustics, linear elasticity, and nonlinear solid mechanics, with applications from musical instruments to shiploaders.

Virtual Elements for Magnetostatic Problems

Lourenco Beirao da Veiga[1]

[1] *University of Milano-Bicocca, Italy* lourenco.beirao@unimib.it

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 with important differences. By avoiding the explicit integration of the shape functions that span the discrete space and introducing an innovative construction of the stiffness matrixes, the VEM acquires very interesting properties and advantages with respect to more standard methods. For instance, the VEM easily allows for general polygonal/polyhedral meshes, even non-conforming and with non-convex elements.

In the present talk we investigate the development of some Virtual Element families for a classical magnetostatic problem in two and three dimensions, that can be considered as a first step towards more complex applications. We start by introducing a first set of Virtual Spaces that constitute a complex (both in 2D and 3D) and detail its application for the discretization of the problem. Afterwards, we also present a modified set of spaces that are more efficient in terms of degrees of freedom, and still constitute a complex. We support the theoretical analysis of the method with a set of numerical tests.

All-at-once versus reduced formulations of inverse problems and their regularization

Barbara Kaltenbacher[1]

[1] *University of Klagenfurt, Austria* Barbara.Kaltenbacher@aau.at

Parameter identification problems typically consist of a model equation, e.g. (systems of) ordinary or partial differential equations, and the observation equation. In the conventional reduced setting, the model equation is eliminated via the parameter-to-state map. Alternatively, one might consider both sets of equations (model and observations) as one large system, to which some regularization method is applied. The choice of the formulation – reduced or all-at-once – can make a considerable difference computationally, depending on which regularization method is used: Whereas almost the same optimality system arises for the reduced and the all-at-once Tikhonov method, the situation is different for iterative methods, especially in the context of nonlinear models. In this talk we will exemplarily provide some convergence results for all-at-once versions of variational, Newton type and gradient based regularization methods. Moreover we will compare the implementation requirements for the respective all-at-one and reduced versions and provide some numerical illustration. Finally we will give an outlook on two further aspects in this context namely

a) all-at-once methods for parameter identification in time dependent PDEs

b) minimization based formulations of inverse problems and their regularization.

The operator preconditioning framework with various applications to interstitial fluid flow and the aging human brain

Kent-Andre Mardal[1]

[1] *University of Oslo, Norway* kent-and@simula.no

The operator preconditioning technique is a constructive framework for designing efficient solution algorithms from the mapping properties of the continuous equations. In this talk we will present the basic framework in an abstract fashion before discussing various applications where the interstitial fluid flow is studied in the central nervous system. In particular, we will consider problems arising in porous media flow in elastic media and multi-scale problems representing the coupling between the vasculature and the extra-cellular space of the human brain. The numerical modelling is motivated by the recently proposed glymphatic system, which is a clearance mechanism where water remove waste associated with Alzheimer disease. The clearance is particularly active during sleep. The numerical investigations employ the finite element method and the software framework FEniCS.

Compatible discretizations in our hearts and minds

Marie E. Rognes[1]

[1] *Simula Research Laboratory, Norway* meg@simula.no

The complexity and fragility of the human physiology matched against the cost and ethical concerns associated with experimental and clinical techniques sets a rich scene for mathematical modelling and simulation. In this talk, I'll focus on numerical and computational aspects of numerical methods for two emerging biomedical applications: (i) the brain's waterscape and (ii) finite collections of biological cells such as cardiac myocytes or pluripotent stem cells. Topics will include generalized poroelasticity, electrical signal propagation, diffusion-reaction problems over interfaces, mixed finite element discretizations, and preconditioning, and be illustrated by theoretical, numerical and computational results.

Dynamical low rank approximation of random time dependent PDEs

Fabio Nobile[1]

[1] *École polytechnique fédérale de Lausanne, Switzerland* fabio.nobile@epfl.ch

Partial differential equations with random coefficients and input data (random PDEs in short) arise in many applications in which the data of the PDE need to be described in terms of random variables/fields due either to a lack of knowledge of the system or to its inherent variability. The numerical approximation of statistics of the solution poses several challenges when the number of random parameters is large and/or the parameter-to-solution map is complex, and effective surrogate or reduced models are of great need in this context.

In this talk we consider time dependent PDEs with few random parameters and seek for an approximate solution in separable form that can be written at each time instant as a linear combination of linearly independent spatial functions multiplied by linearly independent random variables (low rank approximation) in the spirit of a truncated Karhunen-Loève expansion. Since the optimal deterministic and stochastic modes can significantly change over time, we consider here a dynamical approach where those modes are computed on the fly as solutions of suitable evolution equations. From a geometrical point of view, this corresponds to constraining the original dynamics to the manifold of fixed rank functions, i.e. functions that can be written in separable form with a fixed number of terms. Equivalently, the original equations are projected onto the tangent space to the manifold of fixed rank functions along the approximate trajectory, similarly to the Dirac-Frenkel variational principle in quantum mechanics.

We discuss the construction of the method as well as practical numerical aspects for several time dependent PDEs with random parameters, including the heat equation with a random diffusion coefficient; the incompressible Navier-Stokes equations with random Dirichlet boundary conditions; the wave equation with random wave speed. In the latter case, we propose a dynamical low rank approximation that preserves the symplectic structure of the equations.

Thermally Actuated Bilayer Plates

Ricardo Nochetto[1]

[1] *University of Maryland, USA* rhn@math.umd.edu

We present a simple mathematical model of polymer bilayers that undergo large bending deformations when actuated by non-mechanical stimuli such as thermal effects. The model consists of a nonlinear fourth order problem with a pointwise isometry constraint, which we discretize with Kirchhoff quadrilaterals. We prove Γ-convergence of the discrete model and propose an iterative method that decreases its energy and leads to stationary configurations. We investigate performance, as well as reduced model capabilities, via several insightful numerical experiments involving large (geometrically nonlinear) deformations. They include the folding of several practically useful compliant structures comprising of thin elastic layers. This work is joint with S. Bartels and A. Bonito.

Multilevel Monte Carlo and beyond

Rob Scheichl[1]

[1] *University of Bath, UK* r.scheichl@bath.ac.uk

Multilevel Monte Carlo (MLMC) is a recently introduced variance reduction technique for stochastic simulation which greatly reduces the computational cost by employing cheap, coarse-scale models with lower fidelity to carry out the bulk of the stochastic simulations, while maintaining the overall accuracy of the fine scale model through a small number of well-chosen high fidelity simulations.

In this talk, I will first review the ideas behind the approach and discuss a number of applications and extensions that illustrate the generality of the approach. The multilevel Monte Carlo method (in its practical form) has originally been introduced about 10 years ago by Mike Giles for stochastic differential equations in Mathematical Finance and has attracted a lot of interest in the context of uncertainty quantification of physical systems modelled by PDEs. (The first, theoretical paper was by Stefan Heinrich in 1998.) The approach has been extended to Markov chain Monte Carlo, sequential Monte Carlo and other filtering techniques. Among others, its application has been extended to biological/chemical reaction networks, plasma physics, interacting particle systems and more recently to nested simulations.

In the second half of the talk, I will go beyond the classical MLMC framework and use sample-dependent model hierarchies and a posteriori error estimators to efficiently estimate rare events (Multilevel Subset Simulation) as well as to extend the framework from the discrete, level-based approach to a new Continuous Level Monte Carlo (CLMC) method. These latter extensions are work in progress in collaboration with Gianluca Detommaso (Bath), Tim Dodwell (Exeter) and Daniel Elfverson (Umea).

MS01 – Innovative Numerical Methods and their Analysis for Elliptic and Parabolic PDEs

(Ricardo H. Nochetto, Andreas Veeser)

Wednesday, 15:55 – 17:35, Kulturhus

Snorre Christiansen – *Tools for constructing minimal finite element spaces of differential forms*

Lorenzo Tamellini – *A sparse-grid version of IGA methods*

Ragnar Winther – *Local coderivatives and approximation of Hodge Laplace problems*

Thomas Boiveau – *Approximation of parabolic equations by space-time tensor methods*

Thursday, 15:30 – 17:10, Kulturhus

Raphéle Herbin – *The gradient discretization method*

Pietro Zanotti – *Quasi-optimal non-conforming methods for linear variational problems*

Winnifried Wollner – *A priori error analysis for optimization with elliptic PDE constraints*

Andreas Veeser – *Quasi-optimality in parabolic spatial semidiscretizations*

Friday, 08:30 – 10:10, Kulturhus

Christian Kreuzer – *Oscillation in a posteriori error analysis*

Claudio Canuto – *On the convergence and optimality of adaptive hp-FEM*

Alfred Schmidt – *Finite element methods for parabolic problems with time dependent domain*

Shawn W. Walker – *The Ericksen Model of Liquid Crystals with Colloidal and Electric Effects*

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Tools for constructing minimal finite element spaces of differential forms

Snorre H. Christiansen[1]

[1] *Department of Mathematics, University of Oslo, PO Box 1053 Blindern, NO-0316 Oslo, Norway.*
snorrec@math.uio.no

A notion of Finite Element System has been developed to construct finite dimensional spaces of differential forms with good properties, see for instance [1]. The framework guarantees in particular that the spaces come equipped with degrees of freedom that provide projections that commute with the exterior derivative. This is used for the error analysis. Another design principle is that one wants the finite element spaces to contain some pre-specified differential forms, for instance all those that are polynomials of a certain degree. A natural question is then how to construct a *minimal* finite element system containing those. In [2] we developed necessary and sufficient conditions for identifying minimal finite element systems, construction methods to define them, and interpreted some existing finite element spaces as examples of minimal FES. This talk, which is based on joint work with Andrew K. Gillette, will present these results.

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A sparse-grid version of IGA methods

Joakim Beck[1], **Giancarlo Sangalli**[2], **Lorenzo Tamellini**[3]

[1] *KAUST, Saudi Arabia* joakim.beckr@kaust.edu.sa
[2] *Università di Pavia, Italy* giancarlo.sangalli@unipv.it
[3] *IMATI-CNR, Pavia, Italy* tamellini@imati.cnr.it

Sparse grids have been proposed in the early 90's in the context of finite differences (FD) / finite elements (FE) methods to reduce the "curse of dimensionality effect", i.e., the fact that the number of degrees of freedom (DoF) of the approximation grows exponentially in the number of dimensions of the problem.

Roughly speaking, the sparse-grid construction consists in recasting the construction of conventional FE/FD methods in a hierarchical fashion and suitably discarding the components which carry the least amount of information. Under suitable regularity assumptions (slightly more demanding than the usual Sobolev spaces) sparse grids are then able to deliver approximations with essentially the same accuracy of conventional FE/FD methods (i.e., up to a logarithmic factor appearing in the error estimates), using however a much lower number of DoF. Furthermore, the sparse-grid solution can be computed as a linear combination of standard FE/FD solutions on relatively coarse grids (the so-called "combination technique"): this implies that sparse grids can be implemented quite straightforwardly reusing existing solvers and lead to a very natural parallelization of the computation.

In this talk we detail the application of the sparse-grid technology to the h-refined version of the classical IGA method and show some numerical tests that will highlight how sparse IGA performs compared to the classical "full tensor" counterpart.

Local coderivatives and approximation of Hodge Laplace problems

Ragnar Winther[1]

[1] *University of Oslo, Department of Mathematics, Norway* rwinther@math.uio.no

By construction mixed finite element methods introduce nonlocal approximations of the coderivatives. This is true, not only for the standard mixed approximations of second order elliptic prolbems, but also for all the standard mixed finite element approximations of Hodge Laplace problems associated the de Rham complex. Since these methods are based on proper discrete subcomplexes, the exterior derivatives, which are local operators, are computed exactly, while the associated discrete coderivatives are nonlocal. This nonlocal property is an inherent consequence of the mixed formulation of these methods, and can be argued to be an undesired effect of the schemes. As a consequence, more local methods may have improved properties. In the present paper, we construct such methods by relying on a careful balance between the choice of finite element spaces, degrees of freedom, and numerical integration rules.

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Approximation of parabolic equations by space-time tensor methods

Thomas Boiveau[1,2], **Virginie Ehrlacher**[1,2], **Alexandre Ern**[1,2], **Anthony Nouy**[3]

[1] *Université Paris Est, France* thomas.boiveau@enpc.fr
[2] *INRIA Paris, France*
[3] *École Centrale de Nantes, France*

In numerical simulations, the reduction of computational costs is a key challenge for the development of new models and algorithms. In order to approximate the solution of a parabolic evolution equation at a lower cost, model reduction techniques based on tensor methods can be used. The principle is to obtain a separated representation of the solution in space and time. In this work, we consider an approach based on the Proper Generalised Decomposition (see [1, 2] for convergence analysis), we define a rigorous mathematical setting starting from the continuous formulation to define a discrete problem. We note that the parabolic equations have been also considered in [3] where a discrete formulation has been proposed. Here we obtain a different discrete problem. The mathematical framework allows us to formulate a greedy algorithm for the construction of a low-rank approximation through a minimal residual formulation. We perform numerical tests in order to compare the proposed method with the strategy suggested in [3]. An extension of this work would be the coupling between the PGD strategy with adaptivity, in order to improve the accuracy of the decomposition obtained at an even lower cost.

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[1] F. Chinesta, R. Keunings, and A. Leygue. *The Proper Generalized Decomposition for Advanced Numerical Simulations*. Springer Briefs in Applied Sciences and Technology. Springer, Cham, 2014.

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The gradient discretization method

J. Droniou[1] , R. Eymard[2] , T. Gallouët[3], C. Guichard[4] and R. Herbin[3]

[1] *School of Mathematical Sciences, Monash University, Australia*
jerome.droniou@monash.edu
[2] *LAMA, Université Paris-Est, CNRS, France.* Robert.Eymard@u-pem.fr
[3] *Aix Marseille Univ, CNRS, Centrale Marseille, I2M, Marseille, France.*
thierry.gallouet@univ-amu.fr raphaele.herbin@univ-amu.fr
[4] *LJLL, Université Pierre et Marie Curie, Paris, France.* guichard@ljll.math.upmc.fr

The gradient discretization method (GDM) is a framework which contains classical and recent discretisation schemes for diffusion problems of different kinds: linear or non linear, steady- state or time-dependent. The schemes may be conforming or non conforming, and may be built on very general polygonal or polyhedral meshes. In this talk, we shall present the core properties that are required to prove the convergence of a GDM and present the analysis of the method on given linear and non linear model problems. Any scheme entering the GDM framework is then known to converge for these models. Appropriate tools so as to easily check whether a given scheme satisfies the expected properties of a GDM can be identified. Thanks to these tools a number of methods can be shown to enter the GDM framework: some of these methods are classical, such as the conforming Finite Elements, the Raviart-Thomas Mixed Finite Elements, or the non-conforming Finite Elements. Others are more recent, such as the Discontinuous Galerkin methods, the Hybrid Mixed Mimetic or Nodal Mimetic methods, some Discrete Duality Finite Volume schemes, and some Multi-Point Flux Approximation schemes.

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Quasi-optimal nonconforming methods for linear variational problems

Pietro Zanotti[1], **Andreas Veeser**[2]

[1] *Università degli Studi di Milano, Italy* pietro.zanotti@unimi.it
[2] *Università degli Studi di Milano, Italy* andreas.veeser@unimi.it

We consider the approximation of linear elliptic variational problems, symmetric for simplicity. According to the Cea's lemma, conforming Galerkin methods for these problems are quasi-optimal. Conversely, a simple argument reveals that classical nonconforming methods do not enjoy such property. Motivated by this observation, we characterize the quasi-optimality, within a large class of (possibly) nonconforming methods, in terms of suitable notions of stability and consistency. Moreover, we identify the quasi-optimality constant and discuss the ingredients determining it. To illustrate our results, we present the construction of a quasi-optimal Crouzeix-Raviart finite element method for the Poisson problem and show that the corresponding quasi-optimality constant only depends on the shape parameter of the underlying mesh.

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A priori error analysis for optimization with elliptic PDE constraints

Andreas Veeser[1], **Winnifried Wollner**[2]

[1] *Dipartimento di Matematica 'F. Enriques', Università degli Studi di Milano, Via C. Saldini, 50, 20133 Milano, Italy* andreas.veeser@unimi.it
[2] *TU Darmstadt, Department of Mathematics, Dolivostr. 15, 64293 Darmstadt, Germany* wollner@mathematik.tu-darmstadt.de

We consider finite element solutions to quadratic optimization problems, where the state compactly depends on the control via an elliptic partial differential equation. Exploiting that a suitably reduced optimality system satisfies a Gårding inequality, we derive a priori error estimates for state, dual and control variables. The error estimates for state and dual variable are asymptotically independent of the Tikhonov regularization parameter.

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Quasi-optimality in parabolic spatial semidiscretizations

Christian Kreuzer[1], **Francesca Tantardini**[2], **Andreas Veeser**[3]

[1] *Technische Universität Dortmund, Germany* christian.kreuzer@tu-dortmund.de
[2] *Ruhr-Universität Bochum, Germany* francesca.tantardini@ruhr-uni-bochum.de
[3] *Università degli Studi di Milano, Italy* andreas.veeser@unimi.it

We analyze the interplay of the time derivative ∂_t and the space discretization for parabolic initial-boundary value problems like

$$\partial_t u - \Delta u = f \text{ in } \Omega \times (0,T), \quad u = 0 \text{ on } \partial\Omega \times (0,T) \quad u(\cdot,0) = w \text{ on } \Omega.$$

Our focus is on quasi-optimality and best error localization in the spirit of [3], addressing time-independent and time-dependent spatial discretizations.

The key tool of our analysis is the inf-sup theory, with the following formula from [1, 2] for the quasi-optimality constant, which is of independent interest:

$$C_{\text{qopt}} = \sup_{\varphi \in M_2} \frac{\sup_{u \in H_1 : \|u\|_1 = 1} b(u,\varphi)}{\sup_{U \in M_1 : \|U\|_1 = 1} b(U,\varphi)},$$

where b is a continuous bilinear form on the Hilbert spaces H_1 and H_2 satisfying the inf-sup conditions and $M_i \subset H_i$, $i = 1, 2$, are subspaces.

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[3] Andreas Veeser, *Approximating gradients with continuous piecewise polynomial functions*. Found. Comput. Math. 16, 723-750, 2016.

Oscillation in a posteriori error analysis

Christian Kreuzer[1], **Andreas Veeser**[2]

[1] *Technical University of Dortmund, Fakultät für Mathematik Vogelpothsweg 87 44227 Dortmund, Germany* christian.kreuzer@tu-dortmund.de
[2] *Università degli Studi di Milano, Dipartimento di Matematica 'F. Enriques', Via C. Saldini, 50, 20133 Milano, Italy* andreas.veeser@unimi.it

A posteriori error estimators are a key tool for the quality assessment of given finite element approximations to an unknown PDE solution as well as for the application of adaptive techniques.

Typically, the estimators are equivalent to the error up to an additive term, the so called oscillation. It is a common believe that this is the price for the 'computability' of the estimator and that the oscillation is of higher order than the error. Cohen, DeVore, and Nochetto [CoDeNo:2012], however, presented an example, where the error vanishes with the generic optimal rate, but the oscillation does not. Interestingly, in this example, the local H^{-1}-norms are assumed to be computed exactly and thus the computability of the estimator cannot be the reason for the asymptotic overestimation. In particular, this proves both believes wrong in general.

In this talk, we present a new approach to posteriori error analysis, where the oscillation is dominated by the error. The crucial step is a new splitting of the data into oscillation and oscillation free data. Moreover, the estimator is computable if the discrete linear system can essentially be assembled exactly.

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On the convergence and optimality of adaptive hp-FEM

Claudio Canuto[1]

[1] *Dipartimento di Scienze Matematiche, Politecnico di Torino, I-10129 Turin, Italy*
claudio.canuto@polito.it

The design and analysis of adaptive spectral or hp-FEM discretization methods for elliptic equations poses formidable challenges, for at least two reasons: i) the optimality of the approximation should be assessed with respect to specific sparsity classes in which the best N-term approximation error decays exponentially, in addition to the standard classes of algebraic decay which are natural for finite order methods (see [1] for some representative results in this sense); and ii) the choice between applying a mesh refinement or a polynomial enrichment is a quite delicate stage in the refinement process, since early decisions in one of the two directions should be lately amenable to a correction in order to guarantee the final near-optimality of the adaptive discretization for a prescribed accuracy.

In this talk, I will report on recent joint work with R.H. Nochetto, R. Stevenson and M. Verani (see [2, 3]), as well as more recent developments and extensions. We will describe an abstract framework for adaptive finite element discretizations of hp type (hp-AFEM), which incorporates an hp-near best approximation algorithm recently developed by P. Binev. Several practical realizations of hp-AFEM will be discussed. Particular attention will be devoted to the issue of p-robustness, which suggests the adoption of appropriate a-posteriori error estimators (such as equilibrated fluxes). In the analysis of their properties, certain saturation results with respect to the polynomial degree are needed.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS01 – Innovative Numerical Methods and their Analysis for Elliptic and Parabolic PDEs

Finite element methods for parabolic problems with time dependent domain

Alfred Schmidt[1]

[1] *Center for Industrial Mathematics, University of Bremen, Bremen, Germany*
schmidt@math.uni-bremen.de

Time dependent domains arise in many real world situations and applications, examples are free boundary problems like fluid flow with free capillary surface or milling processes with material removal.

We investigate the finite element discretization of parabolic problems on time dependent domains. Approximation of the domain can be done either with a moving mesh approach, or a subdomain approach with or without cut cells. Corresponding FE approximations are studied and numerical simulations are presented.

Applications with industrial background consist typically of coupled systems of PDEs. We consider in particular the simulation and optimization of thermal distortions in milling processes and melting/solidification with free liquid surface.

This is partly joint work with Mischa Jahn, Andreas Luttmann, and Carsten Niebuhr (all from University of Bremen) as well as Eberhard Bänsch (Friedrich-Alexander-Universität Erlangen-Nürnberg).

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS01 – Innovative Numerical Methods and their Analysis for Elliptic and Parabolic PDEs

The Ericksen Model of Liquid Crystals with Colloidal and Electric Effects

Ricardo H. Nochetto[1], **Shawn W. Walker**[2], **Wujun Zhang**[3]

[1] *Department of Mathematics and Institute for Physical Science and Technology, University of Maryland, College Park, MD, USA* rhn@math.umd.edu
[2] *Department of Mathematics and Center for Computation and Technology (CCT) Louisiana State University, Baton Rouge, LA, USA* walker@math.lsu.edu
[3] *Department of Mathematics, Rutgers University, Piscataway, NJ, USA* wujunzhang@gmail.com

We present a robust discretization of the Ericksen model of liquid crystals with variable degree of orientation coupled with colloidal effects (inclusions) and electric fields. The total energy consists of the Ericksen energy, a weak anchoring (or penalized Dirichlet) energy to model colloids, and an electrical energy for a given electric field. We describe our special discretization [1] of the total energy along with a method to compute minimizers via a discrete quasi-gradient flow algorithm which has a strictly monotone energy decreasing property. Numerical experiments are given in two and three dimensions to illustrate that the method is able to capture non-trivial defect patterns, such as the Saturn ring defect [2]. We conclude with a rigorous proof of the Γ-convergence of our discrete energy to the continuous energy.

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MS02 – Mathematical aspects for flows in fractured porous media

(Alessio Fumagalli, Eirik Keilegavlen)

Thursday, 08:30 – 10:10, Hotel Fleischers Osa

Stefano Berrone – *Overcoming mesh constraints in large scale flow and transport simulations in poro-fractured media*

Ivar Stefansson – *Handling of Fractures and Intersections in Finite Volume Discretizations*

Roland Masson – *Hybrid dimensional two-phase flow in fractured porous media*

Runar Berge – *Hydraulic stimulation and friction laws for fracture deformation – a numerical study*

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS02 – Mathematical aspects for flows in fractured porous media

Overcoming mesh constraints in large scale flow and transport simulations in poro-fractured media

Stefano Berrone[1,2], **Andrea Borio**[1,3], **Sandra Pieraccini**[1,4], **Stefano Scialò**[1,5], **Fabio Vicini**[1,6]

[1] *Dipartimento di Scienze Matematiche, Politecnico di Torino, Italy*
[2] stefano.berrone@polito.it, [3] andrea.borio@polito.it,
[4] sandra.pieraccini@polito.it, [5] stefano.scialo@polito.it,
[6] fabio.vicini@polito.it

Large scale subsurface flow and transport simulations are characterized by several modeling, numerical, and computational difficulties. In particular we focus on geometrical complexities of fractured media, uncertainty of geometrical and hydro-geological parameters, and large scale problems. When considering realistic problems in the fields of enhanced Oil & Gas production, geothermal applications, geological storage of either nuclear waste or carbon dioxide, a large number of simulations at the scale of a geological basin are typically necessary. In order to properly take into account the strong and highly variable directionality of the underground flows, an explicit representation of the rock fractures crossing the basin is required, as fractures provide preferable flows paths. The rock fractures usually intersect each other in a dense and chaotic way. In this context, the possibility to apply a Galerkin method for the discretization of the differential models avoiding mesh generation problems is of paramount importance. In [1, 3] the authors propose a PDE-constrained optimization approach to flow simulations on arbitrary DFNs, in which neither fracture/fracture nor fracture/trace mesh conformity is required. The approach totally circumvents the problem of mesh generation, without any need of geometrical modification. Following a more classical approach Virtual Elements have been effectively used when dealing with complex configurations [4]. Ovecoming mesh generation problems is a crucial issue both for addressing computations on huge networks, and for performing massive simulations for uncertainty quantification [4] in stochastically generated networks.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS02 – Mathematical aspects for flows in fractured porous media

Handling of Fractures and Intersections in Finite Volume Discretizations

Ivar Stefansson[1], **Inga Berre**[1], **Eirik Keilegavlen**[1]

[1] *Department of Mathematics, University of Bergen, Norway* ivar.stefansson@uib.no

Finite Volume methods with two- or multi-point flux approximations are among the most widely used discretizations for flow simulations in porous media. The popularity is partly explained by the local mass conservation. For the two-point approximations, the implementation is also reasonably straightforward, making it into the principal workhorse for a range of porous media flow problems. Because of the importance of mass conservation, it is sensible to evaluate flow methods not only in terms of pressure fields, but also indirectly through transport simulations on the flow fields they produce. By examining accumulations of tracer, we aim at revealing details and differences which may be critical to the concentration distribution, but almost indiscernible in pressure comparisons.

When fractures are present in the domain, additional complexity is added to the problem. The two main concerns are complex geometries which challenge the grid generation and the high spatial and parametrical ratios between matrix and fractures. A common approach is to model them as lower-dimensional inclusions. Aligning the faces of the full dimension with the fractures results in hybrid-dimensional methods with conforming meshes. In the implementation framework used in this work, we partition the domain into a number of subdomains of different dimension. We assume that the discretization couplings between two neighbouring subdomains can be performed independently from the rest of the domain. This restricts us from certain coupling discretizations (the MPFA among them). On the other hand, different discretizations in a subdomain and the couplings it participates in is straightforward. This means, for instance, that an existing MPFA code may be "glued together" by a TPFA coupling. We investigate and discuss the assumptions necessary for this simplification to be justified.

The main drawback of the TPFA is its breakdown if the discretization grid is not aligned with the permeability. This is where the MPFA methods should be considered, as they handle anisotropy at the cost of larger discretization stencils and somewhat more involved implementation. Using a method with MPFA in all dimensions (matrix, fractures and intersections) but TPFA in the coupling between them, we will in particular explore the relevance of fracture anisotropy: when and to what extent this justifies the costlier MPFA scheme.

The co-dimension one approach is beneficial compared to the equidimensional one in terms of gridding and cell size. However, the lower-dimensional cells will typically be significantly smaller than the rest, impairing solution matrix condition numbers and, in the case of transport simulations, time step restrictions. Particularly restrictive are the discretization cells at fracture intersections, which typically are several orders of magnitude smaller than the full-dimensional ones.

One remedy for FV schemes is the elimination of these cells introduced by Karimi-Fard et al. in 2004 and extended by Sandve et al. in 2012. While producing satisfactory results in many cases, the procedure does not handle the intersection of fractures of highly varying permeability. We suggest a new approach to this elimination scheme. By discretizing the domain with the intersection cells and then performing a static condensation to remove them, we are able to handle also fractures of different permeability. Moreover, we show how the original scheme can be interpreted as the limiting case of the new interpretation as the intersection permeability goes to infinity. The condensation also provides a natural way of back-calculating the pressure values at the intersections through the condensation matrix.

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September 25 – 29, 2017, Voss, Norway
MS02 – Mathematical aspects for flows in fractured porous media

Hybrid dimensional two-phase flow in fractured porous media

K. Brenner[1], J. Hennicker[2], R. Masson[3], P. Samier[4]

[1] *Université Côte d'Azur, LJAD-Inria-CNRS, Nice, France,* konstantin.brenner@unice.fr
[2] *Université Côte d'Azur, LJAD-Inria-CNRS, Nice, and CSTJF, TOTAL S.A., Pau, France* julian.hennicker@unice.fr
[3] *Université Côte d'Azur, LJAD-Inria-CNRS, Nice, France* roland.masson@unice.fr
[4] *CSTJF, TOTAL S.A., Pau, France* pierre.samier@total.com

In this work, we extend the single phase Darcy flow model proposed in [1,2] to two phase flow. We thus provide a model for two phase Darcy flow through discrete fracture networks (DFN) in porous media, in which the d - 1 dimensional flow in the fractures is coupled with the d dimensional flow in the matrix, leading to the so called hybrid dimensional Darcy flow model.

The model accounts for fractures acting either as drains or as barriers, since it allows pressure jumps at the matrix-fracture interfaces. The model also permits to treat gravity dominated flows as well as discontinuous capillary pressure curves at the material interfaces.

The discretization is presented in the abstract gradient scheme framework accounting for a large range of conforming and non conforming schemes. The convergence of the discrete solution to a weak solution of the model is obtained provided that coercivity, consistency, limit conformity and compacity assumptions are satisfied [3].

Using the Vertex Approximate Gradient scheme, we present several test cases including gravity and capillary effects. They exhibit the importance of keeping the interface unknowns and the nonlinear fluxes continuity at the interface even in the case of fractures acting as drains.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS02 – Mathematical aspects for flows in fractured porous media

Hydraulic stimulation and friction laws for fracture deformation – a numerical study

Runar Lie Berge[1], **Inga Berre**[2], **Eirik Keilegavlen**[2], **Jan Martin Nordbotten**[2]

[1] *University of Bergen, Norway* runar.berge@uib.no
[2] *University of Bergen, Norway* inga.berre@uib.no
[3] *University of Bergen, Norway* Eirik.Keilegavlen@uib.no
[4] *University of Bergen, Norway* Jan.Nordbotten@uib.no

Injection of fluids related to geothermal energy extraction, CO-storage, enhanced oil recovery and energy storage can activate natural fractures due to hydraulic stimulation. For crystalline rock, fractures will dominate subsurface flow patters as well as rock mechanical deformation, and shear displacement of a fracture can increase its permeability by orders of magnitude.

Elevated pressures perturbs the effective stress and reduce the resistance of a fracture to sliding. Focusing on the choice of friction model for deformation of explicitly represented fractures, we present a model for coupled flow, fracture deformation and rock matrix deformation. A finite-volume discretization is used for both mechanics and flow, based on a discrete fracture-matrix model, where fractures are explicitly discretized in a conforming grid. We investigate several test cases, from a simple case to a case motivated by a real fracture network in 3D.

MS03 – Modeling and Simulation of Sea Ice

(Madlen Kimmritz, Thomas Richter)

Thursday, 15:30 – 17:10, Hotel Fleischers Osa

Martin Losch – *A parallel Jacobian-free Newton-Krylov solver for a coupled sea ice-ocean model*

Carolin Mehlmann – *A Newton multigrid solver for viscous-plastic sea ice models*

Madlen Kimmritz – *On explicit methods for solving the sea ice momentum equation using the EVP rheology.*

James Williams – *The effects of increasing spatial resolution on the sea-ice drift speed and energy budget in the viscous-plastic sea-ice model.*

Thursday, 17:25 – 18:15, Hotel Fleischers Osa

Fleurianne Bertrand – *A Least Squares Finite Element Method for Coupled Sea Ice and Subsurface flow*

Timothy Williams – *neXtSIM: A new Lagrangian sea-ice model*

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS03 – Modeling and Simulation of Sea Ice

A parallel Jacobian-free Newton-Krylov solver for a coupled sea ice-ocean model

Martin Losch[1], **Annika Fuchs**[1], **Jean-François Lemieux**[2]

[1] *Alfred-Wegener-Institut, Helmholtz Zentrum für Polar- und Meeresforschung, Postfach 120161, 27515 Bremerhaven, Germany* Martin.Losch@awi.de
[2] *Recherche en Prévision Numérique environnementale/Environnement Canada, 2121 route Transcanadienne, Dorval, Qc, Canada H9P 1J3*

The most common representation of sea ice dynamics in climate models assumes that sea ice is a quasi-continuous non-normal fluid with a viscous-plastic rheology. This rheology leads to non-linear sea ice momentum equations that are notoriously difficult to solve. Recently a Jacobian-free Newton-Krylov (JFNK) solver was shown to solve the equations accurately at moderate costs. This solver is extended for massive parallel architectures and vector computers and implemented in a coupled sea ice-ocean general circulation model for climate studies. Numerical performance is discussed along with numerical difficulties in realistic applications with up to 1920 CPUs. The parallel JFNK-solver's scalability competes with traditional solvers although the collective communication overhead starts to show a little earlier. When accuracy of the solution is required (i.e. reduction of the residual norm of the momentum equations of more that one or two orders of magnitude) the JFNK-solver is unrivalled in efficiency. The new implementation opens up the opportunity to explore physical mechanisms in the context of large scale sea ice models and climate models and to clearly differentiate these physical effects from numerical artifacts.

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS03 – Modeling and Simulation of Sea Ice

A Newton multigrid solver for viscous-plastic sea ice models

C. Mehlmann, T. Richter

Otto-von-Guericke-Universität Magdeburg, Germany carolin.mehlmann@ovgu.edu
thomas.richter@ovgu.de

The sea ice momentum equation with a viscous-plastic (VP) rheology is a strongly nonlinear partial differential equation. The nonlinearity coming form the VP rheology is servere.

$$\begin{aligned} 0 &= \rho_{\text{ice}} H \left(\partial_t \mathbf{v} + f_c \vec{e}_r \times (\mathbf{v} - \mathbf{v}_{ocean})\right) - \operatorname{div} \boldsymbol{\sigma}(\mathbf{v}) - \boldsymbol{\tau}_{\text{ocean}}(\mathbf{v}) - \boldsymbol{\tau}_{\text{atm}} \\ \boldsymbol{\sigma} &= 2\eta(\nabla \mathbf{v} + \nabla \mathbf{v}^T) + (\zeta - \eta)\operatorname{div}(\mathbf{v}) I - \frac{P}{2} I \\ 4\eta = \zeta &= \frac{P}{2}\left((\partial_x \mathbf{v}_1 + \partial_y \mathbf{v}_2)^2 + \frac{1}{4}(\partial_x \mathbf{v}_1 - \partial_y \mathbf{v}_2)^2 + (\partial_x \mathbf{v}_2 + \partial_y \mathbf{v}_1)^2\right)^{-\frac{1}{2}} \end{aligned} \tag{1}$$

The momentum equation is very difficult to solve. The development of fast and robust solvers is still a big issue. In this contribution we present a new efficient Newton multigrid solver.

We use a finite element approach in space and an implicit Euler scheme in time. To approximate the nonlinear problem we apply a modified Newton solver [1]. The idea of the solver is to combine a fixed-point iteration (Picard solver) with a Newton method. We analytically derive the Jacobian matrix and show its positive definiteness. The positive definiteness guarantees global convergence of a properly damped (e.g. line search) Newton iteration. The Jacobian matrix is split into a positive definite part, which is assumed to give stable convergence and a negative semidefinite part, which might be troublesome. The negative semidefinite part is adaptively damped if convergence worsens and the Newton solver turns towards a Picard iteration. We show the improved robustness of the modified Netwon solver on an idealized test case and compare it to a full Newton scheme.

In every Newton step a linear system of equations must be solved. We introduce a geometric multigrid solver [2] as preconditioner to accelerate the solution of the linear problems. We show that the convergence rate of the multigrid method is robust with respect to mesh refinement. This makes it an appealing method for high resolution simulations. We validate the robustness of the linear solver and compare the multigrid preconditioner with an ILU preconditioner. In particular on fine meshes multigrid preconditioning can substantially reduce the computational effort and decreases iteration counts by up to 80%.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS03 – Modeling and Simulation of Sea Ice

On explicit methods for solving the sea ice momentum equation using the EVP rheology.

Madlen Kimmritz[1,2], **Sergey Danilov**[3,4], **Martin Losch**[5]

[1] *Nansen Environmental and Remote Sensing Center, Bergen, Norway* madlen.kimmritz@nersc.no
[2] *Bjerknes Centre for Climate Research, Bergen, Norway*
[3] *Alfred Wegener Institute, Bussestrasse 24, D-27570 Bremerhaven* sergey.danilov@awi.de
[4] *A. M. Obukhov Institute of Atmospheric Physics RAS, Moscow, Russia*
[5] *Alfred Wegener Institute, Bussestrasse 24, D-27570 Bremerhaven* martin.losch@awi.de

Most dynamic sea ice models for climate type simulations are based on the viscous-plastic (VP) rheology. The resulting stiff system of partial differential equations for ice velocity is either solved implicitly at great computational cost, or explicitly with added pseudo-elasticity (elastic-viscous-plastic, EVP). The modification of the EVP (mEVP) approach as done by Bouillon et al., Ocean Modell., 2013 seeks to improve the convergence of the EVP method by re-interpreting it as a pseudotime VP solver.

In this contribution we analyse this scheme focussing on convergence to the VP solution and stability requirements in a simplified setting. We highlight sensitivities to different grid types, and introduce an adaptive version (aEVP) of the mEVP scheme to automatically satisfy local stability constraints such that convergence can be sped up locally.

For an Arctic sea ice simulation we compare the solutions of the explicit solvers (aEVP and mEVP) against each other and against solutions of an implicit VP solver, the Jacobian-free Newton–Krylov (JFNK) solver, which, by construction, provides a converged solution to the equations of viscous-plastic sea ice dynamics. We discuss convergence issues related to the use of the replacement pressure.

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ENUMATH 2017
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MS03 – Modeling and Simulation of Sea Ice

The effects of increasing spatial resolution on the sea-ice drift speed and energy budget in the viscous-plastic sea-ice model.

James Williams[1], **L. Bruno Tremblay**[2]

[1] *NASA Goddard Institute of Space Studies, New York, NY, USA*
James.Williams@mail.mcgill.ca

[2] *McGill University, Montréal , QC, Canada*
Bruno.Tremblay@mcgill.ca

The viscous-plastic sea-ice model is being run at increasingly high spatial and temporal resolution, as the necessary computing resources become readily available. In this study, we show that in the case of pure shear failure, the analytical solution to the model equations is inherently discontinuous due to the use of no-slip boundary conditions. As the model resolution increases this discontinuity becomes better resolved on the model grid, resulting in changes to the energy budget and the domain averaged sea-ice velocity. In particular, we find a 32% increase in the mean sea-ice drift speed when the spatial resolution is increased from 40 km to 5 km. This increase is largely due to a sharpening of the simulated velocity gradient near the boundaries which results in a net increase in input power by the wind, and a net reduction in the relative importance of frictional shear dissipation. We find that at all spatial resolutions the simulated velocity field largely underestimates the analytical free-drift solution, albeit lesser so as the resolution is increased. We show that the sea-ice shear strength can effectively be used to adjust the sea-ice drift speed in the simulation presented. The model equations remain continuous when convergence is the primary mode of failure. In this case, the structure of the thickness and concentration fields effectively sets the velocity gradient near the boundary. Thus there is no significant dependence of the simulated velocity and thickness fields as the spatial resolution is varied given that the plastic wave remains resolved on the model grid. We discuss the relevance of these findings with respect to model calibration and numerical efficiency of high resolution Arctic sea-ice models. Finally, we argue that the application of no-slip boundary boundary conditions to sea-ice dynamics does not have a physical basis.

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MS03 – Modeling and Simulation of Sea Ice

A Least Squares Finite Element Method for Coupled Sea Ice and Subsurface flow

Fleurianne Bertrand[1], **Steffen Münzenmaier**[2]

[1] *University Duisburg-Essen* fleurianne.bertrand@uni-due.de
[2] *University Duisburg-Essen* steffen.muenzenmaier@uni-due.de

Consequently to a research voyage on the SA Agulhas II, samples of the thin layer of ice covering the Antarctic ocean (sea ice) were collected and analysed along two spatial transects into the marginal ice zone (MIZ). The sea ice displacements and drift movements were recorded. Since longitudinal and transverse stresses and vertical stress gradients can be neglected, the sea ice layer can be modelled with the shallow ice equations. These are widely used for the simulation of ice that moves significantly slower than the surrounding environnement. The flows are coupled along an interface where we enforce continuity of pressure and continuity of flux. These assumptions lead to a nonlinear system of equations which can be treated by a (Gauss-)Newton method. The hyperbolic character of the shallow ice equations has to be treated accordingly. A least squares finite element method, providing an inherent error estimator and a positive definite system, is used for the spatial discretization with continuous piecewise polynomials combined with Raviart-Thomas elements.

ENUMATH 2017
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MS03 – Modeling and Simulation of Sea Ice

A sea ice model with wave-ice interactions on a moving mesh

T. Williams[1], **S. Bouillon**[2], **A. Samaké**[3], **P. Rampal**[4], **E. Ólason**[5]

[1] *Nansen Enviromental and Remote Sensing Center, Norway* timothy.williams@nersc.no
[2] *Nansen Enviromental and Remote Sensing Center, Norway* sylvain.bouillon@nersc.no
[3] *Nansen Enviromental and Remote Sensing Center, Norway; University of Bamako, Bamako, Mali* abdoulaye.samake@nersc.no
[4] *Nansen Enviromental and Remote Sensing Center, Norway* pierre.rampal@nersc.no
[5] *Nansen Enviromental and Remote Sensing Center, Norway* einar.olason@nersc.no

The neXtSIM (neXt generation Sea Ice Model) sea ice model runs the Maxwell-EB rheology solved with finite element methods on a triangular mesh. It also has thermodynamic effects and a slab ocean included beneath, as well as wave-ice interactions (ice break-up by waves, ice drift due to the wave radiation stress).

An ALE (Arbitrary Lagrangian/Eulerian) scheme has now been implemented in neXtSIM, so that the mesh is usually moving as time goes on. As part of an investigation about the best strategy for coupling the waves-in-ice module (WIM) to neXtSIM, the WIM may now be run on the neXtSIM mesh.

In this talk we give an overview of both neXtSIM and the WIM, and also some results comparing the different coupling strategies for the WIM.

MS04 – Polyhedral methods and applications

(Paola Antonietti, Stefano Berrone, Daniele Di Pietro, Marco Verani)

Tuesday, 08:30 – 10:10, Hotel Fleischers Kvitanosi

Alexandre Ern – *A Multi-scale Hybrid High-Order method*

Michele Botti – *A Hybrid High-Order method for nonlinear elasticity*

Pierre Cantin – *A compact-stencil scheme on polyhedral meshes for transport equations*

Florent Chave – *A Hybrid High-Order method for Darcy flows in fractured porous media*

Wednesday, 08:30 – 10:10, Hotel Fleischers Kvitanosi

Ilaria Perugia – *Virtual Element Methods for the Helmholtz Problem*

Franco Dassi – *Hitchhiker's guide© to the Virtual Element Method in 3D*

Claudia Chinosi – *A family of virtual elements for the Reissner-Mindlin plate*

Francesca Gardini – *Virtual Element Methods for second order elliptic eigenvalue problems*

Thursday, 15:30 – 17:10, Hotel Fleischers Kvitanosi

Andrew Gillette – *A Plethora of Basis Functions for Quadrilaterals*

Alessio Fumagalli – *Dual virtual element method for fractured geothermal systems*

Andrea Borio – *The Virtual Element Method for the transport of passive scalars in Discrete Fracture Networks*

Daniele Prada – *FETI-DP preconditioners for the Virtual Element Method in two and three dimensions*

ENUMATH 2017
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MS04 – Polyhedral methods and applications

A Multi-scale Hybrid High-Order method

Matteo Cicuttin[1], **Alexandre Ern**[1], **Simon Lemaire**[2]

[1] *Université Paris-Est, CERMICS (ENPC) and INRIA, 77455 Marne-la-Vallée cedex 2, France*
matteo.cicuttin@enpc.fr, alexandre.ern@enpc.fr

[2] *École Polytechnique Fédérale de Lausanne (EPFL), SB-MATH-ANMC, 1015 Lausanne, Switzerland*
simon.lemaire@epfl.ch

Hybrid High-Order (HHO) methods have been recently introduced in the context of linear elasticity [1] and scalar diffusion [2] PDEs. In this work, we devise a multi-scale HHO method. The method hinges on (hybrid) discrete unknowns that are polynomials attached to mesh elements and faces, and on a multi-scale reconstruction operator, that maps onto a fine-scale space spanned by oscillatory basis functions. The method handles arbitrary orders of approximation $k \geq 0$, and is applicable on general meshes. For face-based unknowns that are polynomials of degree k, we devise two versions of the method, depending on the polynomial degree $(k-1)$ or k of cell-based unknowns. We prove, in the case of periodic coefficients, an energy-error estimate of the form $\left(\epsilon^{1/2} + H^{k+1} + \epsilon^{1/2} H^{-1/2}\right)$. More details can be found in [3].

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS04 – Polyhedral methods and applications

A Hybrid High-Order method for nonlinear elasticity

Michele Botti[1], **Daniele A. Di Pietro**[2], **and Pierre Sochala**[3]

[1] *Université de Montpellier, IMAG, Place Eugène Bataillon, 34095 Montpellier, France*
michele.botti@umontpellier.fr

[2] *Université de Montpellier, IMAG, Place Eugène Bataillon, 34095 Montpellier, France*
daniele.di-pietro@umontpellier.fr

[3] *Bureau de Recherches Géologique et Minières, 3 Avenue Guillemin, 45060 Orléans, France*
p.sochala@brgm.fr

We formulate a novel Hybrid High-Order discretization of a class of (linear and) nonlinear elasticity models in the small deformation regime which are of common use in solid mechanics. The proposed HHO discretization is inspired by the recent works on linear elasticity [2] and Leray–Lions operators [1]. The method is valid in two and three space dimensions, it supports general meshes including polyhedral elements and nonmatching interfaces, enables arbitrary approximation order, and has a reduced cost thanks to the possibility of statically condensing a large subset of the unknowns for linearized versions of the problem. Additionally, the method satisfies a local principle of virtual work on each mesh element, with interface tractions that obey the law of action and reaction. For monotone stress-strain relations, convergence to minimal regularity solutions is proved following the ideas of [3]. Moreover, optimal error estimates hold under the additional conditions of Lipschitz continuity and strong monotonicity on the stress-strain law. The performance of the method is investigated on a complete panel of model problems using two types of nonlinear stress-strain laws.

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MS04 – Polyhedral methods and applications

A compact-stencil scheme on polyhedral meshes for transport equations

P. Cantin[1], **J. Bonelle**[2], **E. Burman**[3], **A. Ern**[4]

[1] *Facultad de Matematicas, Pontificia Univ. Catolica de Chile, Chile* pircantin@gmail.com
[2] *EDF R&D, 6 quai de Watier, 78401 Chatou BP 49, France* jerome.bonelle@edf.fr
[3] *Dept. of Mathematics, University College of London, UK* e.burman@ucl.ac.uk
[4] *CERMICS (ENPC), 77455 Marne la Vallée Cedex 2, France* ern@cermics.enpc.fr

In this work [1], we present a new vertex-based scheme for the steady transport problem on polyhedral meshes. This scheme extends the stabilized Lagrange finite element on general meshes while containing the total number of degrees of freedom (dofs), *i.e.* considering only those attached to mesh vertices.

The key idea is to consider scalar dofs attached to both mesh vertices and mesh cells (as for VAG schemes [2]). Then, taking inspiration from the recent analysis of composite finite element schemes in [3], the scheme is only partially stabilized using the Continuous Interior Penalty approach (see [4]) so as to not hamper the possibility to eliminate locally cell-based unknowns. Well-posedness is obtained from an inf-sup condition and a priori error estimates are inferred for smooth and rough solutions. Numerical results are finally presented on three-dimensional polyhedral meshes, and the benefit of our approach is illustrated in terms of computational cost.

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A Hybrid High-Order method for Darcy flows in fractured porous media

Florent Chave[1,2], **Daniele A. Di Pietro**[1], **Luca Formaggia**[2]

[1] *University of Montpellier, Institut Montpelliérain Alexander Grothendieck, 34095 Montpellier, France* florent.chave@umontpellier.fr, daniele.di-pietro@umontpellier.fr

[2] *Politecnico di Milano, MOX, 20133 Milano, Italy* luca.formaggia@polimi.it

We develop a novel Hybrid High-Order method for the simulation of Darcy flows in fractured porous media. The discretization hinges on a mixed formulation in the bulk region and on a primal formulation inside the fracture. Salient features of the method include a seamless treatment of non-conforming discretizations of the fracture, as well as the support of arbitrary approximation orders on fairly general meshes. For the version of the method corresponding to a polynomial degree $k \geq 0$, we prove convergence in h^{k+1} of the discretization error measured in an energy-like norm. In the error estimate, we explicitly track the dependence of the constants on the problem data, showing that the method is fully robust with respect to the heterogeneity of the permeability coefficients, and it exhibits only a mild dependence on the square root of the local anisotropy of the bulk permeability. The numerical validation on a comprehensive set of test cases confirms the theoretical results.

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Virtual Element Methods for the Helmholtz Problem

Ilaria Perugia[1], **Alexander Pichler**[2], **Paola Pietra**[3], **Alessandro Russo**[4]

[1] *Faculty for Mathematics, University of Vienna, Austria* ilaria.perugia@univie.ac.at
[2] *Faculty for Mathematics, University of Vienna, Austria* alex.pichler@univie.ac.at
[3] *IMATI-CNR "Enrico Magenes", Pavia, Italy* pietra@imati.cnr.it
[4] *Department of Mathematics and its Applications, University of Milano Bicocca, Italy* alessandro.russo@unimib.it

The virtual element method (VEM) is a generalization of the finite element method introduced by Beirão da Veiga, Brezzi, Cangiani, Manzini, Marini, and Russo in 2013, which takes inspiration from modern mimetic finite difference schemes, and allows one to use very general polygonal/polyhedral meshes.

This talk is concerned with new methods for the discretisation of the Helmholtz problem based on inserting plane wave basis functions within the VEM framework, in the spirit of the partition of unity method. The main ingredients of these plane wave VEMs are: *i)* a low order VEM space, whose basis functions are associated to the mesh vertices, form a partition of unity, and are not explicitly computed in the element interiors; *ii)* a local projection operator onto a plane wave space; *iii)* an approximate stabilization term. The VEM framework allows to impose interelement continuity, while the plane waves determine high-order accuracy. We will present C^0- and C^1-continuous versions of plane wave VEMs and discuss their numerical performance.

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Hitchhiker's guide© to the Virtual Element Method in 3D

Lourenço Beirão da Veiga[1], **Franco Dassi**[2], **Alessandro Russo**[3]

[1] *University of Milano-Bicocca, Italy, and IMATI-CNR, Italy* lourenco.beirao@unimib.it
[2] *University of Milano-Bicocca, Italy* franco.dassi@unimib.it
[3] *University of Milano-Bicocca, Italy, and IMATI-CNR, Italy* alessandro.russo@unimib.it

The Virtual Element Method (VEM) is a novel way to solve problems in Partial Differential Equations [1]. It is sharing a good degree of success in the recent years due to its flexibility and robustness.

In this talk we will focus on the three dimensional case. In particular, we will show how the developments for the two-dimensional case can be extended to the three-dimensional one with general order of accuracy [2, 3].

This construction will be numerically supported by several examples on different kind of polyhedral meshes and PDEs, from a standard Laplace problem to a more complex convection-reaction-diffusion problem with variable coefficients.

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A family of virtual elements for the Reissner-Mindlin plate

C. Chinosi[1]

[1] *Dipartimento di Scienze e Innovazione Tecnologica (DISIT) Università del Piemonte Orientale Viale Teresa Michel,11-15121 Alessandria, Italy* claudia.chinosi@uniupo.it

The Virtual Element Method (VEM) has been introduced very recently (see [1]) as an extension of Finite Element Methods to general polygonal and polyhedral elements. The interest in numerical methods that can make use of general polytopal meshes has recently grown in the mathematical and engineering literature due to the great advantages related to the use of general grids, such as high flexibility in mesh generation and robustness to distortion. Since its birth the Virtual Element Method has been applied successfully to a wide range of problems (see for instance [3] and the references therein). In particular it has been applied for the approximation of the plate bending problem both in the Kirchhoff-Love formulation (see [4], [5]) as in the Reissner-Mindlin formulation. In this case a family of virtual elements based on the MITC approach of the FEM context (see [2]), has been introduced (see [6]). The theoretical results assure that the introduced elements are locking-free and imply convergence with optimal rate in the H^1-norm, uniformly in the thickness. In order to assess the convergence and the robustness properties of the scheme we have implemented two elements of the family, corresponding to the degree of accuracy $k = 1$ and $k = 2$, respectively. We performed some numerical tests on different families of meshes and we realized a comparison between the virtual elements and the corresponding finite elements. Here we will present the elements of the family and the obtained numerical results that will confirm the theoretical predictions.

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Virtual Element Methods for second order elliptic eigenvalue problems

F. Gardini[1], **G. Vacca**[2]

[1] *Diaprtimento di Matematica, Università degli Studi di Pavia, Italy*
francesca.gardini@unipv.it

[2] *Dipartimento di Matematica e delle Applicazioni, Università degli Studi di Milano Bicocca, Italy*
giuseppe.vacca@unimib.it

The Virtual Element Method (VEM) is a new approximation technique recently introduced in [1] which has been applied to several problems, such as linear elasticity, plate bending, mixed and parabolic problems, just to name a few. In its abstract formulation the method is a generalization of the finite element method which allows, nevertheless, the use of general polygonal and polyhedral meshes without having to integrate complex non-polynomial functions on the elements.

In this talk we analyze the Virtual Element Method applied to elliptic eigenvalue problems. As a model problem we consider the Laplace eigenvalue problem. The discretization of the problem requires the introduction of two discrete bilinear forms, one being the approximated grad-grad form and the other being a discrete version of the L^2-inner product. The latter one is built using the techniques of [2]. It is shown that the Virtual Element Method provides optimal convergence rates both in the approximation of the eigenfunctions and of the eigenvalues. A wide set of numerical tests confirm the theoretical analysis.

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A Plethora of Basis Functions for Quadrilaterals

Andrew Gillette

Department of Mathematics, University of Arizona, USA agillette@math.arizona.edu

Quadrilateral elements serve as a testing ground for the construction of basis functions on more general polygons. In this talk, we will examine some approaches to defining basis functions on general quadrilateral elements with specific applications in mind, such as higher order, vector-valued, serendipity-type, and adaptive elements. We will discuss the comparative advantages of each approach and how they might be leveraged to more general polygons and polyhedra.

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Dual virtual element method for fractured geothermal systems

Alessio Fumagalli[1], **Eirik Keilegavlen**[2], **Pål Næverlid Sævik**[3]

[1] *Department of Mathematics, University of Bergen, Norway* alessio.fumagalli@uib.no
[2] *Department of Mathematics, University of Bergen, Norway* eirik.keilegavlen@uib.no
[3] *Department of Mathematics, University of Bergen, Norway* pal.saevik@uib.no

The presence of a well connected network of fracture is of paramount importance in the exploitation of geothermal energy in deep system. Fractures may behave as open channels dramatically increasing the efficiency of the system, or as barriers excluding parts of the latter. Fractures also boost the heat exchange between the rock matrix and the fluid injected. The development of accurate mathematical models and robust numerical schemes are thus a key ingredient to exploit at best geothermal systems.

Because of economical advantages and accuracy, the collection of fractures is mainly based on the interpretation of outcrops. This approach has some limitations related to local lack of data and poor outcrop exposure. The common technique to generate, based on stochastic realizations, new fractures is seldom consistent with the connectivity of the original system, affecting the flow property of the synthetic network. A topology based approach, [1, 2], is thus essential to include this information and to overcome this problem.

In this work we consider a hierarchy of models, for fluid and heat flow, to employ a discrete fracture matrix model, including matrix, fractures, and intersections. Fractures may impose constraints to the gridding, resulting in high number of cells. We consider a coarsening based on ideas from the algebraic multigrid literature, obtaining cells of arbitrary shapes. On this grid, we discretize the equations using the mixed virtual element method, which is ideally suited to handle the grids produced [3, 4, 5]. Fractures are stochastically generated and properly modified to achieve the target topology. Several numerical tests demonstrate the effectiveness of the proposed approach.

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The Virtual Element Method for the transport of passive scalars in Discrete Fracture Networks

Andrea Borio[1], **Stefano Berrone**[1], **Matías Fernando Benedetto**[2], **Sandra Pieraccini**[1], **Stefano Scialò**[1]

[1] *Politecnico di Torino – Corso Duca degli Abruzzi, 24 – 10129 Torino, Italy.*
andrea.borio@polito.it

[2] *Universidad de Buenos Aires. Facultad de Ingeniería; CONICET - INTECIN, Grupo LMNI. Buenos Aires, Argentina.*

The simulation of flows in fractured media is a very interesting topic, with many industrial applications, for instance in petroleum engineering and geothermal heating systems. In this context, the model of Discrete Fracture Networks is used when the rock matrix can be considered impervious. These domains are stochastically generated sets of intersecting planar polygons, with geometrical configurations that usually a very high computation effort and sometimes cannot be tackled with standard discretization methods. In [1, 2, 4], the Virtual Element method is used to discretize the hydraulic head on each fracture, exploiting its geometrical flexibility to tackle the cited issues. The same approach can be used to simulate the time-dependent evolution of passive scalars within DFN, driven by the Darcy velocity, obtained from the distribution of hydraulic head.

The talk will deal with an efficient approach to the simulation of transport of passive scalars in DFN using mixed virtual elements to obtain a good approximation of the Darcy velocity that is then used as transport velocity in a parabolic advection-reaction-diffusion equation. The latter is discretized with primal virtual elements, using the SUPG stabilized formulation described in [3] to avoid numerical instabilities in convection dominated problems.

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FETI-DP preconditioners for the Virtual Element Method in two and three dimensions

Daniele Prada[1], **Silvia Bertoluzza**[1], **Micol Pennacchio**[1]

[1] *Istituto di Matematica Applicata e Tecnologie Informatiche "Enrico Magenes"*
Consiglio Nazionale delle Ricerche
v. Ferrata 1, 27100 Pavia, Italy

daniele.prada@imati.cnr.it
silvia.bertoluzza@imati.cnr.it
micol.pennacchio@imati.cnr.it

We build and analyze a state-of-the-art domain decomposition method, the Finite Element Tearing and Interconnecting Dual Primal (FETI-DP) approach [1], for the efficient and robust solution of very large linear systems arising from elliptic problems discretized by the Virtual Element Method (VEM) [2].

Our theoretical estimates show that the condition number of the FETI-DP interface problem has a polylogarithmic dependence on the ratio H/h of subdomain and element sizes. The influence of the geometry of the elements on these estimates is discussed. The theory is confirmed by numerical experiments on a linear elliptic problem with highly heterogeneous diffusion coefficients in both two and three dimensions. This demonstrates that the FETI-DP method is numerically scalable with respect to both the problem size and number of subdomains, and its performance is not affected by jumps in the diffusion coefficients, thereby fostering the use of the VEM in real world applications.

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MS05 – Generalized Sampling, Reduced Modeling and sparse recovery

(Olga Mula, Clarice Poon)

Wednesday, 15:55 – 17:35, Hotel Fleischers Bergslien

Simone Brugiapaglia – *Correcting for unknown errors in sparse high-dimensional function approximation*

Elizabeth Qian – *A Certified Reduced Basis Trust Region Approach to PDE-Constrained Optimization*

Albert Cohen – *Measurement selection for reduced model based state estimation*

Jose Luis Romero – *Nonuniform sampling and universality of stable sampling rates.*

Thursday, 17:25 – 18:15, Hotel Fleischers Bergslien

Tommaso Taddei – *A Reduced Basis Technique for Long-Time Unsteady Turbulent Flows*

Vegard Antun – *Uniform recovery guarantees for Walsh sampling and wavelet reconstruction*

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MS05 – Generalized Sampling, Reduced Modeling and sparse recovery

Correcting for unknown errors in sparse high-dimensional function approximation

Ben Adcock[1], **Casie Bao**[2], **Simone Brugiapaglia**[3], **Clayton G. Webster**[4]

[1] *Simon Fraser University, Canada* ben_adcock@sfu.ca
[2] *Simon Fraser University, Canada* cbao@sfu.ca
[3] *Simon Fraser University, Canada* simone_brugiapaglia@sfu.ca
[4] *Oak Ridge National Laboratory, USA* webstercg@ornl.gov

Approximating a high-dimensional function from a finite set of pointwise samples is a fundamental problem in numerical analysis. Recently, much effort has been made in the compressed sensing community on this problem in order to develop new approaches able to lessen the so-called curse of dimensionality (see [2] and references therein).

In this talk, we will review and discuss compressed sensing approaches for high-dimensional function approximation. They take advantage of tools such as orthogonal polynomials, random sampling, structured sparsity in lower (or downward closed) sets, and weighted ℓ^1 minimization. In particular, we will focus on the robustness analysis of these methods when the samples are corrupted by unknown sources of noise, such as truncation, numerical, or discretization error [1, 3].

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A Certified Reduced Basis Trust Region Approach to PDE-Constrained Optimization

Elizabeth Qian[1], **Martin Grepl**[2], **Karen Veroy**[3], **Karen Willcox**[4]

[1] *Department of Aeronautics and Astronautics, MIT, Cambridge, MA, USA* elizqian@mit.edu
[2] *Institute for Geometry and Applied Mathematics, RWTH Aachen University, Aachen, Germany* grepl@igpm.rwth-aachen.de
[3] *Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Aachen, Germany* veroy@aices.rwth-aachen.de
[4] *Department of Aeronautics and Astronautics, MIT, Cambridge, MA, USA* kwillcox@mit.edu

Parameter optimization problems constrained by partial differential equations (PDEs) appear in many science and engineering applications, including design and inverse problems. Solving these optimization problems may require a prohibitively large number of computationally expensive PDE solves, especially if there are many variable parameters. It is therefore advantageous to replace expensive high-dimensional PDE solvers (e.g. finite element) with lower-dimension surrogate models.

In this talk, we use the reduced basis (RB) model reduction method in conjunction with a trust region optimization framework to accelerate PDE-constrained parameter optimizations. New *a posteriori* error bounds on the RB cost and cost gradient for quadratic cost functionals are presented, and used to guarantee convergence to the optimum of the high-fidelity model. The proposed certified RB trust region approach builds the RB model on the fly, solving the high-fidelity model only to update the RB approximation when it is no longer sufficiently accurate. By breaking with the traditional RB offline-online decomposition, the proposed approach requires a minimal number of high-order solves.

We consider problems governed by elliptic and parabolic PDEs and present numerical results for a thermal fin model problem with six parameters.

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MS05 – Generalized Sampling, Reduced Modeling and sparse recovery

Measurement selection for reduced model based state estimation

Peter Binev[2], Albert Cohen[1], Olga Mula[3], James Nichols[4]

[1] *LJLL, University Pierre et Marie Curie, France* cohen@ann.jussieu.fr
[2] *University of South Carolina, Columbia, USA* binev@math.sc.edu
[3] *CEREMADE, University Paris IX Dauphine, France* mula@ceremade.dauphine.fr
[4] *LJLL, University Pierre et Marie Curie, France* james.ashton.nichols@gmail.com

One typical scenario in data assimilation is the following: one observes m linear measurements of a function u which is solution to a PDE where certain parameters are unknown. The measurement functionals are picked from a certain dictionnary $\mathcal{D}$, for example when placing sensors at m chosen locations. The state estimation problem then consists in recovering u from these measurements.

One possible approach to this problem, proposed in [2] and further analysed in [1], exploits the fact that the family of solution for all potential parameter values is well approximated by linear spaces V_n of moderate dimension n. Such spaces are typically obtained by reduced model techniques, such as reduced bases, proper orthogonal polynomial expansions in the parametric variable.

The numerical method achieves a reconstruction which has the accuracy of the best approximation from V_n to the unknown solution u, up to a multiplicative constant $\mu(V_n, W_m) \geq 1$ which takes the form of an inverse inf-sup constant between the space V_n and the space W_m generated by the Riesz representers of the linear forms giving rise to the measurements.

The goal of the work presented in this talk is to select the measurement functionals within $\mathcal{D}$ to maintain $\mu(V_n, W_m)$ of reasonable size, with m as small as possible. In particular, we present a greedy algorithm allowing for a stepwise selection process of reasonable computational cost, and we analyze its properties.

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Nonuniform sampling and universality of stable sampling rates.

José Luis Romero[1]

[1] *Acoustics Research Institute, Austrian Academy of Science, Austria*
jlromero@kfs.oeaw.ac.at

I will present recent results on sampling, focusing on the problem of reconstructing a compactly supported function from non-uniform measurements of its Fourier transform.

We consider a given set of samples, a finite dimensional reconstruction model, and the precise combination of these two ingredients that leads to numerical stability. We show that such balance is largely independent of the geometry of the underlying sampling scheme and is therefore universal among all sampling sets [1]. This allows us to transfer recent results on phase transitions for numerical stability, from one specific sampling set to any sampling set.

A key step is the derivation of weighted bounds for Fourier sampling that are valid for non-uniform sets with density arbitrarily close to the critical value (Nyquist rate) - elaborating on classical results of Beurling. Similar sharp density results have recently been obtained for non-uniform sampling of linear combinations of certain totally-positive functions [2]. I will discuss corresponding applications to the determination of the stable sampling rate.

The talk is based on joint work with Ben Adcock, Milana Gataric, Karlheinz Gröchenig and Joachim Stöckler [1, 2].

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS05 – Generalized Sampling, Reduced Modeling and sparse recovery

A Reduced Basis Technique for Long-Time Unsteady Turbulent Flows

Lambert Fick[1], Yvon Maday[2,3], Anthony T Patera[4], Tommaso Taddei[2],

[1] *Texas A&M University, Department of Nuclear Engineering, USA* lambert.fick@tamu.edu
[2] *Sorbonne Universités, Laboratoire Jacques-Louis Lions, France*
taddei@ljll.math.upmc.fr, maday@ann.jussieu.fr
[3] *Brown University, Division of Applied Mathematics, USA* yvon_jean_maday@brown.edu
[4] *MIT, Department of Mechanical Engineering, USA* patera@mit.edu

For turbulent flows, estimation of the entire solution trajectory through a low-dimensional Reduced Order Model might be unfeasible due to the slow convergence of the Kolmogorov N-width, and due to the sensitivity of the dynamical system to perturbations. Nevertheless, it might still be possible to estimate the time-averaged solution and associated quantities of interest.

In this talk, we propose a Reduced-Basis technique for the estimation of long-time-averaged solutions of parametrized turbulent flows. The key elements of our approach are (i) a Greedy technique for the construction of a low-dimensional reduced space, and (ii) a constrained POD-Galerkin formulation of the reduced solution. The Greedy technique relies on a novel residual indicator for the error in the long-time-averaged solution.

We present a number of numerical examples to illustrate our approach, and to demonstrate the effectivity of the error indicator.

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS05 – Generalized Sampling, Reduced Modeling and sparse recovery

Uniform recovery guarantees for Walsh sampling and wavelet reconstruction

Vegard Antun[1], **Ben Adcock**[2], **Anders Hansen**[3]

[1] *University of Oslo, Norway* vegarant@math.uio.no
[2] *Simon Fraser University, Canada* ben_adcock@sfu.ca
[3] *University of Cambridge, United Kingdom* ach70@cam.ac.uk

Generalized sampling with compressive sensing (GS-CS) [1] provide an attractive model for many real-world inverse problems. In particular it is applicable for any application where the underlying signal is analog, and the samples can be obtained as linear measurements from a sampling operator fixated by the application. Typical examples include most types of medical imaging, such as Magnetic Resonance Imaging (MRI), surface scattering, Computerized Tomography (CT), all of which employ Fourier samples, to fluorescence microscopy and lensless imaging, using binary imaging techniques.

In [2] one derived uniform recovery guarantees for sampling and recovery with finite dimensional orthonormal bases. In our presentation we have extended this to an infinite dimensional framework, by solving a weighted ℓ_1-minimization problem as opposed to the classical unweighed basis pursuit. These recovery guarantees hinges on the local coherence structure of the change of basis matrix between the sampling and recovery basis. Thus, in order to provide any concrete recovery guarantees for this setup we have derived these coherence estimates for Walsh sampling and orthonormal wavelet recovery.

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MS06 – Recent Advances in Space-Time Galerkin Methods and Applications

(Markus Bause, Boris Vexler)

Tuesday, 13:30 – 15:10, Hotel Fleischers Sivle

Monika Balázsová – *Stability of higher-order ALE-STDGM for nonlinear problems in time-dependent domains*

Miloslav Feistauer – *DGM for the solution of nonlinear dynamic elasticity*

Filip Roskovec – *Anisotropic $hp-$space-time discontinuous Galerkin method for the numerical solution of nonlinear problems*

Gunar Matthies – *Numerical studies of higher order variational time stepping schemes for evolutionary Navier–Stokes equations*

Wednesday, 08:30 – 10:10, Hotel Fleischers Sivle

Omar Lakkis – *Aposteriori analysis of time hp-discontinuous Galerkin for fully discretized parabolic problems*

Boris Vexler – *Discrete maximal parabolic regularity and best approximation results for Galerkin finite element solutions of parabolic problems*

Dmitriy Leykekhman – *Best approximation property for the gradient of the finite element solutions for parabolic problems*

Wednesday, 15:55 – 17:10, Hotel Fleischers Sivle

Ilario Mazzieri – *A high-order discontinuous Galerkin approximation to second-order differential equations with applications to elastodynamics*

Markus Bause – *Space-Time Approximation of Wave Problems and Multiphysics Systems*

Johannes Ernesti – *The application of discontinuous Petrov-Galerkin space-time discretizations and inexact Newton methods to seismic imaging*

Manuel Borregales – *Space-time finite elements for non-linear poromechanics*

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS06 – Recent Advances in Space-Time Galerkin Methods and Applications

Stability of higher-order ALE-STDGM for nonlinear problems in time-dependent domains

M. Balázsová[1], **M. Feistauer**[1], **M. Vlasák**[1],

[1] *Charles University, Faculty of Mathematics and Physics, Sokolovská 83, 186 75 Praha 8, Czech Republic*

balazsova@karlin.mff.cuni.cz
feist@karlin.mff.cuni.cz
vlasak@karlin.mff.cuni.cz

Problems in time-dependent domains Ω_t are very important in a number of areas of science and technology. We can mention for example fluid-structure interaction problem, when the flow is solved in a domain deformed due to the coupling with an elastic structure. Very popular technique to solve problems in time-dependent domains is the arbitrary Lagrangian-Eulerian (ALE) method based on a suitable one-to-one ALE mapping of the reference configuration Ω_0 onto the current configuration Ω_t. From different applications the ALE method combined with the space-time discontinuous Galerkin method (ALE-STDGM) seems very robust and accurate.

Papers [1] and [2] are concerned with the stability analysis of the ALE-STDGM applied to a linear convection-diffusion initial-boundary value problem ([2]) as well as to the case of nonlinear convection and diffusion ([1]) with nonhomogeneous Dirichlet boundary condition, using piecewise linear DG time discretization.

In this talk we generalize these results concerning the analysis of the space-time discontinuous Galerkin method applied to the numerical solution of nonlinear convection-diffusion value problem in a time-dependent domain. The problem is reformulated using the 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-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 main attention is paid to the proof of 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, namely its continuity in the $\|\cdot\|_{L^2}$-norm and in special $\|\cdot\|_{DG}$-norm.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS06 – Recent Advances in Space-Time Galerkin Methods and Applications

DGM for the solution of nonlinear dynamic elasticity

Miloslav Feistauer[1], **Martin Hadrava**[1], **Adam Kosík**[2]

[1] *Charles University, Faculty of Mathematics and Physics, Sokolovská 83, 186 75 Praha 8, Czech Republic* feist@karlin.mff.cuni.cz, martin@hadrava.eu
[2] *University of Dortmund, LS III, Vogelpothsweg 87, 44277 Dortmund, Germany*
adam.kosik@gmail.cz

The paper is concerned with the numerical solution of dynamic nonlinear elasticity by the discontinuous Galerkin method (DGM). The deformation of an elastic body is described by the St. Venant-Kirchhoff and Neo-Hookian models. The discretization of the dynamic system is based on splitting the system into two systems of first order in time. They are discretized in space by the DGM. For the time discretization the backward difference formula or time DG method are applied. The developed numerical schemes are analyzed from the point of view of the stability, accuracy and robustness with the aid of several test problems. Attention is also paid to the optimization of penalization parameters. The applications are oriented to fluid-structure interaction (FSI), particularly to the simulation of air flow in a time dependent domain representing vocal tract.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS06 – Recent Advances in Space-Time Galerkin Methods and Applications

Anisotropic $hp-$ space-time discontinuous Galerkin method for the numerical solution of nonlinear problems

Vít Dolejší[1], **Filip Roskovec**[2]

[1] *Charles University, Faculty of Mathematics and Physics, Sokolovská 83, 186 75 Prague, Czech Republic* dolejsi@karlin.mff.cuni.cz
[2] *Charles University, Faculty of Mathematics and Physics, Sokolovská 83, 186 75 Prague, Czech Republic* roskovec@gmail.com

We present an adaptive numerical method for solving non-stationary partial differential equations using the space-time discontinuous Galerkin method. This method is very convenient for adaptation, since it operates with discontinuous polynomials with respect to both space and time variables. Our approach combines the error estimates measuring the dual norm of the residual from [2] with interpolation error estimates to generate anisotropic triangular elements as well as to choose the appropriate polynomial approximation on each element. At each time step we employ the $hp-$version of the continuous mesh and error models, respectively, for the formulation of a mesh optimization problem. Using an iterative algorithm, see [1], we find a suitable anisotropic $hp-$mesh such that the approximate solution has the error estimate below a given tolerance and the resulting number of degrees of freedom is close to the theoretical solution of the mesh optimization problem.

Typically almost no nodes are common for meshes in two consecutive time steps, hence the time discontinuous Galerkin method is more suitable for this kind of adaptation compared e.g. to multistep methods. Moreover, time discontinuous Galerkin method provides high accuracy with respect to time and $hp-$adaptation can be performed not only with respect to space variables but also in time.

The resulting system of nonlinear algebraic equations is solved by inexact Newton-like method in each time step. Further, the residual-based estimate from [2] enables us to identify spatial, temporal and algebraic parts of the computational errors. Then we propose an algorithm which brings all these parts of the total error under control.

We present several numerical examples (both scalar and systems of equations) from various fields of application demonstrating the efficiency of the proposed adaptive strategy.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS06 – Recent Advances in Space-Time Galerkin Methods and Applications

Numerical studies of higher order variational time stepping schemes for evolutionary Navier–Stokes equations

Gunar Matthies[1], **Naveed Ahmed**[2]

[1] *Technische Universität Dresden, Institut für Numerische Mathematik, 01062 Dresden, Germany*
gunar.matthies@tu-dresden.de

[2] *Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Mohrenstr. 39, 10117 Berlin, Germany*
ahmed@wias-berlin.de

We study variational time stepping schemes for evolutionary Navier–Stokes problems using conforming inf-sup stable pairs of finite element spaces for approximating velocity and pressure as spatial discretisation.

Stabilisations based on local projection are used in the case of dominant convection. Higher order continuous Galerkin–Petrov methods (cGP) and discontinuous Galerkin (dG) methods are applied to discretise in time. An adaption of the post-processing given in [1] allows to get for cGP(k) and dG(k) a velocity solution which provides in integral based norms the convergence order $k+2$. In addition, the post-processing leads to numerical solutions which show at the discrete time points for both velocity and pressure the convergence order $2k$ and $2k+1$ for cGP(k) and dG(k), respectively.

Numerical studies for the flow around a circle were performed where the finite element pairs (Q_2, P_1^{disc}) and (Q_3, P_2^{disc}) in space are combined with cGP(k), $k = 2, 3$, and dG(k), $k = 1, 2$, as temporal discretisations. Comparing the values of the benchmark numbers (maximal drag coefficient, maximal lift coefficient, pressure difference between the front and the back of the circle at the final time) with published reference values [2], it can be observed that the higher order time discretisations provide numbers which are close to the reference values even on the coarse spatial grids and large time step lengths. Furthermore, the results obtained with the methods cGP(2) and dG(1) were similar. The same holds for the methods cGP(3) and dG(2).

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS06 – Recent Advances in Space-Time Galerkin Methods and Applications

Aposteriori analysis of time hp-discontinuous Galerkin for fully discretized parabolic problems

Omar Lakkis[1], **Emmanuil H. Georgoulis**[2], **Thomas P. Whiler**[3]

[1] *Free University of Bolzano–Bozen, Italy and University of Sussex, Brighton, England UK*
lakkis.o.maths@gmail.com

[2] *National Technical University of Athens, Greece and University of Leicester, England UK*
Emmanuil.Georgoulis@le.ac.uk

[3] *Universität Bern, Switzerland*
wihler@math.unibe.ch

We derive aposteriori error bounds in $\mathrm{L}_\infty(0,T;\mathrm{L}_2(\Omega))$ 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 $\Omega \times (0,T)$, based on hp-version discontinuous Galerkin time-stepping scheme combined with conforming spatial Galerkin finite element method. The proof is based on the *space-time reconstruction*, which combines the elliptic reconstruction [1, 2, 3] of and the time reconstruction for discontinuous time-Galerkin schemes [4, 5] into a novel tool, allows for the user's preferred choice of aposteriori error estimates in space and careful analysis of mesh-change effects.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS06 – Recent Advances in Space-Time Galerkin Methods and Applications

Discrete maximal parabolic regularity and best approximation results for Galerkin finite element solutions of parabolic problems

Boris Vexler[1], **Dmitriy Leykekhman**[2]

[1] *Faculty for Mathematics, Technical University of Munich, Germany* vexler@ma.tum.de
[2] *Department of Mathematics, University of Connecticut, USA* leykekhman@math.uconn.edu

In this talk we present discrete maximal parabolic regularity results [1] for linear parabolic equations discretized by discontinuous Galerkin methods in time and Lagrange finite elements in space. These results provide a novel flexible technique for establishing optimal error estimates in various non-Hilbertian norms without any coupling conditions between the spatial mesh size and time steps. Especially we present global and interior best approximation type estimates in the $L^\infty((0,T)\times\Omega)$ norm [2]. We also discuss the extension of our results for problems with time-dependent coefficients.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS06 – Recent Advances in Space-Time Galerkin Methods and Applications

Best approximation property for the gradient of the finite element solutions for parabolic problems

Dmitriy Leykekhman[1], **Boris Vexler**[2]

[1] *Department of Mathematics, University of Connecticut, Storrs, CT 06269, USA*
dmitriy.leykekhman@uconn.edu

[2] *Technical University of Munich, Chair of Optimal Control, Center for Mathematical Sciences, Boltzmannstraße 3, 85748 Garching by Munich, Germany,* vexler@ma.tum.de

Besides a purely academic interest, best approximation property for the gradient of the finite element solutions for parabolic problems are desirable in many applications, for example parabolic optimal control problems with gradient constraints. Best approximation property of the gradient of the Galerkin solutions for elliptic problems which is equivalent to the stability of the Ritz projection in W^1_∞ is well investigated. However, no such results are known for the fully discrete solution of parabolic problems. In my talk I will present our global and interior pointwise error estimates for the fully discrete Galerkin solutions which are discretized with continuous elements in space and discontinuous Galerkin methods in time and explain the main points of the proof technique that is based on discrete maximal parabolic regularity in certain weighted norm.

References

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS06 – Recent Advances in Space-Time Galerkin Methods and Applications

A high-order discontinuous Galerkin approximation to second-order differential equations with applications to elastodynamics

P. Antonietti[1], **N. Dal Santo**[2], **I. Mazzieri**[3], **A. Quarteroni**[4]

[1] *MOX-Laboratory for Modeling and Scientific Computing, Department of Mathematics, Politecnico di Milano, P.za Leonardo da Vinci 32, 20133 Milano, Italy* paola.antonietti@polimi.it
[2] *CMCS, École Polytechnique Federale de Lausanne (EPFL), Station 8, 1015 Lausanne, Switzerland* niccolo.dalsanto@epfl.ch
[3] *MOX-Laboratory for Modeling and Scientific Computing, Department of Mathematics, Politecnico di Milano, P.za Leonardo da Vinci 32, 20133 Milano, Italy* ilario.mazzieri@polimi.it
[4] *CMCS, Ècole Polytechnique Federale de Lausanne (EPFL), Station 8, 1015 Lausanne, Switzerland MOX-Laboratory for Modeling and Scientific Computing, Department of Mathematics, Politecnico di Milano, P.za Leonardo da Vinci 32, 20133 Milano, Italy (on leave)* alfio.quarteroni@epfl.ch

In this work we introduce a new DG finite element method for the approximation of a system of second order ordinary differential equations in the form $M\mathbf{u}'' + L\mathbf{u}' + K\mathbf{u} = \mathbf{f}$, where M, L and K are symmetric and positive definite matrices and $\mathbf{f}$ is a source term. Using the energy of the system, we prove the stability of the resulting DG scheme and we perform the a-priori error analysis of the method. After validating these results on some test cases, we present computations obtained on two and three dimensional seismic wave propagation problems.

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MS06 – Recent Advances in Space-Time Galerkin Methods and Applications

Space-Time Approximation of Wave Problems and Multiphysics Systems

Markus Bause[1], **Uwe Köcher**[1]

[1] *Helmut Schmidt University, Holstenhofweg 85, 22043 Hamburg, Gemany* bause@hsu-hh.de
koecheru@hsu-hh.de

Variational space-time discretization schemes are getting of increasing importance for the accurate numerical approximation of highly transient processes like wave propagation phenomena. They offer appreciable advantages like the construction of entire families of schemes, the natural approximation of complex coupled systems of multiphysics by exploiting their weak formulations and the applicability of adaptive finite element techniques. We study three families of continuous, discontinuous and C^1-continuous Galerkin time discretizations. Along with discontinuous Galerkin discretizations of the spatial variables they are used for simulating elastic wave propagation, modeled by

$$\rho\,\partial_t^2 \boldsymbol{u} - \nabla\cdot\boldsymbol{\sigma}(\boldsymbol{u}) = \boldsymbol{f}\,, \qquad \boldsymbol{\sigma} = \boldsymbol{C}(\boldsymbol{x})\boldsymbol{\epsilon}\,, \quad \boldsymbol{\epsilon} = \left(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^\top\right)/2 \tag{2}$$

and rewritten as a system of first order equations in time. In our analyses the acoustic wave equation as the scalar-valued counterpart of Eq. (2) is considered. Various results of our numerical analyses of the space-time discretization of the wave equation are presented. The construction of efficient algebraic solvers for the resulting discrete systems is addressed. Finally, the potential of the schemes for simulating coupled systems of multiphysics involving wave phenomena, like the Biot-Allard system of poroelasticity, is considered.

Parts of the contribution are a joint work with F. Schieweck (University of Magdeburg) and F. Radu (University of Bergen).

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS06 – Recent Advances in Space-Time Galerkin Methods and Applications

The application of discontinuous Petrov-Galerkin space-time discretizations and inexact Newton methods to seismic imaging

Johannes Ernesti[1], **Christian Wieners**[1]

[1] *KIT, Institute of Applied and Numerical Mathematics, Karlsruhe, Germany*
johannes.ernesti@kit.edu
[2] *KIT, Institute of Applied and Numerical Mathematics, Karlsruhe, Germany*
christian.wieners@kit.edu

We introduce a weakly conforming discontinuous Petrov-Galerkin method in space and time for the acoustic wave equation in heterogeneous media. The fully implicit high-order discretization is a minimal residual method for the first-order system with discontinuous test spaces on a decomposition of the space-time cylinder and with trace degrees of freedom on the skeleton of this decomposition.

This is applied to a problem in seismic inversion, where the spatially varying material permeability is recovered approximately from point measurements of the scattered wave. The ill-posed problem in seismic imaging is regularized by an inexact Newton method, where every increment is evaluated by a conjugate gradient iteration. In every Newton step, the residual is computed by solving the wave equation, and every conjugate gradient step additionally requires the solution of the adjoint wave equation with a right-hand side depending on the full space-time solution.

The efficiency of the method is demonstrated by numerical examples in two space dimensions.

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MS06 – Recent Advances in Space-Time Galerkin Methods and Applications

Space-time finite elements for non-linear poromechanics

Manuel Borregales[1], **Florin Adrian Radu**[1], **Kundan Kumar**[1], **Jan Martin Nordbotten**[1].

[1] *University of Bergen, Norway* manuel.borregales@uib.no

Coupled flow and geomechanics, described by Biot's model have several applications including CO_2 sequestration, geothermal energy, and subsidence phenomena. Therefore, the development of robust, efficient and accurate numerical methods to solve Biot's model attracted recently a lot of attention. In particular, a higher order space-time method for the linear Biot model has been proposed and analysed in [1].

In this work, we propose a space-time finite element method for solving a non-linear Biot model. Specifically, we consider the case when the Bulk modulus (Lame coefficient λ) and the fluid compressibility are non-linear functions satisfying certain assumptions. We use a L-scheme, see e.g. [6], for linearization, combined with a fixed stress type splitting [2, 3, 4, 5]. Convergence results sustained by illustrative numerical examples will be presented.

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MS07 – FEM meshes with guaranteed geometric properties

(Sergey Korotov, Jon Eivind Vatne)

Tuesday, 15:30 – 17:10, Hotel Fleischers Kvitanosi

Michal Křížek – *Maximum angle condition for higher dimensional simplicial finite elements*

Jan Brandts – *Properties of and relations between several classes of simplices*

Jon E. Vatne – *Geometrical Properties of Families of Mesh Elements*

Ali Khademi – *On FEM Convergence on Prismatic Meshes*

Thursday, 08:30 – 10:10, Hotel Fleischers Kvitanosi

Tomáš Vejchodský – *Adaptive mesh refinement and robust guaranteed error bounds*

Maria González – *Adaptive solution of convection-diffusion problems using a stabilized mixed finite element method*

Sergey Korotov – *Longest-Edge n-Section Algorithms*

Martin Alkämper – *A weak compatibility condition for Newest Vertex Bisection*

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS07 – FEM meshes with guaranteed geometric properties

Maximum angle condition for higher dimensional simplicial finite elements

Michal Křížek[1], **Sergey Korotov**[2]

[1] *Institute of Mathematics, Czech Academy of Sciences, Žitná 25, CZ-115 67 Prague 1, Czech Republic* krizek@math.cas.cz
[2] *Department of Computing, Mathematics and Physics, Western Norway University of Applied Sciences, Inndalsveien 28, 5020 Bergen, Norway* sergey.korotov@hib.no

We present a survey on the maximum angle condition in the finite element method. In 1968, Miloš Zlámal introduced the minimal angle condition for triangulations that guarantees the optimal interpolation order of triangular finite elements. A more general angle condition, the so-called maximum angle condition for triangular elements, was investigated in the paper [1] by I. Babuška and A. K. Aziz. In 1992, M. Křížek [3] extended the maximum angle condition to linear tetrahedral finite elements. In 2017, A. Hannukainen, S. Korotov, M. Křížek generalized the maximum angle condition to simplicial finite elements in arbitrary space dimension. These authors also showed that the maximum angle condition is not necessary for the convergence of the finite element method.

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Properties of and relations between several classes of simplices

Jan Brandts[1], **Michal Křížek**[2]

[1] *Korteweg-de Vries Institute for Mathematics, University of Amsterdam, Netherlands*
J.H.Brandts@uva.nl

[2] *Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague*
krizek@math.cas.cz

Several special classes of simplices (such as regular, orthocentric, equifacetal, orthogonal, acute, nonobtuse, well-centered, $0/1$) have been identified and studied in the past, not only from the viewpoint of finite element triangulations, but also in the context of the Hadamard Maximal Determinant Conjecture and in abstract algebra [1, 2, 3, 4, 5]. Whereas the relation between some of these classes of simplices is straightforward, others seem unrelated. In this presentation we review some properties of, and relations between, such classes of simplices.

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Geometrical Properties of Families of Mesh Elements

Jon Eivind Vatne[1]

[1] *Department of computing, mathematics and physics, Western Norway university of applied sciences, P.O. Box 7030, 5020 Bergen, Norway* jev@hvl.no

When a mesh is generated in order to solve a partial differential equation by the finite element method, the geometry of the mesh influences both the qualitative and the quantitative properties of the numerical approximation. To make questions about the mesh precise, it is important to have a good parameter space for the shapes of the mesh elements. In this talk several approaches to this problem will be presented. It is important to realize that the choice of parameter space depends on the questions you ask. For instance, in a recent paper [1], the speaker considered simplices parametrized by points on a sphere. This approach is well-suited to study properties related to circumcenters, but it would be a very bad choice for studying degenerations.

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On FEM Convergence on Prismatic Meshes

A. Khademi[1]

[1] *Western Norway University of Applied Sciences, Bergen, Norway* Ali.Khademi@hvl.no

In the talk we will give a new proof for FEM convergence on prismatic meshes. In particular we will present and discuss the "prismatic version" of the maximum angle condition used in the case of triangles and tetrahedra.

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Adaptive mesh refinement and robust guaranteed error bounds

Tomáš Vejchodský[1], **Mark Ainsworth**[2]

[1] *Institute of Mathematics, Czech Academy of Sciences, Prague, Czech Republic*
vejchod@math.cas.cz

[2] *Division of Applied Mathematics, Brown University, Providence, RI, U.S.A.*
Mark_Ainsworth@brown.edu

This talk concerns the standard finite element approximation u_h of the reaction-diffusion problem

$$-\Delta u + \kappa^2 u = f \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \partial\Omega,$$

where $\Omega \subset \mathbb{R}^2$ is a polygonal domain, Δ stands for the Laplacian, f is the density of sources and κ^2 the reaction coefficient. This problem is singularly perturbed if κ is large. We will present a guaranteed upper bound η on the energy norm of the error $|||u - u_h|||$ which is robust even in the singularly perturbed case. This a posteriori error bound is obtained as a sum of local error indicators $\eta^2 = \sum_{K\in\mathcal{T}_h} \eta_K^2$ over elements K in the mesh $\mathcal{T}_h$. Error indicators η_K are suitable for the adaptive mesh refinement, they are locally efficient, and can be computed by a fast algorithm based on robustly equilibrated edge-flux functions g_K, see [1, 2]. In particular, we have

$$\eta_K^2 = \|\boldsymbol{\tau} - \nabla u_h\|_{L^2(K)}^2 + \kappa^{-2}\|\Pi f - \kappa^2 u_h + \operatorname{div}\boldsymbol{\tau}\|_{L^2(K)}^2,$$

where $\boldsymbol{\tau}$ is the robust flux reconstruction of g_K computed in the Raviart-Thomas space.

In contrast to [1, 2], we provide new and considerably simpler flux reconstruction $\boldsymbol{\tau}$. In the talk we will present numerical examples showing the efficiency of this approach for adaptive mesh refinement and a comparison of the newly proposed flux reconstruction with existing approaches.

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Adaptive solution of convection-diffusion problems using a stabilized mixed finite element method

M. González[1], **M. Strugaru**[2]

[1] *Departamento de Matemáticas, Universidade da Coruña, Campus de Elviña s/n, 15071, A Coruña, Spain.* mgtaboad@udc.es
[2] *Basque Center of Applied Mathematics, Alameda Mazarredo 14, 48009, Bilbao, Spain.* mstrugaru@bcamath.org

In this talk, we will consider a linear convection-diffusion equation with mixed boundary conditions and present an extension of the stabilized mixed finite element method introduced in [3]. The approach is based on adding suitable residual type terms to the classical dual-mixed formulation of the problem (see [1, 2, 3]). We will study the well-posedness of the continuous and discrete problems, and we will analyze the convergence of various finite element approximations. In addition, we will derive a fourth-term a posteriori error indicator and prove that it is reliable and locally efficient. We will provide some numerical experiments that illustrate the performance of the method.

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Longest-Edge n-Section Algorithms

S. Korotov[1]

[1] *Western Norway University of Applied Sciences, Bergen, Norway* sergey.korotov@hvl.no

In the talk we will present and discuss main properties of the longest- edge n-section algorithms. These algorithms (in classical and recently designed conforming form) are nowadays used in many applications, including finite element simulations, computer graphics, etc. as a reliable tool for controllable mesh generation. In addition, some hard open problems arising in and around this topic will be outlined.

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A weak compatibility condition for Newest Vertex Bisection

Martin Alkämper[1], **Robert Klöfkorn**[2], **Fernando Gaspoz**[1]

[1] *Martin Alkämper, Fernando Gaspoz*
Institute of Applied Analysis and Numerical Simulation
Chair of Applied Mathematics
Pfaffenwaldring 57
70569 Stuttgart
alkaemper@mathematik.uni-stuttgart.de

[2] *Robert Klöfkorn*
International Research Institute of Stavanger
Thormøhlensgt. 55
5006 Bergen
Norway
Robert.Kloefkorn@iris.no

Newest Vertex Bisection (NVB) is a refinement strategy for simplicial meshes, that is well-known to guarantee geometric properties, such as shape regularity. This is due to the fact, that it is a mere topological refinement procedure and the refined mesh is thus as anisotropic as the initial mesh (up to a constant).

A major drawback of NVB is that it requires a compatibility condition for neighboring simplices, which has to be fulfilled by their relative vertex enumerations. Grids that have been generated by mesh generation software in general cannot be expected to fulfil this condition and it is hard (or impossible) to reorder them accordingly.

We present a weaker compatibility condition and an algorithm to renumber any d-dimensional simplex grid with effort $O(n)$, where n is the number of elements. Additionally we show that some of the nice properties of NVB are preserved and in some special cases the algorithm actually achieves the standard compatibility.

The work presented is joint work with *Robert Klöfkorn (IRIS, Bergen) and Fernando Gaspoz (University of Stuttgart)*.

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MS08 – New frontiers in domain decomposition methods: Optimal control, model reduction, and heterogeneous problems

(Gabriele Ciaramella, Martin J. Gander)

Tuesday, 13:30 – 15:10, Kulturhus

Thomas Carraro – *Adaptive multiple shooting for parabolic optimization problems*

Giulia Fabrini – *Coupling Model Predictive Control and Dynamic Programming Methods for the Computation of Reduced-Order Optimal Feedback Laws*

Faycal Chaouqui – *A New coarse correction for Neumann-Neumann Methods*

Gabriele Ciaramella – *The method of reflections: relations with Schwarz methods and other classical iterative methods*

Thursday, 13:30 – 15:10, Kulturhus

Marco Discacciati – *Domain decomposition methods for the Stokes-Darcy problem*

Tommaso Vanzan – *Optimized Schwarz methods for Stokes-Darcy coupling*

Idoia Cortes Garcia – *Optimized Field/Circuit Coupling for the Simulation of Quenches in Superconducting Magnets*

Julien Salomon – *A decomposition method for the design of propellers and turbines: "The Blade Element Momentum" theory*

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Adaptive multiple shooting for parabolic optimization problems

Thomas Carraro

Institute for Applied Mathematics
Interdisciplinary Center for Scientific Computing (IWR)
Heidelberg University, Germany thomas.carraro@iwr.uni-heidelberg.de

Multiple shooting methods can be interpreted as time domain decomposition methods. In fact, one of the advantages in the application of these techniques is the possible parallelization of the time scheme. An other advantage is the improved robustness of the Newton method due to the so called *lifting* effect. In addition, the decomposition of the time domain limits the intrinsic instabilities of the underlying problem. In particular, multiple shooting methods are required for optimization problems that are highly unstable [1, 2, 3].

In certain cases, it is essential to use systematic adaptive techniques to do a proper time domain decomposition, i.e. it is important to choose the appropriate length of the subintervals to control the inherent instabilities of the problem. We show and compare two different strategies of adaptive multiple shooting to overcome extreme instabilities. The motivation for the development of these techniques, and their possible application, is the optimal control of turbulent flow.

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Coupling Model Predictive Control and Dynamic Programming Methods for the Computation of Reduced-Order Optimal Feedback Laws

Giulia Fabrini[1], **Maurizio Falcone**[2], **Stefan Volkwein**[3]

[1] *University of Konstanz, Department of Mathematics and Statistics, Universitätsstraße 10, D-78457 Konstanz, Germany* Giulia.Fabrini@uni-konstanz.de
[2] *La Sapienza Università di Roma, Dipartimento di Matematica, Roma, Italy* falcone@mat.uniroma1.it
[3] *University of Konstanz, Department of Mathematics and Statistics, Universitätsstraße 10, D-78457 Konstanz, Germany* Stefan.Volkwein@uni-konstanz.de

We consider the approximation of an infinite horizon optimal control problem which combines a first step based on Model Predictive Control (MPC) in order to have a quick guess of the optimal trajectory and a second step where we solve the Bellman equation in a neighborhood of the reference trajectory. The direct global solution approach via the Bellman equation can be rather expensive since we have to set the problem in a domain containing all the possible initial conditions x for the dynamics. Moreover, we have to impose (and choose) the appropriate boundary conditions for the Bellman equation. The main feature of MPC methods is to compute an approximate feedback control for the dynamics starting at a given initial condition x by solving a sequence of finite horizon optimal control problems. Therefore, it seems natural to first solve the problem for a given initial condition via MPC and then compute the value function in a neighborhood of that trajectory in order to reduce the global size of the computational problem. The second step is also necessary to allow for a more stable solution since we use the informations around the reference trajectory and not only those on the reference trajectory. For the computation of the domain in the second step we use an a-posteriori error estimates based on [3]. We will apply our algorithm to the heat equation with convection equation. Since it is well known that the Bellman approach suffer of the so called "curse of dimensionality" a reduced-order modeling is necessary in order to make the problem feasible. In the talk we will also point out how methods from domain decomposition (see [2]) might be useful to make our present approach computationally more efficient.

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A New coarse correction for Neumann-Neumann Methods

Faycal Chaouqui[1], **Martin J.Gander**[2], **Kevin Santugini-Répiquet**[3]

[1] *Université de Genève, Section de mathématiques, Suisse* Faycal.Chaouqui@unige.ch
[2] *Université de Genève, Section de mathématiques, Suisse* Martin.Gander@unige.ch
[3] *Université de Bordeaux, IMB, France* Kevin.Santugini@math.u-bordeaux1.fr

One level iterative domain decomposition methods share only information between neighboring subdomains, and thus do not scale in general. The use of a coarse grid is the only way to transmit global information between distant subdomains and ensure that the algorithm is scalable. The coarse correction can however do more than just make the method scalable: there exists an optimal coarse space in the sense that we have convergence after exactly one coarse step i.e. the method becomes then a direct solver.

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The method of reflections: relations with Schwarz methods and other classical iterative methods

Gabriele Ciaramella[1], **Martin J. Gander**[2]

[1] *Section de Mathématiques 2-4 rue du Lièvre, CH-1211 Genève, Switzerland*
Gabriele.Ciaramella@unige.ch

[2] *Section de Mathématiques 2-4 rue du Lièvre, CH-1211 Genève, Switzerland*
Martin.Gander@unige.ch

The method of reflection is an iterative procedure for solving linear boundary value problems where some "objects" or "holes" are present in the domain. Even though this method seems to be not well-known in the mathematical community, the corresponding literature is quite rich. The method was introduced by Smoluchowski in 1911 [1] for computing (sequentially) an approximate solution of a Stokes problem, where two objects are posed in a fluid in motion. A similar idea was used by Golusin in 1934 [2] to solve (in parallel) a Laplace equation defined on a domain having "holes". A first rigorous mathematical analysis is due to Luke in 1989 [3], where the author defined an alternating (sequential) method of reflections for different types of problems and proved its convergence. Very recently, Salomon et al. [4] studied the method of reflections, in both sequential and parallel forms, and proved its convergence. Even though many other publications can be found in the literature, the method of reflections seems to be still not completely understood from the numerical analysis point of view. This is the main focus of this talk. After introducing the method of reflections in some of its different formulations, as in [3] and [4], we will discuss its relations with classical Schwarz methods and stationary iterative methods. These clarifications will allow us to define new classes of method of reflections with improved convergence behaviors.

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Domain decomposition methods for the Stokes-Darcy problem

Marco Discacciati

Department of Mathematical Sciences, Loughborough University, UK
m.discacciati@lboro.ac.uk

The Stokes-Darcy problem has received a growing attention by the mathematical community over the last decade not only due to its many possible applications, but also to its mathematical nature. Indeed, it is a good example of a multi-physics problem where two different boundary value problems are coupled into a global heterogeneous one. To compute the approximate solution of this problem one could solve it in a monolithic way using either a direct or a suitably preconditioned iterative method. However, its multi-physics nature makes it suitable to splitting methods typical of domain decomposition techniques. These methods allow to recover the solution of the global problem by iteratively solving each subproblem separately and they thus permit to reuse software specifically developed to deal with either incompressible or porous media flows. The difficulty of this approach is to guarantee effective convergence and robustness of the iterations.

In this talk, several domain decomposition methods for the Stokes-Darcy problems will be presented [1, 2, 3]. Their robustness and performance will be analysed and numerical examples will show their effectiveness for practical applications.

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Optimized Schwarz methods for Stokes-Darcy coupling

Tommaso Vanzan[1], **Martin J. Gander**[2]

[1] *Section de Mathématiques 2-4 rue du Lièvre, CH-1211 Genève* tommaso.vanzan@unige.ch
[2] *Section de Mathématiques 2-4 rue du Lièvre, CH-1211 Genève* martin.gander@unige.ch

Optimized Schwarz methods have increasingly drawn attention over the last decades because of their improvements in terms of robustness and computational cost with respect to the classical Schwarz algorithm. Extensive results have been obtained for many different homogeneous problems that is physical phenomena described by a unique differential equation on the whole domain of interest 1,2. However, due to their property of convergence in the absence of overlap, Optimized Schwarz method are even more attractive for heterogeneous problems where the spatial decomposition is provided by the multi-physics of the problem. Moreover, it has been shown that heterogeneity may even improve the performance of algorithms designed first for the homogeneous counterpart3. The Stokes-Darcy coupling has been extensively studied in literature 4, 5 but an optimized algorithm is still missing. We present our theoretical results for several optimized transmission conditions, showing that unexpected results appear when dealing with finite domains.

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Optimized Field/Circuit Coupling for the Simulation of Quenches in Superconducting Magnets

I. Cortes Garcia[1], **S. Schöps**[2], **M. Maciejewski**[3] **and B. Auchmann**[4]

[1] *Institut für Theorie Elektromagnetischer Felder (TEMF), Technische Universität Darmstadt, Germany* cortes@gsc.tu-darmstadt.de
[2] *Institut für Theorie Elektromagnetischer Felder (TEMF), Technische Universität Darmstadt, Germany* schoeps@gsc.tu-darmstadt.de
[3] *Łódź University of Technology, Poland and European Organization for Nuclear Research (CERN), Switzerland* michal.maciejewski@cern.ch
[4] *Paul Scherrer Institut (PSI) and European Organization for Nuclear Research (CERN), Switzerland* bernhard.auchmann@psi.ch

In high-energy particle accelerators, superconducting magnets are used for bending the particle beam's trajectory. For the material to be superconducting, the magnets are operated at very low temperatures (1.9 K) and can quench, that is, become resistive. Uncontrolled release of high magnetic energy stored in the magnets as Joule heating can lead to damage in the magnet and thus the simulation of quench initiation, propagation, as well as of the active protection measures that are put in place, has to be carefully studied. As the protection measures affect both the magnet and the circuit and their mutual influence has to be studied, field/circuit coupling is performed.

After spatially discretising the magnet and representing the circuit in a lumped-element network, we obtain two coupled systems of differential algebraic equations. A waveform relaxation scheme is used for the simulation, that is, the systems are iteratively solved with different simulation tools at different time rates and information is exchanged at certain imposed time steps. This scheme can also be studied in the framework of optimised Schwarz methods as an heterogeneous domain decomposition problem. It allows to improve the convergence of the iteration scheme by choosing optimal transmission conditions between both systems. The obtained expansion of the operator confirms the proposal made in [1] of coupling the magnet as an inductance with a correction term into the circuit and it leaves room for possible improvements in that approach. As quench simulation also involves coupling of other important physical aspects such as the thermal effects, controller circuit and mechanical stresses on the magnet, an analogous analysis can be carried out in order to study the coupling of those systems.

Simulation results of an accelerator dipole magnet with accompanying protection system show the applicability of the proposed approach.

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A decomposition method for the design of propellers and turbines : "The Blade Element Momentum" theory

Julien Salomon[1], **Jérémy Ledoux**[2], **Sebastian Reyes-Riffo**[3]

[1] *Université Paris-Dauphine, PSL Research University, CNRS, CEREMADE, 75016 Paris, France and Inria, ANGE project-team, Rocquencourt - B.P. 105, F78153 Le Chesnay cedex, France*
julien.salomon@dauphine.fr

[2] *Université Paris-Dauphine, PSL Research University, CNRS, CEREMADE, 75016 Paris, France*
ledoux@ceremade.dauphine.fr

[3] *Université Paris-Dauphine, PSL Research University, CNRS, CEREMADE, 75016 Paris, France*
reyesriffo@ceremade.dauphine.fr

The Blade Element Momentum Theory [1, 2, 3] provides a model that enables to evaluate numerically the efficiency of a propeller. The advantage of the related algorithm lies in the decomposition of the computation into two parts : a 2D model that reports lift and drag forces associated with the profile under consideration, and a reduced system of scalar equations that describes the macroscopic forces applied on the propeller. In this talk, we will present necessary assumptions on the 2D model to obtain existence of solution(s) of the latter system. In addition, we prove the convergence of a fixed point algorithm that can be used to solve it numerically.

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MS09 – Discretizations and solvers for multi-physics problems

(Francisco José Gaspar, Carmen Rodrigo)

Tuesday, 08:30 – 10:10, Hotel Fleischers Osa

Massimilano Ferronato – *A stabilized finite volume method for poroelasticity: Numerical challenges and computational efficiency*

Ludmil Zikatanov – *Stabilization techniques for finite element discretizations of Biot's model in poroelasticity*

Xiaozhe Hu – *Robust Preconditioners for the Biot's Model*

Jakub Both – *Numerical investigation of a block-preconditioner for nonlinear Biot's equations*

Wednesday, 08:30 – 10:10, Hotel Fleischers Osa

Johannes Kraus – *Parameter-robust stable discretizations and uniform preconditioners for classical three-field formulation of Biot's consolidation model*

Carmen Rodrigo – *Efficient solvers for the linear thermo-poroelasticity problem*

James Adler – *Energy Minimization and a Deflation Technique for Detecting Multiple Liquid Crystal Equilibrium States*

Prashant Kumar – *A multigrid multilevel Monte Carlo method for transport in Darcy-Stokes system*

Wednesday, 15:55 – 17:35, Hotel Fleischers Osa

Argyrios Petras – *Mathematical and Computational Modeling of the Radiofrequency Ablation for Cardiac Arrhythmias via Open-irrigated Catheter*

Stefan Frei – *Long-term simulation of large deformation, mechano-chemical fluid-structure interactions with application to plaque growth in blood vessels*

Ana Budiša – *A BDDC method for robust discretization of flow in fractured porous media*

Magnus Svärd – *Convergence rates of energy stable finite difference schemes.*

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MS09 – Discretizations and solvers for multi-physics problems

A stabilized finite volume method for poroelasticity: Numerical challenges and computational efficiency

Massimiliano Ferronato[1], **Herminio T. Honorio**[2], **Carlo Janna**[3], **Clovis R. Maliska**[4]

[1] *University of Padova, Padova, Italy* massimiliano.ferronato@unipd.it
[2] *Federal University of Santa Catarina, Florianopolis, Brazil* herminio.eng@gmail.com
[3] *University of Padova, Padova, Italy* carlo.janna@unipd.it
[4] *Federal University of Santa Catarina, Florianopolis, Brazil* clovis.maliska@ufsc.br

The coupled equations of Biot's poroelasticity, consisting of stress equilibrium and fluid mass balance in deforming porous media, still pose severe numerical challenges and recently different discretization methods have been advanced. In this work, they are numerically solved by an Element-based Finite Volume Method (EbFVM) [1]. This discretization method is very flexible, as it allows for the use of unstructured grids made by elements of different types, and provides a conservative approach for both flow and mechanics. Similarly to other discretization techniques, numerical pressure instabilities can arise when undrained conditions take place. A stabilization procedure is advanced following the so-called Physical Influence Scheme (PIS), which was originally introduced for Navier-Stokes equations [2]. The numerical model is validated against classical analytical solutions and realistic three-dimensional problems, providing evidence that the proposed stabilization is able to eliminate the spurious pressure instabilities.

As it typically occurs with coupled multi-physics problems, the algebraic linearized system arising from the numerical discretization is characterized by a block non-symmetric structure. The solution to such system by a monolithic approach is generally characterized by a greater robustness and a faster convergence than sequential methods, provided that an ad hoc block solver is developed. In this work, we investigate the numerical performance obtained by using a multilevel preconditioner where the Schur complement is approximated by using physics-based arguments [3]. The approach is then generalized to a purely algebraic algorithm. Finally, some numerical results in large size realistic applications are presented.

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Stabilization techniques for finite element discretizations of Biot's model in poroelasticity

Carmen Rodrigo[1], **Xiaozhe Hu**[2], **Peter Ohm**[2], **James Adler**[2], **Francisco Gaspar**[1], **Ludmil Zikatanov**[3]

[1] *Department of Applied Mathematics, University of Zaragoza, Spain*
(carmenr|fjgaspar)@unizar.es
[2] *Department of Mathematics, Tufts University, USA*
(Xiaozhe.Hu|Peter.Ohm|James.Adler)@tufts.edu
[3] *Department of Mathematics, The Pennsylvania State University, USA* ludmil@psu.edu

We consider the linear Biot's model in poroelasticity discretized with piece-wise linear finite elements enhanced with face bubbles for the displacement field and piece-wise constants for the pressure field. We show how the face bubbles can be eliminated to obtain new discrete system and we further use this technique to derive a stable discretization for Stokes equation with minimum number of degrees of freedom. We also extend this construction to obtain a three field discretization for the Biot's model. We prove that the resulting scheme is stable in case of low permeabilities and/or small time steps and derive several error estimates for the fully discrete model.

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Robust Preconditioners for the Biot's Model

James H. Adler[1], **Francisco Gaspar**[2], **Xiaozhe Hu**[3], **Carmen Rodrigo**[4], **Ludmil T. Zikatanov**[5]

[1] *Department of Mathematics, Tufts University, Medford, MA 02155, USA*
James.Adler@tufts.edu
[2] *Departamento de Matemática Aplicada, Universidad de Zaragoza, Zaragoza, Spain*
fjgaspar@unizar.es
[3] *Department of Mathematics, Tufts University, Medford, MA 02155, USA*
Xiaozhe.Hu@tufts.edu
[4] *Departamento de Matemática Aplicada, Universidad de Zaragoza, Zaragoza, Spain*
carmenr@unizar.es
[5] *Department of Mathematics, The Pennsylvania State University, University Park, PA 16802, USA*
ludmil@psu.edu

Poroelasticity models the processes of coupled deformable porous media flow which is crucial in many applications. An essential component, and usually the most time-consuming part of simulating coupled PDEs, is solving the large-scale and ill-conditioned linear systems of equations arising from the discretization of the Biot's model. In this work, we generalize the traditional framework of block preconditioners on saddle point systems for the poroelasticity and develop effective preconditioners that are robust with respect to the physical and discretization parameters. Preliminary numerical experiments are presented to support the theory and demonstrate the robustness of our preconditioners.

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Numerical investigation of a block-preconditioner for nonlinear Biot's equations

Jakub W. Both[1], **Kundan Kumar**[1], **Jan M. Nordbotten**[1], **Florin A. Radu**[1]

[1] *Department of Mathematics, University of Bergen, Norway* jakub.both@uib.no
kundan.kumar@uib.no, jan.nordbotten@uib.no, florin.radu@uib.no

The coupling of mechanical deformation and fluid flow in porous media is of emerging interest and relevant for many challenging applications ranging from modeling CO_2 sequestration to understanding swelling and drying-shrinkage of cement-based materials. In this talk, we consider deformable unsaturated porous media under infinitesimal strain, modeled by a three-field formulation of generalized Biot's equations, coupling nonlinearly the equations of linear elasticity and Richards' equation. Due to the nonlinear and coupled character of the model, several numerical challenges arise. We propose a new linearization/splitting scheme, applying simultaneously the L-scheme [1] and the Fixed Stress Splitting scheme [2]. The individual schemes have been originally established for Richards' equation and the linear Biot's equations, respectively. The linearization/splitting scheme employs the natural block structure of the coupled problem and, hence, falls in the category of block-preconditioners. Using several examples, we investigate numerically the robustness and efficiency of the resulting preconditioner for varying material and solver parameters.

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Parameter-robust stable discretizations and uniform preconditioners for classical three-field formulation of Biot's consolidation model

Johannes Kraus[1], **Qingguo Hong**[2]

[1] *Faculty of Mathematics, University of Duisburg–Essen, Thea-Leymann-Str. 9, 45127 Essen, Germany* johannes.kraus@uni-due.de
[2] *Penn State University Mathematics Dept., University Park, State College, PA 16802* huq11@psu.edu

Poroelastic models describe the mechanical deformation and the fluid flow in porous media. They have a wide range of applications in medicine, biophysics and geosciences. A classical and widely used model has been introduced by Biot [1, 2].

In this talk we analyze the stability of a classical three-field formulation of Biot's consolidation model where the unknown variables are the displacements, the fluid flux (Darcy velocity), and the pore pressure. The key to establish the parameter-robust inf-sup stability of the continuous problem is the choice of proper parameter-dependent norms. This allows for the construction of uniform block diagonal preconditioners in the framework of operator preconditioning. Stable discretizations that meet the required conditions for full robustness on a discrete level are discussed and corresponding optimal error estimates proved.

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Efficient solvers for the linear thermoporoelasticity problem

Carmen Rodrigo[1], **Francisco Gaspar**[2]

[1] *Department of Applied Mathematics, University of Zaragoza, Spain.* carmenr@unizar.es
[2] *CWI, Centrum Wiskunde & Informatica, Amsterdam. The Netherlands.* gaspar@cwi.nl

The thermomechanical behavior of fluid saturated porous media is important in a number of diverse areas such as the extraction of geothermal energy, the design of nuclear waste storage sites and the enhanced oil recovery by hot fluid injection. Under common circumstances these problems involve strong coupling among three fields, displacement field, pore pressure field for fluid flow, and temperature field for heat transfer, giving rise to a coupled system of partial differential equations. After discretization, a large linear system of equations has to be solved on each time step. Such a system is characterized by its saddle point type structure, which requires a special treatment for its solution. In this work, the aim is on the numerical solution of the thermoporoelasticity problem by designing efficient solvers based on multigrid methods.

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Energy Minimization and a Deflation Technique for Detecting Multiple Liquid Crystal Equilibrium States

James H. Adler[1], Timothy J. Atherton[1], David B. Emerson[1], Patrick E. Farrell[2], Scott P. MacLachlan[3],

[1] *Tufts University, United States* james.adler@tufts.edu
[2] *University of Oxford*
[3] *Memorial University of Newfoundland*

Multiple equilibrium states arise in many physical systems, including various types of liquid crystal structures. Having the ability to reliably compute such states enables more accurate physical analysis and understanding of experimental behavior. In this talk, we consider adapting and extending a deflation technique for the computation of multiple distinct solutions arising in the context of modeling equilibrium configurations of nematic and cholesteric liquid crystals. The deflation method is applied as part of an overall free-energy variational approach and is modified to fit the framework of optimization of a functional with pointwise constraints. It is shown that multigrid methods designed for the undeflated systems may be applied to efficiently solve the linear systems arising in the application of deflation. For the numerical algorithm, the deflation approach is interwoven with nested iteration, creating a dynamic and efficient method that further enables the discovery of distinct solutions. Finally, we present numerical simulations demonstrating the efficacy and accuracy of the algorithm in detecting important physical phenomena, including bifurcations and disclination behaviors.

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A multigrid multilevel Monte Carlo method for transport in Darcy-Stokes system

Prashant Kumar[1], **Peiyao Luo**[2], **Francisco J. Gaspar**[3], **Cornelis W. Oosterlee**[4]

[1] *CWI – Centrum Wiskunde & Informatica, Amsterdam, The Netherlands, and Faculty of Aerospace Engineering, Delft University of Technology.* pkumar@cwi.nl
[2] *DIAM, Delft University of Technology, The Netherlands.* p.luo@tudelft.nl
[3] *CWI – Centrum Wiskunde & Informatica, Amsterdam, The Netherlands.* gaspar@cwi.nl
[4] *CWI – Centrum Wiskunde & Informatica, Amsterdam, The Netherlands, and DIAM, Delft University of Technology.* c.w.oosterlee@cwi.nl

We describe a finite volume multilevel Monte Carlo (MLMC) method for Uncertainty Quantification of contaminant transport in a coupled Darcy-Stokes system. In particular, we focus on high-dimensional epistemic uncertainty due to an unknown permeability field in the Darcy region. A novel monolithic multigrid algorithm is proposed to efficiently solve the steady-state flow in the Darcy-Stokes domain with highly heterogeneous diffusion coefficient. Further, we analyze different numerical schemes for coupling of transport with random steady-state flow and suggest an optimal combination for the MLMC estimator. Numerical experiments showing asymptotic costs of the proposed method with different regularity of the permeability field are presented.

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Mathematical and Computational Modeling of the Radiofrequency Ablation for Cardiac Arrhythmias via Open-irrigated Catheter

Argyrios Petras[1], **Massimiliano Leoni**[2], **Luca Gerardo-Giorda**[3]

[1] *Basque Center of Applied Mathematics, Bilbao, Spain* apetras@bcamath.org
[2] *Basque Center of Applied Mathematics, Bilbao, Spain* mleoni@bcamath.org
[3] *Basque Center of Applied Mathematics, Bilbao, Spain* lgerardo@bcamath.org

Radiofrequency ablation is an effective treatment process for cardiac arrythmias. Using an open-irrigated catheter, the arrythmogenic tissue is burnt via electrocautery, forming lesions on the tissue at the temperature of $50\,^{\circ}C$. The radiofrequency ablation is generally considered a safe treatment for cardiac arrhithmias, however complications can occur, including the possibility of thrombus formation, in case the blood temperature reaches $80\,^{\circ}C$, and steam pops, in the occurence of overheating of the tissue (around $100\,^{\circ}C$).

We present a mathematical model for the radiofrequency ablation process that uses an open-irrigated catheter. Our model includes the blood-saline interaction through the incompressible Navier-Stokes equation. The temperature change is modelled by Penne's bioheat equation, using a source term for the heat generation due to the thermoelectric effect. The electrical potential generated by the electrodes at the tip of the catheter is considered space and temperature dependent. An elasticity equation is employed to model the deformation of the tissue due to the pressure from the catheter tip at the tissue-catheter contact point.

The system is discretized and solved numerically using the finite element method. Our implementation uses Fenics for the approximation of the solution of the system of equations. A post-processing step, implemented Matlab, calculates the size of the lesion by tracking the $50\,^{\circ}C$ contour of the temperature. The geometric characteristics of the computational lesion, i.e. depth, maximum width etc., are approximated and compared with *in vitro* experimental results. In addition, estimations of possible thrombus occurence and steam pops are presented by tracking the $80\,^{\circ}C$ contour on the blood-tissue interface and the $100\,^{\circ}C$ contour in the tissue respectively.

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Long-term simulation of large deformation, mechano-chemical fluid-structure interactions with application to plaque growth in blood vessels

Stefan Frei[1], **Thomas Richter**[2], **Thomas Wick**[3],

[1] *University College London, United Kingdom* estefan.frei@gmail.com
[2] *University of Magdeburg, Germany* thomas.richter@ovgu.de
[3] *Ecole Polytechnique, Palaiseau, France* thomas.wick@polytechnique.edu

In this talk, we present a numerical framework for mechano-chemical fluid-structure interactions with long-term effects. In particular, we investigate a model for plaque growth in blood vessels including the interaction of the growing solid with the flow in the vessel. The mechano-chemical interaction is modelled by a multiplicative splitting of the deformation gradient.

This application includes two particular difficulties: First, growth may lead to very large deformations, up to full clogging of the fluid domain. Therefore, we use a Fully Eulerian approach, that is able to handle very large deformations up to contact. The second difficulty stems from the different time scales: while the dynamics of the fluid demand to resolve a scale of seconds, growth typically takes place in a range of months. To include both long-scale and short-scale effects appropriately, we propose a temporal two-scale approach using local small-scale problems to compute effective wall stresses that will enter a long-scale problem.

The numerical methodology is substantiated with several numerical tests that include comparisons of the Eulerian approach to an ALE method as well as numerical convergence studies.

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A BDDC method for robust discretization of flow in fractured porous media

Ana Budisa[1], **Eirik Keilegavlen**[2], **Jan M. Nordbotten**[3], **Florin A. Radu**[4]

[1] *University of Bergen,* Ana.Budisa@uib.no
[2] *University of Bergen* eirik.keilegavlen@uib.no
[3] *University of Bergen* jan.nordbotten@uib.no
[3] *University of Bergen* florin.radu@uib.no

Fractured porous media arise in many different applications, such as enhanced geothermal systems, energy storage, and shale gas/oil production. Fractures may provide both high-conducting pathways or barriers to flow and, thus, play a critical role in understanding system behavior. Therefore, it is important to integrate the specific properties of fractured porous media into numerical methods. Our goal is to efficiently solve the flow problem by taking into account the multi-dimensional hierarchy formed by fractures and fracture intersections. In this presentation, we propose a domain decomposition type preconditioner that exploits fractures as a natural interface between subdomains. In the mixed finite element discretization, a mortar method is used to represent the coupling of flow in the fractures with the surrounding domain. Given that, a special focus is set on tailoring the coarse geometry for fracture networks and using constraints and a weighted average across the subdomain interfaces to affect the rate of convergence. This method is verified on several examples of fracture networks to showcase the performance of our solver.

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Convergence rates of of energy stable finite difference schemes.

Magnus Svärd[1], **Jan Nordström**[2]

[1] *Dept. of Mathematics, University of Bergen, P.O. Box 7803, 5020 Bergen, Norway*
Magnus.Svard@uib.no

[2] *Computational Mathematics, Department of Mathematics, Linköping University, Sweden, 581 83 Linköping*
jan.nordstrom@liu.se

It is well-known that stability and consistency of a numerical scheme approximating a well-posed time-dependent linear PDE implies convergence as the grid size approaches zero. The convergence rate is dependent on, but generally not the same as, the order of accuracy of the scheme. Moreover, to obtain a stable scheme, when boundary conditions are included, a lower order of accuracy near the boundary is usually required. A long standing problem is to theoretically deduce the convergence rate from the various approximation orders in the scheme.

The theoretically most versatile tool to analyze convergence rates, is the Laplace-transform analysis (normal-mode analysis). However, the Laplace transform is algebraically complicated to work with. It would be desirable if the convergence properties could be inferred from more readily available estimates. In [1], it was shown that for the heat equation the convergence rate of the boundary errors is 1.5 orders higher than expected. This, however, is not an optimal result as two orders are usually observed. In [2], it was shown that the principal part of the spatial operator dictates the gain in the convergence rate of the boundary errors, with an increase of an order equal to the highest derivative. E.g., for the heat equation, with a second-derivative in space, two orders higher convergence rate is obtained at the boundary. The drawback is that the scheme must be stable in L^∞, which is a very strong stability requirement.

Here, we will weaken this requirement and show that energy stability along with certain accuracy constraints, results in an increase of orders equal to the highest spatial derivative. Furthermore, we will discuss the effect of higher temporal derivatives and exemplify our theory for the second-order wave equation.

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MS10 – Reduced order models for time-dependent problems

(Marie Billaud-Friess, Virginie Ehrlacher, Alexandre Ern)

Tuesday, 08:30 – 10:10, Hotel Fleischers Bergslien

Mario Ohlberger – *The localized reduced basis method for time dependent problems*

Gabriele Santin – *Greedy kernel methods for accelerating implicit integrators for parametric ODEs*

Silke Glas – *Space-time and reduced basis methods*

Stefan Volkwein – *POD-based error control for reduced-order multiobjective PDE-constrained optimization*

Tuesday, 13:55 – 15:10, Hotel Fleischers Bergslien

Amina Benaceur – *A progressive enhanced reduced basis/empirical interpolation method for nonlinear parabolic PDEs*

Gerrit Welper – *Interpolation of functions with parameter dependent discontinuities by transformed snapshots.*

Nicolas Cagniart – *Reduced basis methods for advection dominated problems*

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The localized reduced basis method for time dependent problems

Mario Ohlberger[1], **Stephan Rave**[2], **Felix Schindler**[3]

[1] *Applied Mathematics Münster, Einsteinstr. 62, D-48149 Münster* mario.ohlberger@wwu.de
[2] *Applied Mathematics Münster, Einsteinstr. 62, D-48149 Münster* felix.schindler@wwu.de
[3] *Applied Mathematics Münster, Einsteinstr. 62, D-48149 Münster* stephanrave@wwu.de

Model reduction approaches for parameterized problems have seen tremendous development in recent years. A particular instance of projection based model reduction is the reduced basis (RB) method, which is based on the construction of low-dimensional approximation spaces from snapshot computations, i.e. solutions of the underlying parameterized problem for suitably chosen parameter values. In this talk we will address error control for parabolic problems in general and its application for the localized reduced basis method [3, 2] as well as its usage for the construction of efficient numerical schemes for parameterized single and multiscale problems. Several numerical examples and applications will be shown to demonstrate the efficiency of the resulting approaches. The numerical results were obtained with the newly developed model reduction algorithms implemented in pyMOR (see http://pymor.org and [1]).

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Greedy kernel methods for accelerating implicit integrators for parametric ODEs

B. Haasdonk[1], **G. Santin**[2]

[1] *Institute of Applied Analysis and Numerical Simulation, University of Stuttgart, Germany*
haasdonk@mathematik.uni-stuttgart.de
[2] *Institute of Applied Analysis and Numerical Simulation, University of Stuttgart, Germany*
santinge@mathematik.uni-stuttgart.de

We present a novel acceleration method for possibly arbitrary implicit ODE solvers by means of greedy kernel-based surrogate models. We will first review some basic tools in kernel approximation for the reconstruction of high-dimensional functions, both in input and output. These methods allow to construct approximants to general target functions defined on arbitrary domains by means of scattered samples, i.e., without requiring any structure on the sampling locations. We will then focus on greedy algorithms, in particular the VKOGA ([3]), which constructs approximants based on a small subset of the data sites, thus being faster to evaluate, while still providing a good accuracy, which can even be proven to be quasi-optimal in some cases ([2]). These features make greedy kernel-based algorithms particularly attractive for the construction of surrogate models.

In the context of parametric ODEs, a set of trajectories precomputed with a high-accuracy ODE solver is used to train a kernel model which predicts the next point in the trajectory as a function of the last one. This model is cheap to evaluate, and it is used in the online phase to provide a good initialization point for the nonlinear solver of the implicit integrator. The accuracy of the surrogate model reflects into a significant reduction of the number of required steps of the solver, thus providing an overall speedup of the full simulation. Other than providing an acceleration, this method does not modify the accuracy of the simulation. Indeed, the ODE solver is still used to guarantee the required precision in the trajectory computation, which can now be achieved with possibly much less iterations of the nonlinear solver. Although the method can be potentially applied to a large variety of solvers and different ODEs, we will present in details its use with the implicit Euler method (VKOGA-IE) in the solution of the Lorenz system and the Burgers equation, which result to be meaningful test cases to demonstrate the method's features. In particular, we present refined results over [1].

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Space-time and reduced basis methods

Silke Glas[1], **Karsten Urban**[1]

[1] *Institute for Numerical Mathematics, Ulm University, Germany* silke.glas@uni-ulm.de
karsten.urban@uni-ulm.de

It is well-known that reduced basis methods (RBMs) [2, 3] perform particularly well for problems whose solution depends smoothly on the involved parameters. In this talk, we consider RBMs for instationary problems involving sources of non-smoothness in space, time and parameter. In particular, we are concerned with the Hamilton Jacobi Bellman (HJB) equation, the wave equation and time-dependent obstacle problems. In all these cases, non-smooth effects may vary (travel) in space over time and the evolution is typically unknown, but of great importance.

For the corresponding analysis, we use the space-time variational formulation, in which time is treated as an additional variable within the variational formulation of the problem, [1, 4]. In special cases, certain discretizations of such space-time problems yield time-stepping schemes. Otherwise, recent tensor product solvers may be used.

We discuss recent results in this framework concerning stability, approximation and reduced basis methods including efficient and reliable a posteriori error estimates.

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POD-based error control for reduced-order multiobjective PDE-constrained optimization

S. Banholzer[1], D. Beermann[2], S. Volkwein[3]

[1] *University of Konstanz, Germany* Stefan.Banholzer@uni-konstanz.de
[2] *University of Konstanz, Germany* Dennis.Beermann@uni-konstanz.de
[3] *University of Konstanz, Germany* Stefan.Volkwein@uni-konstanz.de

In the present paper, a bicriterial optimal control problem governed by an abstract evolution problem and bilateral control constraints is considered. To compute Pareto optimal points and the Pareto front numerically, the (Euclidean) reference point method is applied, where many scalar constrained optimization problems have to be solved. For this reason a reduced-order approach based on proper orthogonal decomposition (POD) is utilized. An a-posteriori error analysis ensures a desired accuracy for the Pareto optimal points and for the Pareto front computed by the POD method. Numerical experiments for evolution problems with convection-diffusion illustrate the efficiency of the presented approach.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS10 – Reduced order models for time-dependent problems

A progressive enhanced reduced basis/empirical interpolation method for non-linear parabolic PDEs

Amina Benaceur[1,2,3], **Virginie Ehrlacher**[1,3], **Alexandre Ern**[1,3] **and Sébastien Meunier**[2].

[1] *University Paris-Est, CERMICS (ENPC), 77455 Marne la Vallée Cedex 2, France*
[2] *EDF Lab Les Renardières, 77250 Ecuelles Cedex, France*
[3] *INRIA Paris, 75589 Paris, France* amina.benaceur@enpc.fr

We investigate new developments of the reduced basis method (RBM) for parameterized transient non-linear partial differential equations (PDEs) [3]. In practice, both the treatment of non-affine terms and non-linearities hinge on an empirical interpolation method (EIM). In many cases, the EIM may turn out to be extremely computationally-demanding although it is performed 'offline', since it requires to compute a significant number of non-linear trajectories using the full-order model. In this context, an alternative to the EIM has been recently proposed in [2] so as to alleviate the offline costs of the non-linear RBM through a simultaneous enrichment of both the EIM and the reduced basis spaces. This method solely requires as many full-model computations as the number of functions that span both the RBM and the EIM spaces.

In the present work, we develop a new methodology, the progressive enhanced RBM-EIM method (PREIM), which is inspired from [2]. The PREIM method will be applied to transient PDEs while trying to enhance the accuracy of the approximation. Unlike [2], the offline basis construction in the 'PREIM' is not always based on the RBM approximations. In fact, we take advantage of the full-order parameter-dependent solution if it has already been computed. Otherwise, we resort to the RBM approximation. Furthermore, at every new stage of the 'PREIM', we update the parameter selection after computing the full-order solution for the newly selected parameter. Finally, we present numerical results for a non-linear heat transfer equation using the industrial finite element solver 'code_aster' [1]. The main ideas underlying the 'PREIM' method and some preliminary numerical results were already presented in the MODRED 2017 conference.

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ENUMATH 2017
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MS10 – Reduced order models for time-dependent problems

Interpolation of functions with parameter dependent discontinuities by transformed snapshots.

Gerrit Welper[1]

[1] *University of Southern California, USA* welper@usc.edu

In comparison to elliptic and parabolic problems, our abilities to simulate parametric or stochastic hyperbolic PDEs is still fairly limited. Among several challenges, the efficient approximation of the PDE's solution is largely an open problem. In particular, staple method from the elliptic and parabolic regime such as reduced basis approximations, POD or polynomial chaos expansions, typically show poor performance in the presence of parameter dependent shocks. Namely, these shocks induce jumps with respect to the parameter variables, which then diminish the convergence rates of virtually all established methods. On the other hand, if the jump locations were independent of the parameters, they would be "invisible" in parameter direction and would pose no difficulty for the approximation of the PDE's parametric solution. We therefore propose to reduce the general parameter dependent jumps to this favorable situation by introducing transformations of the physical domain.

To this end, in an offline phase, we first compute the snapshots and suitable transforms of the physical domain for each snapshot. Their intention is to align jump singularities so that the snapshots, evaluated on the transformed physical domain have their jumps in the same parameter independent locations. We are therefore in the favorable situation described above and apply a simple polynomial interpolation of these transformed snapshots in the online phase. In the proposed talk, we discuss how to align the jumps to the right location, which is only known online, and that despite the transforms the final interpolation approximates the actual solution of the parametric PDE.

In order to calculate the transforms, we minimize the L_1-error of the transformed interpolation on a training sample of parameters with respect to the transform itself. On first sight this seems to be a complicated optimization problem and indeed, one can construct simple examples which have unacceptable local minima. Nonetheless, we can split the transform into a series of local contributions that allows us to "localize" the optimization problem and avoid bad local minima, altogether. This is proven rigorously for some $1d$ cases and demonstrated numerically for some $2d$ problems.

The above outlined method works well if we can align all discontinuities which, however, is not always the case. For example, if the number of jumps changes in parameter a proper alignment is not possible. In contrast to the parameter dependent movement of the jumps, which induce singularities for every parameter, changes of the number of jumps (and similar non-align-able cases) are local in parameter space. Therefore, in principle, additional localization methods such as hp-adaption in parameter space can resolve these difficulties. The drawback of this approach is that it does not scale well to high parameter dimensions. To this end, we argue that the "transformed interpolation" above allows us to construct a "tensorized" hp-adaptive method that is more promising for higher parameter dimensions.

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ENUMATH 2017
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MS10 – Reduced order models for time-dependent problems

Reduced basis methods for advection dominated problems

Remi Abgrall[1], **Nicolas Cagniart**[2], **Roxana Crisovan**[1], **Yvon Maday**[2,3], **Benjamin Stamm**[4]

[1] *Institut für Mathematik Universität Zürich Winterthurerstrasse 190 CH-8057 Zürich* remi.abgrall@math.uzh.ch, roxana.crisovan@math.uzh.ch
[2] *Laboratoire Jacques-Louis Lions Université Pierre et Marie Curie Boîte courrier 187 75252 Paris Cedex 05 France* cagniartn@ljll.math.upmc.fr, maday@ann.jussieu.fr
[3] *Institut Universitaire de France, Division of Applied Maths, Brown University, Providence, RI, USA.* [4] *MATHCCES Department of Mathematics RWTH Aachen University Schinkelstr. 2 D-52062 Aachen Germany* best@mathcces.rwth-aachen.de

In the frame of reduced basis techniques, advection dominated problem pose a problem for many reasons : a) stability issues, b) complexity of the solutions, c) moving fronts. In this presentation we shall present some new idea regarding the last item, i.e. how to deal with traveling fronts that linear combination of reduced basis does not allow to tackle. The new idea, introduced in [1], is to add to the classical reduced concept a change of variable moving in time. As regards the first item, the readers may consider [2].

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MS11 – Efficient Propagation of Uncertainties in Hyperbolic Partial Differential Equations

(Per Pettersson, Daniel S. Olderkjær)

Friday, 08:30 – 10:10, Hotel Fleischers Tarald

Per Pettersson – *Level set methods for stochastic discontinuity detection in nonlinear wave propagation problems*

Daniel S. Olderkjær – *A Locally-Reduced-Order-Basis Method for Stochastic Galerkin Formulations of Nonlinear Hyperbolic Problems*

Gabriela Malenová – *Uncertainty quantification for high frequency waves*

Jan Nordström – *Stochastic Galerkin Projection and Numerical Integration for Burgers' equation*

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Level set methods for stochastic discontinuity detection in nonlinear wave propagation problems

Per Pettersson[1], **Alireza Doostan**[2], **Jan Nordström**[3]

[1] *Uni Research, Bergen, Norway* per.pettersson@uib.no
[2] *University of Colorado Boulder, USA* alireza.doostan@colorado.edu
[3] *Linköping University, Linköping, Sweden* jan.nordstrom@liu.se

Nonlinear wave propagation problems governed by conservation laws are frequently subject to large material parameter uncertainties, see e.g., [1] for applications to subsurface CO_2 storage, and [2] for applications in computational fluid dynamics. In many of these problems, the solution is discontinuous in both physical and stochastic space. Efficient stochastic representation (e.g., spectral expansions) of quantities of interest requires knowledge of the location of the discontinuities in stochastic space. However, tracking discontinuities in high-dimensional spaces is a challenging problem and most existing methods are subject to restrictions on the geometry of the discontinuities.

Level set methods can be used to track deforming interfaces and are attractive due to the flexibility with respect to the geometry of the regions separated by the interfaces. In this work, we introduce a level set formulation where a set of sampled solutions of a nonlinear conservation law is treated as an image, and discontinuities are tracked in pseudo-time using the image segmentation techniques introduced in [3].

The stochastic space is tessellated using simplex-shaped stochastic elements, conforming with the geometry of the discontinuities identified by the level set method. This leads to a robust and efficient stochastic representation through localized basis functions. A local random field is identified using polynomial chaos least-squares. Statistics of interest can then be efficiently computed through processing of the local random field parameters.

The proposed methodology will be applied to nonlinear problems from computational fluid dynamics and CO_2 storage, and compared to existing techniques such as multi-element generalized polynomial chaos.

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MS11 – Efficient Propagation of Uncertainties in Hyperbolic Partial Differential Equations

A Locally-Reduced-Order-Basis Method for Stochastic Galerkin Formulations of Nonlinear Hyperbolic Problems

Daniel S. Olderkjær[1,2], **Per Pettersson**[1]

[1] *Uni Research CIPR, Bergen, Norway* daniel.olderkjer@uib.no
[2] *University of Bergen, Bergen, Norway* per.pettersson@uib.no

Nonlinear hyperbolic problems subject to parameter uncertainty frequently arise in modeling of fluid transport in subsurface porous media. The uncertainty stems from limited quality and quantity of prior data, and has traditionally been handled by using sampling based uncertainty quantification techniques such as the Monte Carlo Method (MC). However, in later years the intrusive Stochastic Galerkin (SG) method employing generalized Polynomial Chaos (gPC) expansions [3, 4] to describe stochastic parameters has become increasingly popular.

The SG method transforms the stochastic problem into a larger deterministic system by projecting onto a stochastic basis. The accuracy of the method and size of the new system is dependent on the number of basis functions. When handling discontinuities in nonlinear hyperbolic problems the number of basis functions increases dramatically due to the need of accurately resolving the discontinuities. Hence, efficient methods for decreasing computational cost are in great demand.

As different regions of the stochastic domain may affect the solution at different times and spatial locations, Le Maître et al. [1] proposed an evolving adaptive stochastic basis approach. However, this method decouples the basis, making implementation cumbersome. An alternative approach retains the global basis functions throughout the computations, but seeks to locally reduce the basis order by imposing a threshold on the gPC coefficients. This approach was presented in [5], where it was applied to the Buckley-Leverett equation.

In this work, we extend the locally-reduced-order-basis approach in [5] to the Burgers' equation and the subsurface CO_2 transport model proposed in [2]. An analysis of the computational savings of the method is provided, as well as a comparison between cost and accuracy of the numerical results for the two equations using the MC and SG methods.

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Uncertainty quantification for high frequency waves

Gabriela Malenová[1], **Mohammad Motamed**[2], **Olof Runborg**[1]

[1] *Department of Mathematics and Swedish e-Science Research Center (SeRC), KTH, 100 44, Stockholm, Sweden* {malenova,olofr}@kth.se
[2] *Department of Mathematics and Statistics, The University of New Mexico, Albuquerque, NM 87131, USA* motamed@math.unm.edu

We consider high frequency waves, i.e. solutions to the scalar wave equation with highly oscillatory initial data. The speed of propagation as well as the initial data are considered to be uncertain, described by a finite number of independent random variables with known probability distributions. To compute quantities of interest (QoI) of the solution and their statistics, we combine two methods: the Gaussian beam method to treat the high frequencies and the sparse stochastic collocation to deal with the (possibly high-dimensional) uncertainty.

A crucial assumption for the uncertainty quantification methods to converge fast is the stochastic regularity of the QoI. In particular, the size of the derivatives in the stochastic variable should be bounded independently of the wavelength. We show that QoIs defined as averages of the squared modulus of the wave solution indeed have this property, despite the highly oscillatory character of the waves.

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Stochastic Galerkin Projection and Numerical Integration for Burgers' equation

M. Wahlsten[1], **J. Nordström**[2]

[1] *Linköping University, SE-581 83 Linköping, Sweden.* markus.wahlsten@liu.se
[2] *Linköping University, SE-581 83 Linköping, Sweden.* jan.nordstrom@liu.se

We consider a stochastic analysis of the non-linear Burger's equation and focus on the comparison between intrusive and non-intrusive uncertainty quantification methods. The intrusive approach uses a combination of polynomial chaos and stochastic Galerkin projection. The non-intrusive method uses numerical integration by combining quadrature rules and the probability density functions of the prescribed uncertainties. The two methods applied to a provably stable formulation of the Burgers' equation are then compared. As a measure of comparison, variance size, computational efficiency and accuracy are used.

MS12 – Limiter techniques for flow problems

(Sandra May, Stefan Turek)

Tuesday, 15:30 – 17:10, Kulturhus

Petr Knobloch – *Algebraic flux correction for convection–diffusion problems*

Birte Schmidtmann – *Compact Third-Order Limiter Functions for Finite Volume Methods. Non-Uniform and 2D Grids*

Jesús Bonilla – *High-order monotonicity preserving finite element methods for scalar convection-diffusion problems*

Dmitri Kuzmin – *Flux-Corrected Transport Schemes for Continuous High-Order Bernstein Finite Elements*

Wednesday, 13:30 – 15:10, Kulturhus

Sandra May – *A vector-based slope limiter for finite volume schemes on non-coordinate-aligned meshes*

Deep Ray – *A high-resolution energy preserving method for the rotating shallow water equation*

Francesco Fambri – *Discontinuous Galerkin methods for compressible flows on space-time adaptive meshes with a posteriori sub-cell FV limiting*

Murtazo Nazarov – *Invariant domain preserving continuous finite element methods for system of conservation laws*

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS12 – Limiter techniques for flow problems

Algebraic flux correction for convection–diffusion problems

Gabriel R. Barrenechea[1], **Volker John**[2], **Petr Knobloch**[3]

[1] *University of Strathclyde, Department of Mathematics and Statistics, 26 Richmond Street, Glasgow G1 1XH, UK* gabriel.barrenechea@strath.ac.uk
[2] *Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstr. 39, 10117 Berlin, Germany* john@wias-berlin.de
[3] *Charles University, Faculty of Mathematics and Physics, Sokolovská 83, 18675 Praha 8, Czech Republic* knobloch@karlin.mff.cuni.cz

This contribution is devoted to the application of algebraic flux correction (AFC) finite element schemes to the numerical solution of scalar steady-state convection–diffusion problems. In contrast to the most finite element stabilization techniques, which are based on variational formulations, the idea of AFC schemes is to modify the algebraic system corresponding to the discrete problem. The basic philosophy of AFC schemes was formulated already in the 1970s. In the last fifteen years, these methods have been intensively developed by Dmitri Kuzmin and his coworkers, see, e.g., [4, 5]. In [1, 2, 3], we investigated the solvability of the nonlinear discrete problems obtained using the AFC methodology, proved the validity of the discrete maximum principle under various assumptions and derived a priori error estimates.

In this contribution, we review some of our theoretical results and then we concentrate on formulating general conditions on the limiters assuring the discrete maximum principle. We present several examples of limiters and discuss the properties of the corresponding schemes, both theoretically and computationally. In particular, we discuss the validity and consequences of the linearity preservation.

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ENUMATH 2017
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MS12 – Limiter techniques for flow problems

Compact Third-Order Limiter Functions for Finite Volume Methods. Non-Uniform and 2D Grids

Birte Schmidtmann[1], **Pawel Buchmüller**[2], **Manuel Torrilhon**[1]

[1] *MathCCES, RWTH Aachen University, Germany*
schmidtmann@mathcces.rwth-aachen.de

[2] *Institute of Mathematics, Heinrich-Heine University Düsseldorf, Germany*

We want to solve hyperbolic conservation laws using finite volume methods. In this context, we are interested in the reconstruction of interface values which are used as input values of the numerical flux function. The reconstruction is necessary for obtaining higher-order accuracy. Towards this end, we present limiter functions remaining in the setting of the most compact stencil, consisting of only nearest neighbors. This means three cells in one and five cells in two space dimensions, thus we are aiming at third-order accurate solutions.

The main aspect of the reconstruction is that the resulting scheme is high-order accurate in smooth parts and does not develop spurious oscillations at discontinuities, large gradients, or shocks. Furthermore, we want to avoid the so-called extrema clipping, i.e. the order reduction at smooth extrema, as encountered by TVD methods.

We recently developed a third-order limiter function fulfilling these requirements [1]. The function contains a decision criterion distinguishing between discontinuities and smooth extrema. This criterion does not contain tuning parameters but only uses information of the initial condition. In [1], we developed and analyzed the limiter function on one-dimensional equidistant grids. Here, we present the extension of the limiter to non-equidistant grids in one dimension. Furthermore, we make the limiter applicable for test cases on two-dimensional Cartesian grids with adaptive mesh refinement (AMR) [3]. This is achieved by the common approach of dimensional splitting. In order to apply this technique without loss of third-order accuracy, the order-fix developed in [2] is incorporated into the scheme. Several numerical test cases validate the excellent performance of the limiter and show that the extended formulation still yields the expected third-order accuracy.

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High-order monotonicity preserving finite element methods for scalar convection-diffusion problems

Jesús Bonilla[1], **Santiago Badia**[2]

[1] *Centre Internacional de Mètodes Numèrics en Enginyeria (CIMNE)*
Universitat Politècnica de Catalunya, Spain jbonilla@cimne.upc.edu
[2] *Centre Internacional de Mètodes Numèrics en Enginyeria (CIMNE)*
Universitat Politècnica de Catalunya, Spain sbadia@cimne.upc.edu

Many problems satisfy some sort of maximum principle (MP) or positivity at the continuous level. For steady problems, the MP implies that the solution at the interior is bounded by the solution at the boundary. However, these properties might not be readily satisfied at the discrete level. The violation of the MP by the discrete solution may lead to nonphysical results or even disable nonlinear solvers. Therefore, it is essential to provide numerical schemes that inherit such monotonicity properties, namely discrete maximum principle (DMP) preserving schemes.

Although many DMP-preserving methods for explicit time integration are currently available, monotonic schemes for steady or transient problems with implicit time integration are scarce and not so well developed. Implicit time integration is highly desired for problems with fast time scales without engineering/scientific interest. Nevertheless, several improvements have been developed recently to provide accurate DMP-preserving schemes for implicit time integration [1, 2, 3]. In particular, in [1] a stabilized continuous Galerkin (cG) finite element (FE) method is supplemented with an artificial diffusion operator to yield a scheme that is DMP-preserving for strictly acute meshes and piecewise continuous FE. In [2] the scheme is generalized for arbitrary meshes and a novel differentiable artificial diffusion operator is presented. This last development allows us to dramatically improve the nonlinear convergence of the scheme. Finally in [3] we extend the previous results to the framework of piecewise linear discontinuous Galerkin FE method.

However, all the schemes previously cited need a piecewise linear spatial discretization and are only unconditionally DMP-preserving for first order time integration. Currently, our work focuses on the extension of the previous works to high order discretizations both in space and time.

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ENUMATH 2017
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MS12 – Limiter techniques for flow problems

Flux-Corrected Transport Schemes for Continuous High-Order Bernstein Finite Elements

Christoph Lohmann[1], Dmitri Kuzmin[1], John N. Shadid[2], Sibusiso Mabuza[2]

[1] *Institute of Applied Mathematics (LS III)*
TU Dortmund University, Germany
[2] *Computational Mathematics Department*
Sandia National Laboratories, USA

christoph.lohmann@math.tu-dortmund.de
kuzmin@math.uni-dortmund.de
jnshadi@sandia.gov
smabuza@sandia.gov

This talk presents the first extension of the flux-corrected transport (FCT) methodology to continuous high-order finite element discretizations of scalar conservation laws on simplex meshes. Using Bernstein polynomials as local basis functions, we constrain the variation of the numerical solution by imposing local discrete maximum principles on the coefficients of the Bézier net. The design of accuracy-preserving FCT schemes for high-order Bernstein-Bézier finite elements requires a major upgrade of algorithms tailored for linear and multilinear Lagrange elements. The proposed ingredients include (i) a new discrete upwinding strategy leading to low order approximations with compact stencils, (ii) a variational stabilization operator based on the difference between two gradient approximations, and (iii) new localized limiters for antidiffusive element contributions. The optional use of a smoothness indicator based on a second derivative test makes it possible to avoid unnecessary limiting at smooth extrema and achieve optimal convergence rates for problems with smooth solutions. The accuracy of the proposed schemes is assessed in numerical studies for the linear transport equation.

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MS12 – Limiter techniques for flow problems

A vector-based slope limiter for finite volume schemes on non-coordinate-aligned meshes

S. May[1], **M. Berger**[2]

[1] *Department of Mathematics, TU Dortmund, Vogelpothsweg 87, 44227 Dortmund, Germany*
sandra.may@math.tu-dortmund.de

[2] *Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, NY 10012, United States*
berger@cims.nyu.edu

In this talk we present a robust and accurate slope limiter for finite volume schemes on non-coordinate-aligned meshes. The limiter was specifically designed for Cartesian embedded boundary ('cut cell') meshes but can also be used on general unstructured meshes. It is inherently multi-dimensional and linearity preserving. Traditionally, a *scalar* limiter is used on these meshes due to its simplicity: one computes a trial gradient and then reduces all components of the gradient by the same scalar $\Phi \in [0, 1]$.

We present a more multi-dimensional approach: in two dimensions, we limit the gradient in x and y direction separately using factors $\Phi_x, \Phi_y \in [0, 1]$, respectively. This approach has the benefit of being less diffusive but the downside of resulting in a coupled problem. This approach cannot be implemented by sequentially limiting each edge of a cell, since changing the components of the gradient individually rotates the gradient. We formulate the limiting problem as a linear program (LP): retain as much of the unlimited gradient as possible (measured in the L^1 norm) while satisfying certain monotonicity constraints.

This formulation results in a tiny LP to be solved at each cut cell at each time step with just two unknowns in two dimensions. Standard LP algorithms are at the other end of the spectrum - one problem with thousands of unknowns (or more). We use a little known variant of the Simplex algorithm that is much more efficient for our tiny problems. Our vector limiter is only a factor of 2-3 more expensive than the standard scalar limiter while being significantly more accurate [1].

In this talk, we discuss the main features of our vector-based slope limiter and the algorithm we use to solve the resulting LPs. We present numerical results in two dimensions on both unstructured and cut cell meshes. We conclude with a discussion of extending the limiter to three dimensions.

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A high-resolution energy preserving method for the rotating shallow water equation

Deep Ray[1], **Praveen Chandrashekar**[2]

[1] *TIFR - Centre for Applicable Mathematics, Bangalore, India* deep@math.tifrbng.res.in
[2] *TIFR - Centre for Applicable Mathematics, Bangalore, India* praveen@tifrbng.res.in

The shallow water equations with additional Coriolis source terms due to the Earth's rotation, are used in several meteorological models to simulate planetary waves. This system is known to have an infinite number of invariants, provided the solutions are smooth. Thus, it is important to construct numerical methods that are able to preserve most of these invariants, in order to capture the physical dynamics of the model.

We consider the vector-invariant form of the shallow water equations, and propose a high-order finite difference scheme that ensures the preservation of total energy. The central numerical flux is constructed using the ideas of entropy conservative fluxes for conservation laws. Since most of the model invariants depend on vorticity, we directly solve for vorticity by approximating the associated scalar conservation law using a high-order WENO finite difference method with flux splitting. Although central fluxes are used to evolve the $h - \mathbf{u}$ variables, the upwinded WENO scheme for vorticity is able to implicitly introduce dissipation without hindering the preservation of total energy, thus making the coupled scheme suitable for long time simulations.

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MS12 – Limiter techniques for flow problems

Discontinuous Galerkin methods for compressible flows on space-time adaptive meshes with a posteriori sub-cell FV limiting

Francesco Fambri[1], **Michael Dumbser**[1], **Olindo Zanotti**[1] , **Arturo Hidalgo**[2]

[1] *Department of Civil, Environmental and Mechanical Engineering, University of Trento, Via Mesiano, 77 - 38123 Trento, Italy* francesco.fambri@unitn.it
[2] *Departamento de Matemática Aplicada y Métodos Informáticos, Universidad Politécnica de Madrid, Madrid, Spain*

In this work the numerical discretization of the partial differential governing equations for compressible flows is dealt within the discontinuous Galerkin (DG) framework along space-time adaptive meshes. It is a well known fact that a major weakness of high order DG methods lies in the difficulty of limiting discontinuous solutions, which generate spurious oscillations. Over the years, different kinds of *limiters* have been proposed to cope with this problem. In this work, within the detected troubled cells, the DG-polynomials of the previous time step are scattered along a suitable finer *subgrid*. Then, a more reliable numerical solution is *recomputed a posteriori* by employing an ADER-WENO FV scheme on the *sub-grid* averages within that troubled cells. Finally, a high order DG polynomial is reconstructed back from the evolved sub-cell averages. The presented method has been applied to the *Euler*, the *ideal MHD* [1], A *ideal SRMHD equations* [2], but also the the case of *diffusive fluids*, i.e. fluid flows in the presence of *viscosity*, *thermal conductivity* and *magnetic resistivity* [3]. The adopted formalism is quite general, leading to a novel family of adaptive ADER-DG schemes suitable for hyperbolic systems of partial differential equations in which the numerical fluxes also *depend on the gradient of the state vector*. The numerical results show clearly that the *shock-capturing capability* of the news schemes are significantly enhanced within the cell-by-cell *Adaptive Mesh Refinement* (AMR) implementation together with time accurate local time stepping (LTS), leading to an unprecedented ability in resolving even the finest details in the dynamics of the fluid. The resolution properties of the new scheme have been shown through a wide number of test cases performed in two and in three space dimensions, from low to high Mach numbers, from low to high Reynolds regimes.

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Invariant domain preserving continuous finite element methods for system of conservation laws

Murtazo Nazarov[1]

[1] *Division of Scientific Computing, Department of Information Technology, Uppsala University, Sweden* murtazo.nazarov@it.uu.se

When solving conservation laws numerically it is important that the numerical solution satisfies an invariant domain property. The invariant property is a key property for the analysis of nonlinear conservation equations and greatly facilitates the stability or convergence analysis of the related algorithms. Designing high order finite element stabilization techniques that satisfy the invariant domain property in arbitrary space dimensions and mesh types is a nontrivial task.

In this talk we present a new stabilized method that satisfies the invariant domain property for system of conservation laws for arbitrary unstructured meshes, see e.g. [1, 2]. We prove that the method converges to the unique entropy solution for scalar conservation laws in any space dimensions.

The method can be made high order in time by using Strong Stability Preserving Runge-Kutta (SSP-RK) methods and high order in space using Flux-Corrected Transport (FCT) techniques, see for example [3]. Some numerical results of the method for scalar conservation laws and system of compressible Euler equations will be presented.

This is a joint work with Jean-Luc Guermond and Bojan Popov.

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MS13 – Monge-Ampère solvers with applications to illumination optics

(Jan ten Thije Boonkkamp, Wilbert IJzerman)

Monday, 15:50 – 17:55, Hotel Fleischers Tarald

Jan ten Thije Boonkkamp – *The Monge-Ampère equation for freeform optics*

Jean-David Benamou – *Optimal Transportation Solvers for FreeForm Optics*

Elisa Friebel – *Galerkin Methods for the Monge–Ampère: Equation arising in Lens Design*

Omar Lakkis – *Galerkin methods for the Monge–Ampère equation with transport boundary conditions*

Nitin K. Yadav – *A Least-Squares Method for the Design of Optical Systems and the Relation with Optimal Mass Transport*

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The Monge-Ampère equation for freeform optics

J.H.M. ten Thije Boonkkamp[1], **R. Beltman**[1], **W.L. IJzerman**[1,2]

[1] *Department of Mathematics and Computer Science, Eindhoven University of Technology, PO Box 513, 5600 MB, Eindhoven, The Netherlands*
j.h.m.tenthijeboonkkamp@tue.nl
r.beltman@tue.nl

[2] *Philips Lighting, High Tech Campus 7, 5656 AE Eindhoven, The Netherlands*
wilbert.ijzerman@philips.com

Freeform optics is concerned with the computation of an optical surface, either a reflector or a lens, that converts a given light distribution of a source $\mathcal{S}$ into a desired distribution at the target $\mathcal{T}$. The governing physical principles are the laws of geometric optics (law of reflection, Snell's law) and conservation of luminous flux. This problem is an example of an inverse problem and gives rise to an elliptic Monge-Ampère equation coupled with a transport boundary condition.

Assume, the optical surface is given by the relation $z = u(\boldsymbol{x})$ with $\boldsymbol{x} \in \mathcal{S}$, then the Monge-Ampère boundary value problem reads

$$\det\big(\mathrm{D}^2 u\big) = f(\boldsymbol{x}, \nabla u), \quad \boldsymbol{x} \in \mathcal{S}, \tag{3a}$$

$$\nabla u\big(\partial\mathcal{S}\big) = \partial\mathcal{T}, \tag{3b}$$

for some $f(\boldsymbol{x}, \nabla u) \geq 0$, where $\mathrm{D}^2 u$ denotes the Hessian matrix of u. In [1] we have developed a least-squares method for the numerical solution of the boundary value problem (3), which consists of two stages. First, we compute a mapping $\boldsymbol{m}$, representing ∇u, from the equation $\det\big(\mathrm{D}\boldsymbol{m}\big) = f(\boldsymbol{x}, \boldsymbol{m})$, where $\mathrm{D}\boldsymbol{m}$ denotes the Jacobi matrix of $\boldsymbol{m}$, and corresponding boundary condition $\boldsymbol{m}(\partial\mathcal{S}) = \partial\mathcal{T}$. We solve this problem iteratively by minimizing the corresponding least-squares functionals. In each iteration we have to update the functional for the interior domain and the for boundary, which can be done point-wise, after which we compute an update for the mapping $\boldsymbol{m}$. This latter step requires the solution of two Poisson equations for the components of $\boldsymbol{m}$. Second, upon convergence we compute the location of the optical surface from $\boldsymbol{m}$, also in a least-squares sense.

The method is very efficient and can handle very complicated target distributions. As an example, we have applied the method to a source with a given emittance (lumininous flux per area) emitting a parallel bundle of light which is converted into a desired intensity (luminous flux per solid angle) in the far field. Examples are given for both a reflector and a lens.

References

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Optimal Transportation Solvers for FreeForm Optics

Jean-David Benamou[1]

[1] *INRIA Paris and CEREMADE U. Paris Dauphine, France.*
Jean-David Benamou@inria.fr

Following the pioneering works of Caffarelli, Oliker and Wang, the inverse problem of freeforming a convex (or concave) reflector which sends prescribed idealized sources to a target intensity is known to be particular instance of optimal transportation problems. This is, for example, a promising approach to automatize the industrial design of optimized energy efficient reflectors (car/public lights for instance). The INRIA Mokaplan team [1] has recently developed several efficient numerical methods for optimal transportation problems. I will summarize these recent advances and present their application in freeform optics[2].

[1] https://team.inria.fr/mokaplan/
[2] https://project.inria.fr/mokabajour/

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Galerkin Methods for the Monge–Ampère Equation arising in Lens Design

K. Brix[1], **W. Dahmen**[2], **E. Friebel**[3],

[1] *RWTH Aachen, Germany* brix@igpm.rwth-aachen.de
[2] *RWTH Aachen, Germany* dahmen@igpm.rwth-aachen.de
[3] *RWTH Aachen, Germany* friebel@igpm.rwth-aachen.de

Given a point light source and a target, we investigate how to design a lens represented by a free-form surface such that this lens creates a desired light intensity distribution on the target, e.g., a projected image on a screen. The mathematical formulation of this so called inverse refractor problem (IRP) is related to optimal transport problems. Hence, a lens surface can similarly be defined by the solution of a fully nonlinear Monge–Ampère (MA) type equation complemented by a certain type of boundary conditions, also known as transport boundary equations.
Recently first Galerkin methods for the standard MA equation $\det(D^2u) = f$ with Dirichlet boundary conditions have been developed[1, 2, 3]. This talk deals with the development of related Galerkin concepts for MA type equations in the IRP, i.e. handling more complex right-hand sides, as well as transport boundary conditions. Specifically, we discuss a particular challenge, namely the appropriate treatment of the convection-diffusion equations with possibly varying Péclet numbers arising during the Newton update.

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Galerkin methods for the Monge–Ampère equation with transport boundary conditions

Ellya Kawecki[1], **Omar Lakkis**[2], **Tristan M. Pryer**[2]

[1] *University of Oxford, England UK* kawecki@maths.ox.ac.uk
[2] *Free University of Bolzano–Bozen, Italy and University of Sussex, England UK* lakkis.o.maths@gmail.com
[3] *University of Reading, England UK* T.Pryer@reading.ac.uk

The Monge–Ampère partial differential equation (MA) plays a central role in the solution of the Monge–Kantorovich optimal mass transportation problem with function data and when the cost functional is the squared Euclidean norm-based Wasserstein distance [3]. In this context, the MA arises naturally with *transport boundary conditions* (also known as second boundary conditions) that can be thought of as nonlinear oblique Neumann type conditions. Following the approach of [6], the resulting boundary value problem for a function u, may be written as

$$\begin{aligned} g(\nabla u(\boldsymbol{x}))\det \mathrm{D}^2 u(\boldsymbol{x}) &= f(\boldsymbol{x}) \text{ for } \boldsymbol{x}\in\Omega \\ b(\nabla u(\boldsymbol{x})) &= 0 \text{ for } \boldsymbol{x}\in\partial\Omega. \end{aligned} \tag{4}$$

where Ω is a bounded convex domain and b a convex function such that $\Omega = \{b<0\}$, and $f, g \geq 0$ are continuous functions with $\operatorname{Sprt} f = \Omega$ and $\int f = \int g$. The numerical approximation of (4) with transport boundary conditions is important in application such as illumination optics. Previous numerical studies include [1] and the more recent approach of [2]. I will present a new Galerkin method as an alternative that provides numerical accuracy, efficiency of computation and simplicity of implementation. Thanks to the finite element approach this method's highlight are geometric flexiblit, high orders of approximation for smooth solutions and potential for adaptive mesh refinement when solutions are singular (e.g., viscosity). The methodology we employ is that of Hessian recovery combined with Newton's method as introduced by [4] and a careful treatment of gradient terms via recovery. The versatility of our approach is supported by a publicly available solver script in Python–FEniCS [5].

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A Least-Squares Method for the Design of Optical Systems and the Relation with Optimal Mass Transport

N.K. Yadav[1], **J.H.M. ten Thije Boonkamp**[1], **W.L. IJzerman**[1,2]

[1] *CASA, Department of Mathematics and Computer Science, Eindhoven University of Technology, PO Box 513, 5600 MB Eindhoven, The Netherlands.* n.k.yadav@tue.nl
[2] *Philips Lighting, High Tech Campus 7, 5656 AE Eindhoven, The Netherlands.*
j.h.m.tenthijeboonkkamp@tue.nl, wilbert.ijzerman@philips.com

The optical system design problem is an *inverse problem:* "Find an optical system which contains reflectors and/or lenses that gives the desired light output at the target for a given input at the source". We present a new generalized methodology to design such optical systems.

Every optical system needs to satisfy two basic physical principles: energy conservation and the laws of geometrical optics. The key tool for the design of such an optical system is to find a mapping $\mathrm{y} = \boldsymbol{m}(\mathrm{x}) : \mathcal{S} \to \mathcal{T}$, where $\mathcal{S}$ and $\mathcal{T}$ are the source and target domains, respectively, that satisfies the energy conservation. Using the laws of geometric optics (reflection/refraction) we can derive a generalized mathematical structure for optical systems as follows, i.e.,

$$u_1(\mathrm{x}) + u_2(\mathrm{y}) = c(\mathrm{x}, \mathrm{y}), \quad \text{with } \mathrm{y} = \boldsymbol{m}(\mathrm{x}), \tag{5}$$

where $u_1(\mathrm{x})$, $u_2(\mathrm{y})$ represent the geometry of the optical system, and $c(\mathrm{x}, \mathrm{y})$ is the distance function, depending on the optical system, and called the cost function in the mass transport problem [2].

We can show that under certain assumptions the mapping $\boldsymbol{m}$ is implicitly given by the relation $\nabla_{\mathrm{x}} c(\mathrm{x}, \boldsymbol{m}(\mathrm{x})) = \nabla_{\mathrm{x}} u_1(\mathrm{x})$. Substituting the mapping in the energy conservation relation, we obtain

$$f(\mathrm{x}) = g(\boldsymbol{m}(\mathrm{x}))J(\mathrm{x})|\det(\mathrm{D}\boldsymbol{m}(\mathrm{x}))|, \ \ \forall \mathrm{x} \in \mathcal{S}, \tag{6}$$

where $\mathrm{D}\boldsymbol{m}$ is the Jacobian matrix of the mapping $\boldsymbol{m}$ and $J(\mathrm{x})$ is the Jacobian of the coordinate transformation depending on the optical system, and both f and g are either an emittance (luminous flux per area) or intensity (luminous flux per solid angle) of the source and the target, respectively. Now the problem is to calculate the mapping $\boldsymbol{m}$ using relations (5) and (6).

We solve this type of optical design problem by extending the least-squares method introduced in [1]. The algorithm is an iterative minimization procedure. In each iteration we have to update the functional for the interior domain and the for boundary, which can be done point-wise, after which we compute an update for the mapping $\boldsymbol{m}$. This latter step requires the solution of two Poisson equations for the components of $\boldsymbol{m}$. Second, upon convergence we compute the location of the optical surfaces from $\boldsymbol{m}$, also in a least-squares sense.

We find that under certain assumptions the optical design problem is equivalent to the mass transport problem: given a (mass) density function f defined on a space $\mathcal{S}$ and a density g defined on $\mathcal{T}$, find a mapping $\boldsymbol{m}$, referred to as the transport plan, such that the total mass contained in $\mathcal{S}$ equals the total mass in $\mathcal{T}$, and the mapping $\boldsymbol{m}$ minimizes the total transport cost $c(\mathrm{x}, \mathrm{y})$ [2]. Thus, we conclude that the optical design problem is equivalent to solving the optimal mass transport problem.

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MS14 – Biomembranes, Elastic Shells, and Complex Interfaces Symposium

(Shawn W. Walker, Thomas Yu)

Wednesday, 08:30 – 10:10, Hotel Fleischers Bergslien

Thomas Yu – *Numerical Solution and Uniqueness of the Canham-Evans-Helfrich Model for Biomembranes*

Antoine Laurain – *Controlling the footprint of droplets*

Steven Ruuth – *An implicit formulation of the closest point method using RBF-FD and applications to PDEs on moving surfaces*

Nung Kwan Yip – *Convergence of various thresholding schemes*

Thursday, 08:30 – 10:10, Kulturhus

Ricardo Cortez – *Microorganisms swimming through a viscoelastic network*

Lisa Fauci – *Bacterial motility in confined environments*

Chandrasekhar Venkataraman – *Asymptotic limits of models for receptor-ligand dynamics*

David Landa Marbán – *An upscaled model for permeable biofilm formation in a thin strip*

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Numerical Solution and Uniqueness of the Canham-Evans-Helfrich Model for Biomembranes

Thomas Yu[1], **Jingmin Chen**[2], **Sara Grundel**[3], **Robert Kusner**[4]

[1] *Department of Mathematics, Drexel University, U.S.A.* yut@drexel.edu
[2] *Citigroup Global Markets Inc., U.S.A.* jingmchen@gmail.com
[3] *Max Planck Institute for Dynamics of Complex Technical Systems, Germany* grundel@mpi-magdeburg.mpg.de
[4] *Department of Mathematics, University of Massachusetts at Amherst, U.S.A.* kusner@math.umass.edu

The Canham-Evans-Helfrich model of biomembranes suggests that lipid-bilayers membranes tend to minimize its Willmore energy $W = \int H^2 dA$ while subjected to certain surface area, volume and inner-outer surface area difference constraints. We present numerical methods for solving this class of variational problems based on a technique known as subdivision surface and compare it with existing approaches based on piecewise linear (PL) surfaces. In contrast to PL surfaces, the (honest) Willmore energy of a subdivision surface exists; moreover, its value together with its first variation (w.r.t. the control vertex positions) can be efficiently computed.

In the arguably most ubiquitous case of spherical, or genus 0, membranes, we develop also a flexible C^2 and higher order subdivision scheme, and present experiments that suggest its superior performance over the more standard Loop subdivision method for the biomembrane problem. Overall, subdivision methods occur to be not only more accurate but also more robust than methods based on PL surfaces. The former is hardly surprising, but we are struggling in understanding the latter. The author hopes to mobilize some interest in understanding these geometric numerical methods more deeply.

Part of the difficulty in understanding the numerical methods intertwines with the fact that the geometric variational problems themselves are not well-understood at an analytic level. For instance, it is well-known that the Willmore ernergy is invariant under not only Euclidean rigid motions and scaling, but also sphere inversions; under what situations would the extra constraints (area, volume, area difference) uniquely pin down the Euclidean shape of the Willmore minimizer? We shall present some of our preliminary results in this wide-open uniqueness problem.

(The speaker thanks undergraduate Co-ops Andrew Zigerelli, Yilin Yang, and Patrick Brogan for their extensive effort in algorithm developments and numerical experiments.)

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Controlling the footprint of droplets

Antoine Laurain[1], **Shawn W. Walker**[2]

[1] *Instituto de Matemática e Estatística, Universidade de São Paulo, Rua do Matão, 1010, CEP 05508-090 - São Paulo - SP, Brazil.* laurain@ime.usp.br
[2] *Department of Mathematics, Louisiana State University, Baton Rouge, LA 70803-4918.* walker@math.lsu.edu

The development of engineered substrates has progressed to an advanced level, which allows for control of the shape of sessile droplets on these substrates. Controlling local droplet shape via substrate surface tensions has various applications, such as directing the growth of bio-films and cell cultures, depositing a film of material onto a substrate in a particular pattern, or creating lenses with focal properties controlled by locally modifying substrate tensions.

We present an optimal control of a free boundary problem. Specifically, we show how to direct the shape of the droplet-substrate interface, also called "droplet footprint", by controlling the substrate surface tension. We use shape differential calculus to derive a gradient flow approach to compute equilibrium shapes for sessile droplets on substrates. We prove a shape sensitivity result with respect to the substrate surface tensions for the free boundary problem associated with the footprint. We then develop a gradient based optimization method to find the substrate surface tension yielding an equilibrium droplet shape with a desired footprint. The results are published in [1].

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An implicit formulation of the closest point method using RBF-FD and applications to PDEs on moving surfaces

Argyrios Petras[1], **Steve Ruuth**[2]

[1] *Basque Center for Applied Mathematics, Spain* apetras@bcamath.org
[2] *Department of Mathematics, Simon Fraser University, Canada* sruuth@sfu.ca

The closest point method [1] is an embedding method developed to solve a variety of partial differential equations (PDEs) on smooth surfaces using a closest point representation of the surface and standard Cartesian grid methods in the embedding space. Recently, an explicit closest point method was proposed that uses finite differences derived from radial basis functions (RBF-FD) [2]. Here we propose an implicit formulation of this method, using a least squares formulation to impose the constant extension of the solution off the surface in the normal direction. Our proposed method is particularly flexible with respect to the choice of the computational grid in the embedding space. In particular, we may compute over a computational tube that includes deactivated nodes. This fact enables us to combine the proposed method with the grid based particle method [3] to obtain a numerical method for approximating PDEs on moving surfaces. We present a number of examples to illustrate the numerical convergence properties of our method.

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Convergence of various thresholding schemes

Tim Laux[1], **Nung Kwan Yip**[2]

[1] *Max Planck Institute for the Mathematical Sciences, Leipzig, Germnay*
tim.laux@mis.mpg.de

[2] *Purdue University, West Lafayatte, Indiana, USA*
yip@math.purdue.edu

We present rigorous convergence proof for different versions of the classical thresholding scheme - alternating linear diffusion and projection. The scheme was first introduced by Merriman-Bence-Osher in the 90's and henceforth called the MBO scheme. Though it was originally formulated for the motion of a hypersurface by its mean curvature, recently it has found wide applications in simulating the motion of grain boundaries and junctions. We will discuss these recent advances, in particular we will prove their convergence to the underlying (geometric) motions for vortices, filaments and hypersurfaces. The key idea is the recent variational formulation and interpretation (by Esedoglu-Otto, Laux-Otto) of the MBO scheme as a gradient flow.

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Microorganisms swimming through a viscoelastic network

Ricardo Cortez[1], **Lisa Fauci**[2], **Jacek Wrobel**[3]

[1] *Tulane University, USA* rcortez@tulane.edu
[2] *Tulane University, USA* fauci@tulane.edu
[3] *Raytheon, USA* jwrobel@tulane.edu

In many physiological settings, microorganisms must swim through viscous fluids with suspended polymeric networks whose length scales are comparable to that of the organism. I will present a model of a flagellar swimmer moving through a compliant viscoelastic network immersed in a three-dimensional viscous fluid. The swimmer moves with a prescribed gait, exerting forces on the fluid and the heterogeneous network. The viscoelastic structural links of this network are stretched or compressed in response to the fluid flow caused by these forces, and these elastic deformations also generate forces on the viscous fluid. We track the swimmer as it leaves a region of Newtonian fluid, enters and moves through a heterogeneous network, and finally exits the network region back to the Newtonian space. We find that stiffer networks give a boost to the velocity of the swimmer. In addition, we find that the efficiency of swimming is dependent upon the evolution of the compliant network as the swimmer progresses through it.

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Bacterial motility in confined environments

Lisa J. Fauci[1], **John Lagrone**[1], **Ricardo Cortez**[1]

[1] *Tulane University, New Orleans, Louisiana, USA* fauci@tulane.edu

The ability of bacteria to swim through pores within soil or sediment that may be contaminated by oil is essential for their role in remediation. It is known that bacteria can move preferentially towards a chemoattractant by adjusting their run-and-tumble dynamics - the probability of their reorientation decreases as they move up the gradient. A tumbling event is characterized by a disruption of the flagellar bundle, where individual flagella may reverse their spin direction and move apart. We are interested in examining the dynamics of flagellar bundling within a pore whose diameter is on the scale of a flagellar length. As a step towards this goal, we consider a single elastic helical flagellum confined in a cylindrical tube. We examine its swimming performance when it is driven by an applied torque, balanced by an opposite torque on a virtual cell body. We also examine trajectories of the swimmer when its axis is initially not parallel to the axis of the cylinder.

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Asymptotic limits of models for receptor-ligand dynamics

Chandrasekhar Venkataraman[1], **Charles M. Elliott**[2], **Thomas Ranner**[3]

[1] *University of St Andrews, UK* cv28@st-andrews.ac.uk
[2] *University of Warwick, UK* c.m.elliott@warwick.ac.uk
[3] *University of Leeds, UK* t.ranner@leeds.ac.uk

We consider coupled bulk-surface systems of partial differential equations, with nonlinear coupling, that arise in mathematical models for receptor-ligand interactions. We motivate the consideration of a number of asymptotic limits of the models as they arise in biologically relevant regimes. We develop a mathematical theory for the treatment of the original problem and the resulting limits and discuss the approximation of the problems with a bulk-surface finite element method. Throughout the talk, the theoretical results will be supported by computations.

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MS14 – Biomembranes, Elastic Shells, and Complex Interfaces Symposium

An upscaled model for permeable biofilm formation in a thin strip

D. Landa Marbán[1], **F. A. Radu**[2], **I. S. Pop**[3], **K. Kumar**[4]

[1] *University of Bergen, Department of Mathematics, Norway* david.marban@uib.no
[2] *University of Bergen, Department of Mathematics, Norway* florin.radu@uib.no
[3] *University of Bergen, Department of Mathematics, Norway* iuliu.pop@uib.no
[4] *University of Bergen, Department of Mathematics, Norway* kundan.kumar@uib.no

The purpose of microbial enhanced oil recovery is the use of bacterial products to improve the oil extraction. After some time of injecting water to a reservoir, the water will flow through main paths and the oil production will stop. We can use the biomass in order to clog these main paths. Then, the water will flow through new paths, increasing the oil recovery. A mathematical model that realistically describes the biologically regulated mechanism of adaptive bio-plugging is needed to qualify the technology for field implementation. The focus of this work is the derivation of a core-scale model for permeable biofilm formation with variable biofilm density. We start building a pore-scale model in which the local geometry of the pore is represented as a thin strip [1]. We include in the model the composition of the biofilm: active biomass, EPS and water [2]. We apply homogenization techniques to obtain the upscaled model. We perform numerical simulations with both models (we implement the pore-scale model in COMSOL Multiphysics and the core-scale model in MRST) and we compare with laboratory experiments. We discuss all the results and propose further work.

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MS15 – Uncertainty Propagation

(Alexey Chernov, Oliver Ernst, Sebastian Krumscheid, Fabio Nobile)

Tuesday, 13:30 – 15:10, Hotel Fleischers Tarald

Dirk Nuyens – *Quasi-Monte Carlo (QMC) sampling*

Frances Kuo – *Quasi-Monte Carlo for stochastic wave propagation*

Alexey Chernov – *Multilevel Monte Carlo approximation of covariance functions*

Benjamin Peherstorfer – *Multifidelity methods for rare event simulation*

Wednesday, 08:30 – 10:10, Hotel Fleischers Tarald

Sebastian Krumscheid – *Multilevel Monte Carlo approximation of functions*

Anthony Nouy – *Higher-order principal component analysis for the approximation of functions in tree-based low-rank formats*

Colin Fox – *Bounding Errors in Estimates from Computational MCMC*

Martin Eigel – *A sampling-free adaptive Bayesian inversion with hierarchical tensor representations*

Thursday, 08:30 – 10:10, Hotel Fleischers Tarald

Markus Bachmayr – *Space-parameter-adaptive approximation of affine-parametric elliptic PDEs*

Akil Narayan – *Compressed sensing with sparse corruptions: Fault-tolerant sparse collocation approximations*

Harri Hakula – *Stochastic Galerkin approximation of the Reynolds equation with random film thickness*

Marc Schmidlin – *Uncertainty Quantification for PDEs with Anisotropic Random Diffusion*

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Quasi-Monte Carlo (QMC) sampling

Dirk Nuyens[1]

[1] *NUMA, KU Leuven, Belgium* dirk.nuyens@cs.kuleuven.be

Monte Carlo (MC) sampling is used in many uncertainty quantification problems. If MC sampling is used in the context of estimating expected values by averaging samples of the integrand function, then the convergence is rather slow, $O(N^{-1/2})$ for N samples of the integrand, but the bound comes (mostly) without the curse of dimensionality.

Quasi-Monte Carlo (QMC) sampling is a deterministic version of MC sampling, but can achieve higher rates, $O(N^{-\alpha})$, $\alpha > 1/2$, of convergence, for integrands with *mixed dominating smoothness* α. One such method is that of *interlaced polynomial lattice rules*, see, e.g., [1, 2]. In contrast to MC sampling, QMC sampling mostly does suffer from the curse of dimensionality, unless the method can be framed in a *weighted function space*. It is therefore interesting to analyse the problem and find a matching weighted function space of dominating mixed smoothness.

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Quasi-Monte Carlo for stochastic wave propagation

Frances Y. Kuo[1], **Mahadevan Ganesh**[2], **Ian H. Sloan**[3]

[1] *School of Mathematics and Statistics, UNSW Sydney, Australia* f.kuo@unsw.edu.au
[2] *Department of Applied Mathematics & Statistics, Colorado School of Mines, Golden, USA* mganesh@mines.edu
[3] *School of Mathematics and Statistics, UNSW Sydney, Australia* i.sloan@unsw.edu.au

The standard Galerkin variational formulation of the deterministic wave propagation model governed by the Helmholtz partial differential equation is indefinite for large wavenumbers. The lack of coercivity (indefiniteness) of the sesquilinear form in the standard Galerkin problem and associated finite element method models is one of the major difficulties for simulating and analyzing wave propagation models. This difficulty is markedly augmented when the input data in the wave propagation model, such as the refractive index, is a random field. We develop the analysis of quasi-Monte Carlo finite element methods for efficient simulation of such stochastic Helmholtz models.

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Multilevel Monte Carlo approximation of covariance functions

Alexey Chernov

Carl von Ossietzky University, Oldenburg, Germany alexey.chernov@uni-oldenburg.de

The problem of numerical estimation of statistical moments in complex PDE systems with uncertain parameters has received a substantial attention in the recent years. Frequently, realistic PDE models involve uncertain parameters with small spatial correlation length, or feature solutions having low stochastic regularity. In such cases a Monte Carlo simulation is a typical method of choice for numerical propagation of uncertainty [1] . The Multilevel Monte Carlo Method (MLMC) is an improvement of the Monte Carlo simulation that takes advantage of the hierarchical decomposition of the physical space. It combines coarse and therefore cheap samples of the solution with gradually more accurate samples obtained on refined grids in such a way that the overall complexity is significantly reduced preserving the same level of accuracy.

In this talk we focus on the numerical approximation of the covariance function by MLMC. A specific difficulty here is that the covariance function is a high-dimensional object defined in a spatial domain of double dimension. This significantly increases the cost of evaluation and storage requirements. The remedy proposed in [2] employs a sparse tensor product approximation of the covariance function. This approach involves an auxiliary decomposition in a hierarchical wavelet basis, a technical tool that is not easy to implement. We propose an alternative approximation that avoids hierarchical wavelet decomposition, develop an error analysis and comment on the performance of the proposed approach.

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Multifidelity methods for rare event simulation

Benjamin Peherstorfer[1], **Boris Kramer**[2], **Karen Willcox**[2]

[1] *University of Wisconsin-Madison, USA* peherstorfer@wisc.edu
[2] *Massachusetts Institute of Technology, USA* {bokramer,kwillcox}@mit.edu

In many situations across computational science and engineering, multiple computational models are available that describe a system of interest. These different models have varying evaluation costs and varying fidelities. Typically, a computationally expensive high-fidelity model describes the system with the accuracy required by the current application at hand, while lower-fidelity models are less accurate but computationally cheaper than the high-fidelity model. Sampling-based uncertainty propagation typically requires multiple model solves at many different inputs, which often leads to computational demands that exceed available resources if only the high-fidelity model is used. We present multifidelity methods for rare event simulation that leverage low-cost low-fidelity models for speedup and occasionally make recourse to the expensive high-fidelity model to establish unbiased estimators. Our methods combine low-fidelity models of any type, including projection-based reduced models, data-fit models and response surfaces, coarse-grid approximations, and simplified-physics models. Our numerical results demonstrate that our multifidelity methods achieve significant speedups while providing unbiased estimators, even in the absence of error control for the low-fidelity models.

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Multilevel Monte Carlo approximation of functions

S. Krumscheid[1], **F. Nobile**[2]

[1] *CSQI, Institute of Mathematics, EPFL, Switzerland* sebastian.krumscheid@epfl.ch
[2] *CSQI, Institute of Mathematics, EPFL, Switzerland* fabio.nobile@epfl.ch

Many applications across sciences and technologies require a careful quantification of non-deterministic effects to a system output, for example when evaluating the system's reliability or when gearing it towards more robust operation conditions. At the heart of these considerations lies an accurate yet efficient characterisation of uncertain system outputs. For the approximation of moments of said outputs, the multilevel Monte Carlo method has been established as a computationally efficient sampling method that is applicable to a wide range of applications. While a characterisation of the uncertain output in terms of a few moments may be sufficient in some applications, many applications would, however, require many (possibly infinitely many) moments for an accurate approximation of an output's distribution. That is, a moment-based characterisation of an uncertain output (e.g. via a truncated Edgeworth series expansion) is often unfeasible. As a matter of fact, in some practically relevant cases, for example when the system output follows a Lévy distribution (also known as a van der Waals profile), moments do not even exist, so that a moment-based characterisation is even impossible here.

In this talk we will introduce novel multilevel Monte Carlo techniques for an efficient characterisation of an uncertain system output's distribution. These techniques rely on accurately approximating general parametric expectations, i.e. expectations that depend on a parameter, uniformly on some interval. The resulting multilevel Monte Carlo estimators of such functions enable to derive efficient approximations of various means to characterise a system output's distribution, for example an approximation to the characteristic function or to the cumulative distribution function. A further important consequence of these results is that they allow to construct multilevel Monte Carlo estimators for various robustness indicators, such as for quantiles (also known as value-at-risk) or for the conditional value-at-risk. It is noteworthy that these robustness indicators cannot be expressed as moments. Consequently, they are out of reach for an efficient treatment via standard multilevel Monte Carlo methods, although first specialised multilevel techniques for some robustness indicators have been introduced recently. Here, we will present the construction and the analysis of general multilevel Monte Carlo methods for functions and discuss their applications to the estimation of various robustness indicators. Moreover, we will illustrate the performance of the developed multilevel methodologies using different benchmark examples, before, if time permits, addressing problems arising in the context of robust design in aeronautics.

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Higher-order principal component analysis for the approximation of functions in tree-based low-rank formats

Anthony Nouy[1]

[1] *Ecole Centrale Nantes, France* anthony.nouy@ec-nantes.fr

We present an algorithm for the approximation of high-dimensional functions using tree-based low-rank approximation formats (tree tensor networks). A multivariate function is here considered as an element of a Hilbert tensor space of functions defined on a product set equipped with a probability measure, the function being identified with a multidimensional array when the product set is finite. The algorithm only requires evaluations of functions (or arrays) on a structured set of points (or entries) which is constructed adaptively. The algorithm is a variant of higher-order singular value decomposition which constructs a hierarchy of subspaces associated with the different nodes of a dimension partition tree and a corresponding hierarchy of interpolation operators. Optimal subspaces are estimated using empirical principal component analysis of interpolations of partial random evaluations of the function. The algorithm is able to provide an approximation in any tree-based format with either a prescribed rank or a prescribed relative error, with a number of evaluations of the order of the storage complexity of the approximation format.

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Bounding Errors in Estimates from Computational MCMC

Colin Fox[1]

[1] *University of Otago, New Zealand* colin.fox@otago.ac.nz

Computational sample-based inference typically iterates a numerical approximation to the Metropolis-Hastings scheme. In statistics the standard practice is to assume that all calculations and the detailed-balance condition are computed exactly, while the numerical analyst is duty-bound to observe that this cannot be true. The good news is that detailed balance must be somehow robust to numerical error – otherwise statisticians would have complained a long time ago. More formally, we ask: what is the error in estimates induced by computational MCMC? We present analyses to treat deterministic and random numerical approximation.

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A sampling-free adaptive Bayesian inversion with hierarchical tensor representations

Martin Eigel[1], **Manuel Marschall**[2], **Reinhold Schneider**[3]

[1] *WIAS Berlin, Germany* martin.eigel@wias-berlin.de
[2] *WIAS Berlin, Germany* manuel.marschall@wias-berlin.de
[3] *TU Berlin, Germany* schneidr@math.tu-berlin.de

Based on a parametric deterministic representation of a linear forward model, a sampling-free approach to Bayesian inversion with an explicit representation of the parameter densities is developed. The approximation of the involved randomness inevitably leads to several high-dimensional expressions, which are often tackled with classical (slowly converging) sampling methods such as MCMC. As an alternative, a complete functional treatment of the inverse problem is derived, with *functional representations of the parametric forward solution as well as the probability densities* of the calibration parameters, determined by Bayesian inversion. The proposed sampling-free approach is discussed in the context of hierarchical tensor representations, which are employed for the adaptive evaluation of a random PDE (the forward problem) in generalized chaos polynomials [1] and the subsequent high-dimensional quadrature of the log-likelihood, which involves an adaptive Runge-Kutta method in tensor format. This modern compression technique alleviates the curse of dimensionality by hierarchical subspace approximations of the respective solution manifolds. A crucial point is that all required computations can then be carried out efficiently in the low-rank format. A priori convergence of the posterior is examined, considering all approximations that occur in the method [2].

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Space-parameter-adaptive approximation of affine-parametric elliptic PDEs

Markus Bachmayr

Universität Bonn, Hausdorff Center for Mathematics & Institute for Numerical Simulation, Wegelerstr. 6, 53115 Bonn, Germany bachmayr@ins.uni-bonn.de

We consider the approximation of PDEs with parameter-dependent coefficients by sparse polynomial approximations in the parametric variables combined with suitable discretizations in the spatial domain. Here we are especially interested in problems with countably many parameters, as they arise when coefficients with uncertainties are modelled as random fields. For the resulting fully discrete approximations of the corresponding solution maps, we obtain convergence rates in terms of the total number of degrees of freedom. In particular, in the case of affine parametrizations, we find that independent adaptive spatial approximation for each term in the polynomial expansion yields improved convergence rates. Moreover, we give a construction of near-optimal adaptive solvers for finding such approximations.

This talk is based on joint works with Albert Cohen, Wolfgang Dahmen, Dinh Dũng, Giovanni Migliorati, and Christoph Schwab.

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Compressed sensing with sparse corruptions: Fault-tolerant sparse collocation approximations

Akil Narayan[1], **Ben Adcock**[2], **Anyi Bao**[2], **John D. Jakeman**[3]

[1] *Department of Mathematics, Scientific Computing and Imaging (SCI) Institute, University of Utah, USA* akil@sci.utah.edu
[2] *Department of Mathematics, Simon Fraser University, Canada* ben_adcock@sfu.ca
[3] *Computer Sciences Research Institute, Sandia National Laboratories, USA* jdjakem@sandia.gov

The recovery of approximately sparse or compressible coefficients in a Polynomial Chaos Expansion is a common goal in modern parametric uncertainty quantification (UQ). However, relatively little effort in UQ has been directed toward theoretical and computational strategies for addressing the sparse *corruptions* problem, where a small number of measurements are highly corrupted. Such a situation has become pertinent today since modern computational frameworks are sufficiently complex with many interdependent components that may introduce hardware and software failures, some of which can be difficult to detect and result in a highly polluted simulation result. [2]

In this presentation we present a novel compressive sampling-based theoretical analysis for a regularized ℓ^1 minimization algorithm that aims to recover sparse expansion coefficients in the presence of measurement corruptions [1]. Our recovery results are uniform, and prescribe algorithmic regularization parameters in terms of a user-defined *a priori* estimate on the ratio of measurements that are believed to be corrupted. We also propose an iteratively reweighted optimization algorithm that automatically refines the value of the regularization parameter, and empirically produces superior results. Our numerical results test our framework on several medium-to-high dimensional examples of solutions to parameterized differential equations, and demonstrate the effectiveness of our approach.

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Stochastic Galerkin approximation of the Reynolds equation with random film thickness

Harri Hakula[1]

[1] *Department of Mathematics and Systems Analysis, Aalto University, Finland*
Harri.Hakula@aalto.fi

Consider the equations governing an isothermal flow of an incompressible viscous fluid,

$$\rho\left(\frac{\partial \boldsymbol{v}}{\partial t} + (\nabla \boldsymbol{v})\boldsymbol{v}\right) = -\nabla p + 2\mu \operatorname{div} \boldsymbol{D}(\boldsymbol{v}) + \rho \boldsymbol{b}, \quad \operatorname{div} \boldsymbol{v} = 0,$$

where $\boldsymbol{v}$ is the unknown velocity field, $\rho > 0$ is the constant density, $\mu > 0$ is the constant viscosity and $\boldsymbol{b}$ corresponds to the body force. Moreover, $\boldsymbol{D}(\boldsymbol{v}) = \frac{1}{2}(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T)$ denotes the symmetric part of the velocity gradient and p is a scalar field associated with the incompressibility constraint—often referred to as the mechanical pressure [1]. We consider stationary flows while assuming that the inertial effects and contribution of the body force can be neglected. This reduces the governing equations to the following Reynolds equation via an intermediate Stokes system:

$$\frac{\partial}{\partial x}\left(h^3 \frac{\partial p}{\partial x}\right) = \frac{\partial h}{\partial x}. \tag{7}$$

The irregularity of the channel height will be introduced through a perturbation of h by a suitable random field. Formally the stochastic Reynolds equations becomes: Let (Ω, Σ, P) be a probability space. Find a random pressure field $p \in L^2_P(\Omega, H^1_0(D))$ such that

$$\frac{\partial}{\partial x}\left(\big[h(\omega, x)\big]^3 \frac{\partial p(\omega, x)}{\partial x}\right) = \frac{\partial h(\omega, x)}{\partial x}, \quad \text{in } D, \tag{8}$$

$$p(\omega, x) = 0, \quad \text{on } \partial D. \tag{9}$$

In this talk, different modeling options in realistic geometries are discussed. Special emphasis is on non-affine KL-expansion of $h(\omega, x)$. In practical problems low-frequency perturbations correspond to manufacturing imperfections, for instance in casting, and are more important than the high-frequency ones typically related to damage and wear. The effectiveness of the Galerkin approach is demonstrated using a series of numerical experiments.

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Uncertainty Quantification for PDEs with Anisotropic Random Diffusion

Helmut Harbrecht[1], **Michael D. Peters**[2], **Marc Schmidlin**[3]

[1] *University of Basel, Switzerland* helmut.harbrecht@unibas.ch
[2] *EPF Lausanne, Switzerland* michael.peters@epfl.ch
[3] *University of Basel, Switzerland* marc.schmidlin@unibas.ch

We will consider elliptic diffusion problems with an anisotropic random diffusion coefficient. More specifically, we will model diffusion in a medium comprised of very thin fibres, where the diffusion strength in fibre direction is notably different to the diffusion strength perpendicular to the fibres – thus we may describe the diffusion strength in fibre direction and the actual fibre direction by a vector field $\mathbf{V}$. Any uncertainty regarding the vector field $\mathbf{V}$ then propagates, yielding uncertainty in the diffusion coefficient and therefore also in the solution of our elliptic diffusion problem.

Using the vector field $\mathbf{V}$'s Karhunen-Loève expansion we can reformulate the elliptic diffusion problem into a parametric form with a random parameter. We then derive that the regularity of the solution's dependence on the random parameter is entirely determined by the decay of the vector field $\mathbf{V}$'s Karhunen-Loève expansion. This result allows for sophisticated quadrature methods, such as the quasi-Monte Carlo method or the anisotropic sparse grid quadrature, to be used to approximate quantities of interest, like the solution's mean or its variance. Numerical examples will be presented to supplement the theoretical results.

References

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MS16 – Mixed and nonsmooth methods in numerical solid mechanics

(Fleurianne Bertrand, Oliver Sander)

Monday, 15:50 – 17:30, Hotel Fleischers Osa

Jad Dabaghi – *Adaptive inexact semi–smooth Newton methods for a contact between two membranes*

Bernhard Kober – *Strong vs. Weak Symmetry in Stress-Based Mixed Finite Element Methods for Linear Elasticity*

Marcel Moldenhauer – *Stress reconstruction for the nonconforming P2 finite element method and a posteriori error estimation*

Ingo Münch – *Evolution of load-bearing structures with phase field modeling*

Tuesday, 15:30 – 17:10, Hotel Fleischers Osa

Thomas Richter – *An accelerated Newton multigrid method for nonlinear materials in structure mechanics and fluid mechanics*

Oliver Sander – *Nonsmooth multigrid methods for plasticity and phasefield problems*

Gerhard Starke – *Stress-Based Mixed Finite Element Methods with Weakly Enforced Symmetry for Elasto-Plasticity*

Nils Viebahn – *Pros and Cons of some mixed Galerkin and Least-Squares Finite Element schemes*

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Adaptive inexact semi–smooth Newton methods for a contact between two membranes

Jad Dabaghi[1], **Martin Vohralík**[2], **Vincent Martin**[3]

[1] *Inria Paris, 2 rue Simone Iff, 75589 Paris, & Université Paris-Est, CERMICS (ENPC), 77455 Marne-la-Vallée 2, France* jad.dabaghi@inria.fr
[2] *Inria Paris, 2 rue Simone Iff, 75589 Paris, & Université Paris-Est, CERMICS (ENPC), 77455 Marne-la-Vallée 2, France* martin.vohralik@inria.fr
[3] *Université technologie de Compiègne (UTC), 60200, France* vincent.martin@utc.fr

We propose an adaptive inexact version of a class of semi-smooth Newton methods. As a model problem, we consider the system of variational inequalities describing the contact between two membranes and its finite element discretization. Any iterative linearization algorithm like the Newton-min, Newton-Fisher Burmeister is taken into account, as well as any iterative linear algebraic solver. We prove an a posteriori error estimate between the exact solution and the approximate solution valid on any step of the linearization and algebraic resolution. This estimate is based on discretization and algebraic flux reconstructions, where the latter one is obtained on a hierarchy of nested meshes. The estimate distinguishes the discretization, linearization, and algebraic components of the error and allows us to formulate adaptive stopping criteria for both solvers. Numerical experiments for the semi-smooth Newton-min algorithm in combination with the GMRES solver confirm the efficiency of the method.

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Strong vs. Weak Symmetry in Stress-Based Mixed Finite Element Methods for Linear Elasticity

Bernhard Kober[1], **Gerhard Starke**[2]

[1] *Fakultät für Mathematik, Universität Duisburg-Essen, 45127 Essen*
bernhard.kober@stud.uni-due.de

[2] *Fakultät für Mathematik, Universität Duisburg-Essen, 45127 Essen*
gerhard.starke@uni-due.de

In stress-based mixed finite element methods the approximation of the stress ideally fulfills two requirements: First, to satisfy the conservation of angular momentum, the stress tensor should be symmetric, and second, to satisfy the conservation of momentum, the normal component across cell interfaces should be continuous. Since the implementation of finite element spaces that satisfy both requirements is less efficient than other mixed methods, relaxing either one of the two constraints is an expedient and often used approach. We study the relationship and properties of two such approaches: In [2] stress is approximated in the $H(\mathrm{div})$-conforming Raviart-Thomas space while symmetry is (only weakly) enforced by a Lagrange multiplier approximating the unsymmetric part of the displacement gradient. In [2], on the other hand, the stress approximation is symmetric while only the first moments of its normal component are continuous across cell interfaces. We propose a simple way to construct a finite element space that is easy to implement and that contains both the Raviart-Thomas and the nonconforming symmetric space. Using this space, we can apply the method of [2] to obtain the approximation of [2] and compare and assess the two approaches.

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Stress reconstruction for the nonconforming P2 finite element method and a posteriori error estimation

Marcel Moldenhauer[1], **Gerhard Starke**[2], **Fleurianne Bertrand**[3]

[1] *Fakultät für Mathematik, Universität Duisburg-Essen, Thea-Leymann-Straße 9, 45127 Essen, Germany* marcel.moldenhauer@uni-due.de
[2] *Fakultät für Mathematik, Universität Duisburg-Essen, Thea-Leymann-Straße 9, 45127 Essen, Germany* gerhard.starke@uni-due.de
[3] *Fakultät für Mathematik, Universität Duisburg-Essen, Thea-Leymann-Straße 9, 45127 Essen, Germany* fleurianne.bertrand@uni-due.de

We want to build upon the framework given in [1] and present an a posteriori error estimator for the nonconforming P2 finite element method of the nonlinear hyperelasticity problem based on the approximation of the first Piola-Kirchhoff stress tensor.
In [2] a nonconforming P2 finite element method was used with success to reconstruct an H(div)-conforming flux with application to a posteriori error estimation. We want to study the positive characteristics of nonconforming P2 elements in the framework of [1] and confirm the quality of our stress reconstruction and effectiveness of our error estimator with numerical examination of the Cooks membran problem. See also [3].

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS16 – Mixed and nonsmooth methods in numerical solid mechanics

Evolution of load-bearing structures with phase field modeling

Ingo Münch[1]

[1] *Karlsruhe Institute of Technology, Germany* ingo.muench@kit.edu

We suggest an algorithm to generate the topology of load-bearing structures automatically. Such algorithms are of great practical importance since most real-world problems cannot be solved analytically. Since Bendsøe and Kikuchi [1] proposed the material distribution concept instead of discrete values for voids and material, numerical methods for topology optimization have been investigated extensively and reached the stage of application in industrial software [2].

In our approach, the desired filling level is the main parameter of the objective function. On the basis of phase field modeling the boundary value problem is solved within the Finite Element framework. The phase field parameter couples to the density and stiffness of the material. An Allen-Cahn equation describes the phase transition such that the steady state yields the final topology. We drop mass conservation and couple the von Mises stress to the nucleation density in the design domain. Negative nucleation density leads to the reduction of material, whereas positive nucleation density increases the density of material. The model is tuned to evolve continuous regions of voids or dense material. Voids retain an infinitesimal residual stiffness, which is by factor 10^{-6} lower than the stiffness of the dense material. However, FEM-remeshing is not required. The complexity of the resulting topology is controlled by two parameters, which we discuss in several numerical experiments.

Due to the bright spectrum of mechanical applications, the objective function for topology optimization lies in the eye of the beholder. From a practical point of view, the complexity of the topology is limited by aspects of manufacturing. From a mechanical point of view, the minimal compliance case of a structure is attractive, see among the others [3]. In [4] the objective function minimizes the overall stress field σ. However, our algorithm homogenizes the von Mises stress within the evolving structure. The specific material can be considered a posteriori, e.g., steel with appropriate elastic limit.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS16 – Mixed and nonsmooth methods in numerical solid mechanics

An accelerated Newton multigrid method for nonlinear materials in structure mechanics and fluid mechanics

T. Richter

Otto-von-Guericke-Universität Magdeburg, Germany thomas.richter@ovgu.de

We analyze a modified Newton method that was first introduced by Turek and coworkers [1]. The basic idea of the acceleration technique is to split the Jacobian $A(x)$ into a "good part" $A_1(x)$ (possibly positive definite) and into a troublesome part $A_2(x)$. During the course of convergence, this second part is adaptively damped, such that the solver is a blend between a Picard iteration and the full Newton scheme.

For prototypical problems with similarities to non Newtonian fluid models, viscous-plastic materials like sea ice (see [2] for an application of this Newton scheme) or Bingham plastics we will provide an analysis of this technique and show, how a proper combination of the adaptive Newton scheme with global damping will lead to fast convergence, where traditional solvers fail or converge very slowly.

The linear problems are approximated with a geometric multigrid solvers. Linear tolerances are adaptively coupled to the nonlinear Newton convergence. By a special blocking of different solution unknowns a very good robustness is obtained for complex nonlinear problems.

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MS16 – Mixed and nonsmooth methods in numerical solid mechanics

Nonsmooth multigrid methods for plasticity and phasefield problems

Oliver Sander[1], **Carsten Gräser**[2]

[1] *Institut für Numerische Mathematik, TU Dresden, Germany*
oliver.sander@tu-dresden.de
[2] *Fachbereich Mathematik und Informatik, FU Berlin, Germany* graeser@mi.fu-berlin.de

Various problems in mechanics lead to nonsmooth (almost) convex minimization problems. Besides contact and friction problems, this structure is exhibited by primal plasticity models and phase-field models of fracture formation. Such problems are typically solved using predictor–corrector or operator-splitting methods. These are expensive, because they solve sequences of linear problems. Also, their convergence behavior is not always clear.

We propose a nonsmooth multigrid method that can solve these problems roughly in the time of one linear problem. For primal plasticity problems this means that solving one spatial problem can be done in the time of a single predictor–corrector iteration. This is shown experimentally, and we prove that the method converges for any initial iterate and any associative smooth or nonsmooth yield law.

The energies used in phase-field models of fracture formation are frequently biconvex rather than convex. Nevertheless, numerical experiments show clear superiority of the multigrid method over traditional operator-splitting schemes. Additionally, a slightly generalized convergence result shows global convergence of the multigrid solver to a stationary point of the energy.

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MS16 – Mixed and nonsmooth methods in numerical solid mechanics

Stress-Based Mixed Finite Element Methods with Weakly Enforced Symmetry for Elasto-Plasticity

Gerhard Starke[1]

[1] *Fakultät für Mathematik, Universität Duisburg-Essen, 45127 Essen*
gerhard.starke@uni-due.de

A large number of stress-based mixed finite element approaches have been proposed in recent decades and studied for linear elasticity computations. Among those methods with weakly enforced symmetry by Lagrange multipliers those using Raviart-Thomas spaces are particularly appealing. One of the reasons for this is that their behaviour is quite similar in two and three space dimensions. We study the finite element combinations based on next-to-lowest order Raviart-Thomas spaces by [2] and [3] for elasto-plasticity with a von Mises yield criterion. In fact, looking at the original PEERS paper by [1] which started the history of weakly symmetric stress methods, it is interesting to note that the treatment of plasticity was one of their main motivations. In our approach, the plasticity constraint is treated with a semi-smooth Newton method leading to a sequence of linear saddle-point problems for the stresses. A displacement reconstruction in H^1 gives rise to a least-squares functional which constitutes an a posteriori error estimator using results from [4]. The effectiveness of the resulting adaptive refinement strategy will be examined by computational results.

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ENUMATH 2017
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MS16 – Mixed and nonsmooth methods in numerical solid mechanics

Pros and Cons of some mixed Galerkin and Least-Squares Finite Element schemes

Jörg Schröder[1], **Nils Viebahn**[1], **Karl Steeger**[1]

[1] *Institut für Mechanik, Universität Duisburg-Essen, Germany* nils.viebahn@uni-due.de

Numerical simulations of physical phenomena require efficient finite element formulations which provide reliable results for all physical quantities needed. In solid mechanics often used standard Galerkin displacement elements could provide unphysical results under certain circumstances, as e.g. incompressibility. To overcome this deficiency, mixed methods are a suitable choice. For an overview over mixed elements, the reader is referred to [1]. Basis for mixed Galerkin finite elements are, in general, functionals of Hu-Washizu or Hellinger-Reissner type. Unfortunately, these mixed methods should fulfill several mathematical requirements, especially the LBB-condition (Ladyzhenskaya-Babuška-Brezzi-condition), see e.g. [2]. This inf-sup condition demands to balance the polynomial orders of the chosen interpolations for the different field variables. Another approach to construct mixed finite elements is the least-squares finite element method (LSFEM), compare e.g. [3], which is a minimization problem and not restricted by the LBB-condition. The L_2-norm minimization of the residuals of the given first-order system of differential equations (balance of momentum and constitutive relation) and the choice of suitable weights lead to a functional depending on displacements and stresses. In the present contribution the arising solution spaces and the conforming and non-conforming discretization of the field quantities will be discussed for both element types. Furthermore, the mixed Galerkin finite elements will be compared to mixed LSFEMs with regard to reliability and performance for geometrically linear and nonlinear problems and structural stability problems, see also [4] and [5].

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MS17 – A posteriori error estimation, adaptivity and approximation

(Christian Kreuzer, Andreas Veeser, Pietro Zanotti)

Thursday, 08:30 – 10:10, Hotel Fleischers Sivle

Peter Binev – *Tree Approximation and Adaptive Methods*

Andreas Veeser – *Best error localization with piecewise polynomials in a Sobolev Hilbert triple*

Fernando Gaspoz – *H^1-stability of the L^2-projection and applications to adaptive methods*

Markus Weimar – *Explicit regularity estimates for solutions to quasi-linear PDEs*

Thursday, 13:30 – 15:10, Hotel Fleischers Kvitanosi

Lars Diening – *Local estimates for the discrete (p-)harmonic functions for fully adaptive meshes*

Karsten Urban – *Reduced Basis Methods and Adaptivity*

Alexander Haberl – *Adaptive FEM and adaptive BEM for the Helmholtz equation*

Patrik Daniel – *An adaptive hp-refinement strategy with computable guaranteed error reduction factors*

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MS17 – A posteriori error estimation, adaptivity and approximation

Tree Approximation and Adaptive Methods

Peter G. Binev[1]

[1] *Department of Mathematics, University of South Carolina, Columbia, SC 29208, USA*
binev@math.sc.edu

Adaptive methods for approximation can be formally described through the process of growing a full binary tree T that represents a coarse-to-fine partitioning of the domain. Each element Δ of the partition is related to a leaf-node of the tree T, also denoted by Δ. The set $\mathcal{L}(T)$ of leaf-nodes represents the entire partition. If $e(\Delta)$ is the local error at Δ or its estimate, then $\sum_{\Delta\in\mathcal{L}(T)} e(\Delta)$ is used as the total error of approximation. The goal is to build a tree T with a given number of nodes such that its total error is as small as possible by using only the information about $e(\Delta)$ of the current nodes. This setup is often employed for the h-adaptive finite elements methods.

To extend this framework for the case of hp-adaptivity, we introduce *ghost* subtrees $\mathcal{T}_\Delta$ each of which is rooted at a leaf-node $\Delta \in \mathcal{L}(T)$. The number of leaves of the ghost tree $\mathcal{T}_\Delta$ assigns the number of degrees of freedom to be used in the approximation of the element Δ. The entire tree structure $\mathcal{T}$ – the partition tree T together with the attached ghost trees $\mathcal{T}_\Delta$ – represents the local distribution of the number of degrees of freedom on the domain. For finding $\mathcal{T}$ we introduce a greedy-type algorithm with respect to quantities based on a modification of the local approximation errors. The partition tree T is received by trimming $\mathcal{T}$ in an optimal way with respect to the total hp-type error.

We prove that the proposed algorithms have near-best performance and near-optimal complexity in both cases of h- and hp-adaptivity in different approximation setups.

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MS17 – A posteriori error estimation, adaptivity and approximation

Best error localization with piecewise polynomials in a Sobolev Hilbert triple

Francesca Tantardini[1], **Andreas Veeser**[2], **Rüdiger Verfürth**[3]

[1] *Ruhr-Universität Bochum, Germany* francesca.tantardini@ruhr-uni-bochum.de
[2] *Università degli Studi di Milano, Italy* andreas.veeser@unimi.it
[3] *Ruhr-Universität Bochum, Germany* ruediger.verfuerth@ruhr-uni-bochum.de

Consider the problem of approximating some function from a Sobolev space by continuous functions that are piecewise polynomial with fixed total degree. Best error localization means that the best error over the whole domain is equivalent to an l_2-norm of best errors over small subdomains, which ideally are mesh elements. The equivalence may depend on the shape regularity of the underlying mesh, but is independent of the regularity of the involved target function. Such a basic approximation result is an attractive departure point for error bounds as well as useful in the context of adaptivity.

In this talk we shall present best error localizations in H^1_0, L_2 and H^{-1}. We will compare them, outline differences, and discuss also simultaneous best error localization in this Hilbert triple.

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H^1-stability of the L^2-projection and applications to adaptive methods

Fernando Gaspoz[1], **Claus-Justus Heine, Kunibert Siebert**

[1] *University of Stuttgart, Germany* fernando.gaspoz@ians.uni-stuttgart.de

The L^2-projection onto discrete spaces plays an essential role in the analysis of finite element discretizations. On uniform grids H^1-stability of the L^2-projection can easily be deduced by an inverse estimate. This simple proof hinges on the fact that the minimal mesh-size is comparable to the maximal mesh-size. We provide a technique that sidestep this restriction and prove the stability in H^1 of the L^2-projection for piecewise continuous Finite Element Spaces for a class of adaptive meshes. We also present some new applications of this estimate.

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MS17 – A posteriori error estimation, adaptivity and approximation

Explicit regularity estimates for solutions to quasi-linear PDEs

M. Weimar[1]

[1] *Ruhr-Universität Bochum, Germany* markus.weimar@rub.de

It is well-known that the rate of convergence of numerical schemes which aim to approximate solutions to operator equations is closely related to the maximal regularity of these solutions in certain scales of smoothness spaces of Sobolev and Besov type. For linear elliptic PDEs on Lipschitz domains, a lot of results in this direction already exist. In contrast, it seems that not too much is known for nonlinear problems.

In this talk, we are mainly concerned with the p-Laplace operator which has a similar model character for quasi-linear equations as the ordinary Laplacian for linear problems. It finds applications in models, e.g., for turbulent flows of a gas in porous media, radiation of heat, as well as in non-Newtonian fluid theory. We discuss a couple of local regularity estimates for the gradient of the unknown solutions. These assertions are then used to derive global smoothness properties by means of wavelet-based proof techniques. Finally, the presented results imply that adaptive algorithms are able to outperform (at least asymptotically) their commonly used counterparts based on uniform refinement.

The material extends assertions which were obtained earlier in joint work with S. Dahlke, L. Diening, C. Hartmann, and B. Scharf [1, 2].

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Local estimates for the discrete (p-)harmonic functions for fully adaptive meshes

L. Diening[1], **T. Scharle**[2]

[1] *University of Bielefeld, Germany* lars.diening@uni-bielefeld.de
[2] *Oxford University, Great Britain* toni.scharle@queens.ox.ac.uk

It is well known that harmonic functions and p-harmonic functions have higher interior regularity. In 1957 De Giorgi introduced a new technique that allows for example to estimate the maximum of the solution on a ball by an mean integral of the solution on an enlarged ball. A similar result holds for p-harmonic functions. The proof is based on subtle Cacciopoli estimates using truncation operators. In this talk we present similar estimates for discretely harmonic and p-harmonic functions. Our solutions can be scalar valued as well as vector valued, which makes a big difference for p-harmonic functions.

Such estimates are of strong interest, since these estimates provide an alternative approach to L^∞-estimates of the error $u - u_h$, which is a future project. Various results already exist in this direction for harmonic functions, e.g. [2]. However, the main obstacle in this direction even in the linear case is adaptivity. All of the results obtained so far, require that the mesh size does not vary too much locally. This puts certain undesired assumptions on the refinement algorithm.

Our approach differs in such that we allow for arbitrary highly graded meshes (still shape regular). However, our approach uses certain properties of the Lagrange basis functions. This restrict our approach at the moment to acute meshes and linear elements. The proof of our result is based on a discretized version of the De Giorgi technique.

Let us mention also that there is a strong relation to the discrete maximum principle. In particular, in the case of p-harmonic functions, similar truncation operators and similar mesh requirements (non-obtuse) appear, see [1].

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MS17 – A posteriori error estimation, adaptivity and approximation

Reduced Basis Methods and Adaptivity

Karsten Urban[1]

[1] *Ulm University, Inst. of Numerical Mathematics, Helmholtzstr. 20, 89081 Ulm, Germany*
karsten.urban@uni-ulm.de

The reduced basis method (RBM) has become a standard tool for the efficient numerical solution of parameterized partial differential equations (PPDEs). Typically, the RBM relies on a detailed (high fidelity) discretization (sometimes called 'truth'), which is used for all parameters. The reduced model is then determined based upon this truth.

Of course, the reduced model can only be as good as the detailed model, which immediately raises the question why not to use adaptive methods (in space, time and/or dimension) to construct the reduced model. In this talk, we discuss some results in that direction.

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MS17 – A posteriori error estimation, adaptivity and approximation

Adaptive FEM and adaptive BEM for the Helmholtz equation

Alex Bespalov[1], Alexander Haberl[2] and Dirk Praetorius[2]

[1] *School of Mathematics, University of Birmingham, UK* a.bespalov@bham.ac.uk
[2] *Institute for Analysis and Scientific Computing, TU Wien, Austria*
alexander.haberl@asc.tuwien.ac.at
dirk.praetorius@asc.tuwien.ac.at

Given $f \in \mathcal{H}^*$, we consider adaptive FEM and BEM for weak formulations of the type

$$a(u,v) + \langle \mathcal{K}u, v\rangle = \langle f, v\rangle \quad \text{for all } v \in \mathcal{H}, \tag{10}$$

where $a(\cdot,\cdot)$ is an elliptic and symmetric bilinear form on $\mathcal{H} := H^1_0(\Omega)$ for FEM, or $\mathcal{H} := H^{-1/2}(\partial\Omega)$ for BEM and $\mathcal{K} : \mathcal{H} \to \mathcal{H}^*$ is a continuous and compact linear operator. We suppose that (10) is well-posed and hence admits a unique solution $u \in \mathcal{H}$. This setting is met, e.g., for the Helmholtz equation. For a standard conforming FEM and BEM discretization of (10) by piecewise polynomials, usual duality arguments show that the underlying triangulation has to be sufficiently fine to ensure the existence and uniqueness of the Galerkin solution.

Extending the abstract approach of [1], we prove in [4] that adaptive mesh-refinement is capable of overcoming this preasymptotic behavior and eventually leads to convergence with optimal algebraic rates. Unlike previous works [2, 3], one doesn't have to deal with the *a priori* assumption that the initial mesh is sufficiently fine. The overall conclusion of our results thus is that adaptivity has stabilizing effects and can, in particular, overcome preasymptotic and possibly pessimistic restrictions on the meshes.

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An adaptive hp-refinement strategy with computable guaranteed error reduction factors

Patrik Daniel[1], **Alexandre Ern**[2], **Iain Smears**[1], **Martin Vohralík**[1]

[1] *Inria Paris, 2 rue Simone Iff, 75589 Paris, France & Université Paris-Est, CERMICS (ENPC), 77455 Marne-la-Vallée 2, France* patrik.daniel@inria.fr
iain.smears@inria.fr
martin.vohralik@inria.fr

[2] *Université Paris-Est, CERMICS (ENPC), 77455 Marne-la-Vallée 2, France & Inria Paris, 2 rue Simone Iff, 75589 Paris, France* alexandre.ern@enpc.fr

We propose a new practical adaptive refinement strategy for hp-finite element approximations of elliptic problems. Following some recent theoretical developments in polynomial-degree-robust a posteriori error analysis, we solve two complementary classes of discrete local problems on the vertex-based patches. The first class involves the solution on each patch of a mixed finite element problem with homogeneous Neumann boundary conditions, which leads to an $\mathbf{H}(\mathrm{div}, \Omega)$-conforming equilibrated flux. This in turns yields a guaranteed upper bound on the error and serves to mark elements for refinement via a Dörfler bulk criterion. The second class of local problems involves the solution, on each marked patch only, of two separate primal finite element problems with homogeneous Dirichlet boundary conditions, which serve to decide between h-, p-, or hp-refinement. Altogether, we show that these ingredients lead to a computable error reduction factor; we guarantee that while performing the hp-adaptive refinement as suggested, the error will be reduced at least by this factor on the next hp-mesh. In a series of numerical experiments in two space dimensions, we first study the accuracy of our predicted reduction factor: in particular, we measure the ratio of the predicted reduction factor relative to the true error reduction, and we find that it is very close to the optimal value of one for both smooth and singular exact solutions. Finally, we study the overall performance of the proposed hp-refinement strategy on several test cases, for which we observe exponential convergence rates.

MS18 – Noncommutative stochastic differential equations: Analysis and simulation

(Kurusch Ebrahimi-Fard, Simon J.A. Malham, Anke Wiese)

Tuesday, 08:30 – 10:10, Hotel Fleischers Tarald

Anne Kværnø – *Stochastic B–series and order conditions for exponential integrators*

Charles Curry – *Noncommutative stochastic exponentials: analytic and geometric perspectives*

Kurusch Ebrahimi-Fard – *Non-commutative stochastic exponentials from a shuffle algebra viewpoint*

Thomas Cass – *A Stratonovich-to-Skorohod conversion formula for integrals with respect to Gaussian rough paths*

Wednesday, 15:55 – 17:35, Hotel Fleischers Tarald

Anke Wiese – *The exponential Lie series for continuous semimartingales*

Yvain Bruned – *Renormalisation of singular SPDEs*

Laure Coutin – *Invariance for rough differential equations.*

Simon Malham – *Stochastic differential systems and efficient integrators*

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MS18 – Noncommutative stochastic differential equations: Analysis and simulation

Stochastic B–series and order conditions for exponential integrators

A. A. Arara[1], **K. Debrabant**[2], **A. Kværnø**[3]

[1] *School of Mathematics and Statistics, Hawassa University, Hawassa, Ethiopia*
alemayehu_arara@yahoo.com

[2] *Kristian Debrabant, Department of Mathematics and Computer Science, University of Southern Denmark, 5230 Odense M, Denmark*
debrabant@imada.sdu.dk

[3] *Department of Mathematical Sciences, Norwegian University of Science and Technology - NTNU, NO-7491 Trondheim, Norway.*
anne.kvarno@ntnu.no

We will discuss B–series for the solution of a stochastic differential equation of the form

$$\mathrm{d}X(t) = \Big(AX(t) + g_0\big(X(t)\big)\Big)\mathrm{d}t + \sum_{m=1}^{M} g_l(X(t)) \star \mathrm{d}W_m(t), \quad X(0) = x_0,$$

for which the exact solution can be written as

$$X(t) = e^{tA}x_0 + \int_0^t e^{(t-s)A} g_0(X(s))\mathrm{d}s + \sum_{m=1}^{M} \int_0^t e^{(t-s)A} g_m(X(s)) \star \mathrm{d}W_m(s)$$

Based on this, we will derive an order theory for exponential integrators for such problems. The integral w. r. t. the Wiener process has to be interpreted e. g. as an Itô or a Stratonovich integral. This is an extention of the stochastic B–series theory developed in [1].

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MS18 – Noncommutative stochastic differential equations: Analysis and simulation

Noncommutative stochastic exponentials: analytic and geometric perspectives

Ch. Curry[1]

[1] *Department of Mathematical Sciences, Norwegian University of Science and Technology – NTNU, NO-7491 Trondheim, Norway* charles.curry@ntnu.no

We explore different situations in which noncommutative stochastic exponentials arise, including stochastic exponentials on Lie groups and other manifolds [3, 4, 5, 7], free stochastic exponentials [1, 2], and exponentials in quantum stochastic calculus [6, 8]. In doing so we lay the foundations for algebraic treatments of these separate cases.

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MS18 – Noncommutative stochastic differential equations: Analysis and simulation

Non-commutative stochastic exponentials from a shuffle algebra viewpoint

K. Ebrahimi-Fard[1]

[1] *Department of Mathematical Sciences, Norwegian University of Science and Technology – NTNU, NO-7491 Trondheim, Norway* kurusch.ebrahimi-fard@math.ntnu.no

Based on joint work [2], where a formula is given for the logarithm of the solution of a linear matrix-valued SDE driven by arbitrary semimartingales, we consider left and right stochastic exponentials for general noncommutative semimartingales [1, 3, 5, 7], and study them from the point of view of quasi-shuffle algebras. The central aim of this work is to present and analyse explicit expressions for stochastic exponentials using the fine structure of quasi-shuffle algebras [4], and to relate them to the classical Magnus expansion [6].

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A Stratonovich-to-Skorohod conversion formula for integrals with respect to Gaussian rough paths

Thomas Cass[1]

[1] *Department of Mathematics, Imperial College, London, UK* thomas.cass@imperial.ac.uk

Lyons' theory of rough paths allows us to solve stochastic differential equations driven by a Gaussian processes X of finite p-variation. The rough integral of the solutions against X again exists. We show that the solution also belong to the domain of the divergence operator of the Malliavin derivative, so that the 'Skorohod integral' of the solution with respect to X can also be defined. The latter operation has some properties in common with the Ito integral, and a natural question is to find a closed-form conversion formula between this rough integral and its Malliavin divergence. This is particularly useful in applications, where often one wants to compute the (conditional) expectation of the rough integral. In the case of Brownian motion our formula reduces to the classical Stratonovich-to-Ito conversion formula. There is an interesting difference between the formulae obtained in the cases $2 <= p < 3$ and $3 <= p < 4$, and we consider the reasons for this difference. We elaborate on the connection with previous work in which the integrand is generally assumed to be the gradient of a smooth function of X_t; we show that our formula can recover these results as special cases.

This is joint work with Nengli Lim.

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The exponential Lie series for continuous semimartingales

A. Wiese[1], **K. Ebrahimi-Fard**[2], **S.J.A. Malham**[3], **F. Patras**[4]

[1] *Maxwell Institute for Mathematical Sciences and School of Mathematical and Computer Sciences, Heriot-Watt University, Edinburgh, UK* A.Wiese@hw.ac.uk
[2] *Department of Mathematical Sciences, Norwegian University of Science and Technology, Trondheim, Norway* kurusch.ebrahimi-fard@math.ntnu.no
[1] *Maxwell Institute for Mathematical Sciences and School of Mathematical and Computer Sciences, Heriot-Watt University, Edinburgh, UK* S.J.A.Malham@hw.ac.uk
[4] *Laboratoire J.A. Dieudonné, Université de Nice Sophia-Antipolis, Nice, France* patras@unice.fr

We consider stochastic differential systems driven by continuous semimartingales and governed by non-commuting vector fields. We derive an explicit formula for the logarithm of the Itô flowmap. The derivation relies on the lift to the quasi-shuffle algebra of products of multiple integrals. We also prove that the logarithm of the flowmap is an exponential Lie series. This relies on a natural change of basis to vector fields for the associated quadratic covariation processes, analogous to Stratonovich to Itô corrections. Such exponential Lie series are important in the development of strong Lie group integration schemes that ensure approximate solutions lie on any homogeneous manifold on which the solution evolves.

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Renormalisation of singular SPDEs

Yvain Bruned[1]

[1] *University of Warwick, UK* Y.bruned@warwick.ac.uk

The regularity structures introduced by Martin Hairer in [4] allow us to describe the solution of a singular SPDEs by a Taylor expansion with new monomials. Two Hopf algebras are used in this theory in [2, 4] for recentering these monomials and proving their convergence: the Connes-Kreimer Hopf algebra and the extraction-contraction Hopf algebra. These Hopf algebras are considered with decorations in [2] and twisted antipodes define two kinds of renormalisation. A cointeraction similar to the one obtained in [3] is also proved with these new decorations. The recent work [1] shows a precise counterpart in the rough path context for SDEs. The use of a pre-Lie structure in [1] seems to be a promising approach for describing the renormalised SPDEs.

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Invariance for rough differential equations.

Laure Coutin[1]

[1] *Institut Mathématique de Toulouse, Université Paul Sabatier, 118, Route de Narbonne, 31062 TOULOUSE, Cedex 4, FRANCE* laure.coutin@math.univ-toulouse.fr

In 1942, Nagumo has obtain a necessary and sufficient condition for un convex compact set to be invariant under the solution of an ordinary differential equations. This result was extend by Aubin and Da Prato to the case of stochastic differential equations. The object to this talk is to state and prove the same result for rough differential equtations, with some application to fractional Brownian motion. It is based on a join work with N. Marie.

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Stochastic differential systems and efficient integrators

Simon J.A. Malham[1]

[1] *Department of Mathematics, Heriot–Watt University, Edinburgh EH14 4AS, UK*
S.J.A.Malham@hw.ac.uk

We investigate efficient integrators for nonlinear stochastic differential systems. These are approximations that generate strong numerical integration schemes that are more accurate than the corresponding stochastic Taylor approximation, independent of the governing vector fields and to all orders. We discuss the the algebraic structure underlying the stochastic Taylor solution expansion for stochastic differential systems and how to exploit it to produce efficient integrators. We will also discuss extensions of these results to more general scenarios. The material presented is based on work with multiple authors [1, 2, 3].

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MS19 – Kernel methods for large scale problems: Algorithms and applications

(Elisabeth Larsson, Gabriele Santin)

Wednesday, 08:30 – 10:10, Kulturhus

Jeremy Levesley – *Convergence rate of multilevel sparse grid quasi-interpolation on the torus*

Emma Perracchione – *Anisotropic weights for RBF-PU interpolation with subdomains of variable shapes.*

Victor Shcherbakov – *A Meshfree Approach to Simulations of Ice Flow: Application to the Haut Glacier d'Arolla.*

Francisco Bernal – *A Radial Basis Function - Partition of Unity method for the incompressible Navier-Stokes equations.*

Wednesday, 15:55 – 17:35, Hotel Fleischers Bergslien

Elisabeth Larsson – *Parameter Estimation in Finance Using Radial Basis Function Methods*

Christian Rieger – *Kernel methods for high dimensional pdes*

Slobodan Milovanović – *RBF-FD with Polyharmonic Splines for Multi-Dimensional PDEs in Finance*

Ali Safdari-Vaighani – *Radial basis function approximation method for pricing of basket options under jump diffusion models*

Friday, 08:30 – 09:45, Hotel Fleischers Bergslien

Barbara Zwicknagl – *Kernel methods for multiscale approximation*

Dominik Wittwar – *On uncoupled separable matrix-valued kernels*

Gabriele Santin – *Greedy methods for kernel-based approximation*

Tommaso Taddei – *An Adaptive Parametrized-Background Data-Weak approach to Variational Data Assimilation*

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MS19 – Kernel methods for large scale problems: Algorithms and applications

Convergence rate of multilevel sparse grid quasi-interpolation on the torus

Jeremy Levesley[1], **Simon Hubbert**[2], **Xingping Sun**[3]

[1] *University of Leicester* jl1@le.ac.uk
[2] *Birkbeck, University of London* s.hubbert@bbk.ac.uk
[3] *Missouri State University* XSun@MissouriState.edu

Sparse grid algorithms have become an efficient tool for beating the curse of dimentionality as the dimension of the approximating space only grows algebraically (up to a Logarithmic factor) with the dimension of the ambient space. Tensor product spline algorithms have been used both for approximation and the solution of partial differential equations. As dimension grows functions appear smoother due to the difficulty of finding localised bad behaviour. Approximating these smooth functions with a finite order basis, such as splines, leads to saturation in approximation order. Thus smooth kernels are a good choice for approximation.

In this paper we analyse multilevel sparse grid quasi-interpolation on a torus using Gaussians. The torus is chosen as Fourier methods can be used. In earlier work [1] the first two authors have shown that the multilevel method on the torus converges. However the convergence rate established therein is not as fast as observed in most of our numerical simulations. In the current paper, we will show that sparse grid quasi-interpolation with Gaussian achieves a comparable convergence rate to tensor product spline approximation schemes.

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Anisotropic weights for RBF-PU interpolation with subdomains of variable shapes.

E. Perracchione[1], **R. Cavoretto**[2], **A. De Rossi**[3], **G.E. Fasshauer**[4]

[1] *Department of Mathematics, University of Padua* emma.perracchione@math.unipd.it
[2] *Department of Mathematics, University of Turin* roberto.cavoretto@unito.it
[3] *Department of Mathematics, University of Turin* alessandra.derossi@unito.it
[4] *Department of Applied Mathematics and Statistics, Colorado School of Mines, Golden, CO* fasshauer@mines.edu

The Partition of Unity (PU) method, performed by means of local Radial Basis Function (RBF) approximants, has been proved to be an efficient and accurate numerical tool for interpolating large data sets [4]. Such method decomposes the domain into several *subdomains* or *patches*, which, in the context of interpolation, usually consist of hyperspheres of a fixed radius forming a covering of the original domain, and computes the PU interpolant as the weighted sum of several local approximants.

In [2], an approach via the PU method that selects *optimal* local interpolants is proposed. Optimal in the sense that both the shape parameters governing the flatness of the local RBFs and the radii of the hyperspherical PU subdomains are selected by minimizing *a priori* error estimates. Such approach allows to effectively deal with points with highly varying densities.

However, the fact that the proposed technique only works for hyperspherical subdomains is limiting if points follow dissimilar distributions along the different dimensions, such as the track data (see e.g. [1]). For this case, we develop a novel technique that basically consists in choosing patches centred at the tracks so that they contain only few points of the nearest tracks. In this sense, ellipsoidal patches perform better and moreover the choice of anisotropic kernels naturally follows [3].

Computational aspects devoted to efficiently select both the shape parameters and the semi-axes of the subdomains via a priori error estimates, such as leave one out cross-validation schemes, are also considered. Finally, we provide applications to real world data sets.

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A Meshfree Approach to Simulations of Ice Flow: Application to the Haut Glacier d'Arolla.

Victor Shcherbakov[1], **Josefin Ahlkrona**[2]

[1] *Uppsala University, Sweden* victor.shcherbakov@it.uu.se
[2] *University of Kiel, Germany* ahlkrona@math.uni-kiel.de

Numerical models of glacier and ice sheet dynamics traditionally employ finite difference or finite element methods. Although these are highly developed and mature methods, they suffer from some drawbacks, such as inability to handle complex geometries (finite differences) or a costly assembly procedure for nonlinear problems (finite elements). Additionally, they are mesh-based, and therefore moving domains become a challenge.

We introduce a meshfree approach based on a radial basis function (RBF) method. The meshfree nature of RBF methods enables efficient handling of moving margins and free ice surface. RBF methods are also accurate, easy to implement, and allow for reduction the computational cost associated with the linear system assembly, since stated in strong form.

To demonstrate the global RBF method we model the velocity field of ice flow in the Haut Glacier d'Arolla, which is governed by the nonlinear First Order Stokes equations. We test the method for different basal conditions and for a free moving surface. We also compare the global RBF method with its localised counterpart—the RBF partition of unity method (RBF-PUM)—that allows for a significant gain in the computational efficiency, while maintaining similar accuracy. Both RBF methods are compared with the classical finite element method in terms of accuracy and efficiency. We find that the RBF methods are more efficient than the finite element method and well suited for ice dynamics modelling, especially the partition of unity approach.

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A Radial Basis Function - Partition of Unity method for the incompressible Navier-Stokes equations.

Francisco Bernal[1], **Elisabeth Larsson**[2], **Alfa R.H. Heryudono**[3]

[1] *École Polytechnique, Paris (France)* francisco.bernal@polytechnique.edu
[2] *Uppsala University (Sweden)* elisabeth.larsson@it.uu.se
[3] *University of Massachusetts Dartmouth (USA)* aheryudono@umassd.edu

The flow of a viscous fluid past a cylinder is a benchmark for the simulation of fluid-structure interaction and for the assessment of numerical methods in computational fluid dynamics. In this work, we solve it by combining the novel radial basis function-based partition of unity method (RBF-PUM) [1] and the trust-region algorithm for RBF collocation [2]. The proposed method is well suited to tackling both the far-field boundary conditions away from the cylinder, and to adaptive discretization in the region of the wake immediately past it. Preliminary numerical results are reported.

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Parameter Estimation in Finance Using Radial Basis Function Methods

Josef Höök[1], Elisabeth Larsson[2], Erik Lindström[3], and Lina von Sydow[2]

[1] *Swedbank, Sundbyberg, Sweden* josefhook@gmail.com
[2] *Department of Information Technology, Scientific Computing Uppsala University, Sweden*
elisabeth.larsson@it.uu.se, lina.vom.sydow@it.uu.se
[3] *Centre for Mathematical Sciences, Mathematical Statistics, Lund University, Sweden*
erikl@maths.lth.se

Given time series market observations for a price process, the parameters in an assumed underlying model, such as a stochastic diffusion process, can be determined through maximum likelihood estimation [1, 3]. Transition probability densities then need to be estimated between each pair of data points. A common approach is to use a stochastic simulation of the transition process [2]. We show that Gaussian radial basis function approximation [4] of the deterministic Fokker-Planck equations [5] for the densities leads to a convenient mathematical representation. We present numerical results for one and two factor interest rate models [6], and show that the deterministic method has significantly better performance in terms of computational cost than a particle filter approach.

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Kernel methods for high dimensional pdes

Michael Griebel[1], **Christian Rieger**[2]

[1] *Fraunhofer-Institut für Algorithmen und Wissenschaftliches Rechnen SCAI, Schloss Birlinghoven, 53754 Sankt Augustin, Germany, and Institut für Numerische Simulation, Universität Bonn, Wegelerstr. 6-8, 53115 Bonn, Germany* griebel@ins.uni-bonn.de
[2] *Institut für Numerische Simulation, Universität Bonn, Wegelerstr. 6-8, 53115 Bonn, Germany* rieger@ins.uni-bonn.de

In this talk, we focus on parametric partial differential equations and some associated numerical reconstruction tasks. Such differential equations often arise in the modeling of unresolved physical quantities. It is sometimes convenient to design a stochastic surrogate model which leads to a (possibly infinite) parametric problem after choosing a fixed basis expansion. The solution of such a parametric equation is a function of the spatial variables and the parameters, and hence the evaluation of such a function for a fixed parameter involves the solution of a spatial pde. The numerical costs of such a function evaluation motivate why one is interested in algorithms which need only a small number of parameter values to describe the function as a function of the parameters to a prescribed accuracy. That this is possible in many cases is due to the usually high regularity of the function depending on the parameters. We discuss such regularity results and how they can be exploited in kernel based regularized reconstruction methods. Here, we focus on kernel-based methods in the parameter space, where common mesh-generation techniques seem not to be appropriate. Further, we make use of the built-in regularizing effects of kernel-based methods since we automatically have inexact data due to the numerical error in the solution of the spatial pde. Finally, we present some a priori error analysis.

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RBF-FD with Polyharmonic Splines for Multi-Dimensional PDEs in Finance

Slobodan Milovanović[1], **Lina von Sydow**[2]

[1] *Uppsala University, Sweden* slobodan.milovanovic@it.uu.se
[2] *Uppsala University, Sweden* lina.von.sydow@it.uu.se

We aim at using radial basis function generated finite differences (RBF-FD) [1] to solve multi-dimensional PDEs that arise when pricing multi-asset financial derivatives [2]. Being mesh-free while generating a sparse differentiation matrix, this method exploits the best properties from both finite difference (FD) methods and radial basis function (RBF) methods [3]. Moreover, RBF-FD is expected to be advantageous for high-dimensional problems compared to: Monte Carlo (MC) methods which converge slowly, global RBF methods since they produce dense matrices, and FD methods because they require regular grids [4]. A recent progress in research related to RBF-FD [5, 6], which showed the benefits of using polyharmonic splines (PHS) as RBFs augmented with polynomials, has sparked a great potential for applying this method in e.g. financial engineering. We demonstrate the performance of the method with new implementational features (e.g. smoothing of the initial conditions) while pricing European and American basket options with discrete or continuous dividends under the standard Black-Scholes-Merton model with up to three underlying assets. The results highlight RBF-FD as a sparse method, capable of achieving high accuracy with a small number of nodes.

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Radial basis function approximation method for pricing of basket options under jump diffusion models

Ali Safdari-Vaighani

Department of Mathematics, Faculty of Mathematical Sciences and Computer, Allameh Tabataba'i University, Tehran, Iran asafdari@atu.ac.ir

Pricing financial contracts on several underlying assets are received more and more interest as a demand for complex derivatives. The option pricing under asset price involve jump diffusion processes leads to the partial integral differential equation (PIDEs), which is an extension of the Black-Scholes PDE with a new integral term. The aim of this talk is to show how basket option prices in the jump diffusion models, mainly on the Merton model, can be computed using RBF based approximation methods. The RBF-PU method [1, 2] is applied for numerical solution of the resulting PIDEs form the two-asset European vanilla put options as well as three-asset case. It is shown that using the tailored node distribution helps to increase the accuracy of the approximation in the regoin near the exercise price in compared to uniform node distribution. The numerical experiments show the accuracy and efficiency of the proposed method in the acceptable computational time.

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Kernel methods for multiscale approximation

Michael Griebel[1], **Christian Rieger**[2], **Barbara Zwicknagl**[3],

[1] *Fraunhofer-Institut für Algorithmen und Wissenschaftliches Rechnen SCAI, Schloss Birlinghoven, 53754 Sankt Augustin, Germany, and Institut für Numerische Simulation, Universität Bonn, Wegelerstr. 6-8, 53115 Bonn, Germany* griebel@ins.uni-bonn.de
[2] *Institut für Numerische Simulation, Universität Bonn, Wegelerstr. 6-8, 53115 Bonn, Germany* rieger@ins.uni-bonn.de
[3] *Institut für Mathematik, Universität Würzburg, Emil-Fischer-Str. 40, 97074 Würzburg, Germany* barbara.zwicknagl@mathematik.uni-wuerzburg.de

Many approximation problems have an intrinsic multiscale structure. In particular, problem-induced reproducing kernels are often not given in a closed form expression but in a multiscale decomposition. To work practically with such multiscale kernels, a careful approximation of the kernel function is required, which does not spoil the good approximation properties of the kernel-based trial spaces. In this talk, we will discuss some quantitative approximation and stability properties of the resulting algorithms based on properly approximated kernel functions, including inverse Bernstein-type estimates for the finite-dimensional trial spaces, and estimates on the condition numbers of kernel matrices. Typical examples include regularized reconstruction algorithms in generalized Besov spaces (see [3]).

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS19 – Kernel methods for large scale problems: Algorithms and applications

On uncoupled separable matrix-valued kernels

D. Wittwar[1], **B. Haasdonk**[2]

[1] *Institute of Applied Analysis and Numerical Simulation, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany* dominik.wittwar@mathematik.uni-stuttgart.de
[2] *Institute of Applied Analysis and Numerical Simulation, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany* bernard.haasdonk@mathematik.uni-stuttgart.de

We are interested in approximating vector-valued functions on a domain Ω. Instead of generating individual approximations for each function component, we consider Reproducing kernel Hilbert spaces $\mathcal{H}_k \subset \{f : \Omega \to \mathbb{R}^m\}$ of vectorial functions which, similar to the scalar case, admit a unique reproducing kernel k. It can be shown, c.f. [1] that for any $x, y \in \Omega$ the kernel can be represented by a matrix $k(x, y) \in \mathbb{R}^{m\times m}$. These spaces seem promising, when modelling correlations between the target function components.

In this talk we study uncoupled separable kernels, i.e. the kernel k has a representation

$$k(x, y) = \sum_{i=1}^{p} k_i(x, y)Q_i, \quad \text{with} \quad \sum_{i=1}^{p} \operatorname{rank}(Q_i) = \operatorname{rank}\left(\sum_{i=1}^{p} Q_i\right), \tag{11}$$

where k_i are strictly positive definite scalar-valued kernels and $Q_i \in \mathbb{R}^{m\times m}$ are symmetric positive semidefinite matrices. We extend tools from the scalar to the matrix-valued case, in particular, we investigate conditions for the strict positive definiteness. Furthermore, we introduce interpolation operators, Power functions and error bound [3]. In comparison to [2] we use a more versatile notion of Power function which facilitates a-priori error bounds.

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MS19 – Kernel methods for large scale problems: Algorithms and applications

Greedy methods for kernel-based approximation

G. Santin[1], **B. Haasdonk**[2]

[1] *Institute of Applied Analysis and Numerical Simulation, University of Stuttgart, Germany*
santinge@mathematik.uni-stuttgart.de
[2] *Institute of Applied Analysis and Numerical Simulation, University of Stuttgart, Germany*
haasdonk@mathematik.uni-stuttgart.de

Kernel methods provide powerful and flexible methods to approximate functions defined on general domains, with possible high-dimensional input and output space, and using samples at scattered locations.

Thanks to this high flexibility, kernel methods have been increasingly used in the recent times to produce surrogate models, i.e., cheap approximate models which are used to replace highly accurate but expensive simulations.

In this context, greedy methods have proven to be particularly effective ([4]). Indeed, they allow to construct good approximants based on small, thus cheap to evaluate expansions. The approximant is constructed using a small set of kernel centers, which are selected in an efficient way by picking at each iteration the point which maximizes a certain selection criterion.

We will review in this talk the main greedy strategies used in this context and recall their application to the approximation of vector-valued functions. We will present some recent results on their convergence rate, which can be proven to be quasi-optimal in some case ([2, 3]).

Moreover, we will introduce a new non-symmetric greedy algorithm which constructs kernel interpolants with centers possibly different from the data sites (see [1]). This method allows to construct an expansion with bases which are centered arbitrarily on the domain and not bounded to be selected from the available data locations.

Experimentally, we demonstrate the potential of the new algorithm on artificial examples as well as on real world applications.

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An Adaptive Parametrized-Background Data-Weak approach to Variational Data Assimilation

Yvon Maday[1,2], **Anthony T Patera**[3], **Tommaso Taddei**[1],

[1] *Sorbonne Universités, Laboratoire Jacques-Louis Lions, France*
taddei@ljll.math.upmc.fr, maday@ann.jussieu.fr
[2] *Brown University, Division of Applied Mathematics,* yvon_jean_maday@brown.edu
[3] *MIT, Department of Mechanical Engineering,* patera@mit.edu

We present an Adaptive Parametrized-Background Data-Weak (APBDW) approach to the steady-state variational data assimilation (state estimation) problem for systems modeled by partial differential equations. The variational formulation is based on the Tikhonov regularization of the PBDW formulation [Y Maday, AT Patera, JD Penn, M Yano, Int J Numer Meth Eng, 102(5), 933-965] for pointwise noisy measurements. We propose an adaptive procedure based on *a posteriori* estimates of the L^2 state-estimation error to improve performance. We also present *a priori* estimates for the L^2 state-estimation error that motivate the approach and guide the adaptive procedure. We illustrate our method through a number of numerical experiments.

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MS20 – Advanced discretization methods for computational wave propagation

(Julien Diaz, Marcus Grote)

Tuesday, 15:30 – 17:10, Hotel Fleischers Sivle

Helene Barucq – *Trefftz methods based on shaped functions locally computed with Discontinuous Galerkin methods. Application to the Helmholtz equation.*

Théophile Chaumont-Frelet – *Finite element approximation of electromagnetic waves with non-fitting meshes*

Claire Scheid – *The Multiscale Hybrid Mixed method for time dependent propagation of electromagnetic waves.*

Elvira Shishenina – *Trefftz-DG approximation for elasto-acoustics*

Thursday, 13:30 – 15:10, Hotel Fleischers Sivle

Marlis Hochbruck – *Error analysis of an ADI splitting for discontinuous Galerkin discretizations of linear Maxwell's equations*

Andreas Sturm – *Locally implicit time integration for linear Maxwell's equations*

Marcus Grote – *Convergence Analysis of Energy Conserving Explicit Local Time-stepping Methods for the Wave Equation*

Sébastien Imperiale – *High order local time discretization for wave equations based on domain decomposition methods.*

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Trefftz methods based on shaped functions locally computed with Discontinuous Galerkin methods. Application to the Helmholtz equation.

Hélène Barucq[1], **Abderrahmane Bendali**[2], **Julien Diaz**[3], **Sébastien Tordeux**[4]

[1] *MAGIQUE-3D Inria Team-Project and University of Pau and Pays de l'Adour, France* helene.barucq@inria.fr
[2] *INSA of Toulouse, France* abderrahmane.bendali@insa-toulouse.fr
[1] *MAGIQUE-3D Inria Team-Project and University of Pau and Pays de l'Adour, France* julien.diaz@inria.fr
[4] *LMA UMR 5142 and MAGIQUE-3D Inria Team-Project* sebastien.tordeux@inria.fr

Finite element approximations of Helmholtz problems are subject to *pollution effect*, in particular when set in very large domains. One approach is to increase the number of nodes but the capabilities of storage computer run the risk of being reached quickly. Discontinuous Galerkin (DG) methods have demonstrated a stronger durability than standard continuous FEMs. Trefftz methods for which the local shape functions are wave functions (cf., for example, [1]) have also proved to perform well and so does Boundary Integral Equations (BIE). Recently, FEMs in which local shape functions are obtained as BIE solutions have been investigated. In this context, [3] uses an improved approximation of the Dirichlet-to-Neumann (DtN) operator for matching the local solutions at the interfaces of the mesh that are combined to define a DG solution to the Helmholtz equation. It is called BEM Symmetric Trefftz DG method (BEM-STDG). BIEs are used to compute the DtN operator within each element of the DG formulation mesh which means that the contribution of the BIEs is element-wise only. The degrees of freedom of the discrete problem to be solved are then located on the boundaries of the elements and the approximations are ultimately performed in terms of piecewise polynomial functions on a BEM mesh. In contrast to usual Trefftz methods, h or p refinements are as simple and efficient as in a standard FEM or DG.
Here, we investigate the idea of approximating the DtN operator with FEM instead of BEM. By comparing with BEM-STDG, we test the capability of high-order FEM DtN approximations to resist to *pollution effect*.

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MS20 – Advanced discretization methods for computational wave propagation

Finite element approximation of electromagnetic waves with non-fitting meshes

T. Chaumont-Frelet[1], **S. Nicaise**[2] **D. Pardo**[3,1]

[1] *Basque Center for Applied Mathematics, Spain* tchaumont@bcamath.org
[2] *University of Valenciennes, France* snicaise@univ-valenciennes.fr
[3] *University of the Basque Country (UPV/EHU), Spain* dzubiaur@gmail.com

We aim at solving borehole logging applications, for which we need to approximate the magnetic field generated by a dipole. As it is customary for these applications, we consider 3D Maxwell's equations in a convex domain featuring constant permittivity and permeability, but a piecewise constant conductivity.

We analyze a discretization technique for Maxwell's equations based on Nedelec's edge elements with non-fitting meshes. The term *non-fitting* describes meshes for which the parameters defining the physical properties of the medium of propagation can take different values inside one cell. As a result, these parameters are allowed to exhibit discontinuities inside the mesh cells.

Since the faces (or edges in 2D) of non-fitting meshes do not need to be aligned with the physical interfaces of the propagation medium, they are simpler to generate than fitting meshes. In particular, simple mesh topologies such as cartesian grids are possible. Additionally, one can select cells that are larger than the small scale details contained in the propagation medium. As a result, the use of non-fitting meshes might simplify the implementation, and even reduce the number of degrees of freedom required to solve the problem by using larger cells.

It is well known that the use of non-fitting meshes might decrease the convergence rate of the associated finite element method, since the electric field normal component is discontinuous across physical interfaces. Indeed, using non-fitting meshes amounts to approximate a discontinuous field by locally continuous shape functions.

In this work, we derive new error estimates for first order Nedelec's elements that take advantage of the constant permeability assumption. The key result state that magnetic field approximation converges faster than the electric field for both fitting and non-fitting meshes. Moreover, we prove that the convergence rate of the magnetic field is the same for fitting and non-fitting meshes.

In the second part of the presentation, we analyze different strategies to accurately and efficiently integrate the linear system coefficients. The best choice of integration technique depends on the mesh size and the used polynomial order. Numerical experiments illustrate the aforementioned error-estimates and the performance of each quadrature technique.

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The Multiscale Hybrid Mixed method for time dependent propagation of electromagnetic waves.

S. Lanteri[1], D. Paredes[2], C. Scheid[1,3], F. Valentin[4]

[1] *INRIA Sophia Antipolis, 2004, route des Lucioles - BP 93, 06902 Sophia Antipolis Cedex, France.* Stephane.Lanteri@inria.fr

[2] *Instituto de Matemáticas, Pontificia Universidad Catòlica de Valparaìso - IMA/PUCV, Chile.* diego.paredes@ucv.cl

[3] *Côte d'Azur University, J. A. Dieudonné Laboratory, Parc Valrose, 06108 Nice, Cedex 02, France.* Claire.Scheid@unice.fr

[4] *Applied Mathematics Department, National Laboratory for Scientific Computing – LNCC, Av. Getulio Vargas, 333, 25651-070 Petropolis - RJ, Brazil.* valentin@lncc.br

A nanoscaled structure that is illuminated by light (at optical frequencies) offers a lot of nice features that physicists try to exploit in the context of nanophotonics. Indeed, one is able to obtain very efficient light enhancement and focusing properties that may be used in several applicative contexts from nanolasers to biomedical applications. In this area, numerical simulations are central for the physicists in order to design the correct nanostructure that would give best effects. The numerical framework has to be build carefully to meet the needs of the physicists and has to be reliable enough to tackle all the specific difficulties encountered in nanophotonics. In particular, the geometry of the structure can be quite complicated, and the media highly heterogeneous. With this in mind, in this work, we focus on the numerical modelling of time dependent wave propagation problems with possibly strong multiscales characteristics. We investigate the possibility of using the so-called Multiscale Hybrid Mixed (MHM) method that has been introduced in [1, 2] for stationary problems. The latter rely on the concept of multiscale basis functions that reconstruct by themselves a part of high-contrast features of the problem. The algorithm rely on a two level discretization. The basis functions being computed at the second (finer) level allow for the reconstruction of the solution via the communication at the first (coarser) level on the skeleton of the mesh by introducing a new hybrid variable. We propose to extend and study (theoretically and numerically) the viability of this approach for time dependent electromagnetic wave propagation problems; we thus concentrate on the first order time-dependent Maxwell's equations. We will explain the resolution strategy with several time integration schemes and present numerical results assessing the validity of the approach.

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Trefftz-DG approximation for elasto-acoustics

H.Barucq[1], **H.Calandra**[2], **J.Diaz**[1], **E.Shishenina**[1]

[1] *Team-Project Magique-3D, Inria, France* elvira.shishenina@inria.fr
[2] *Total S.A., USA*

Discontinuous finite element methods have proven their numerical accuracy and flexibility, but they are still criticized for requiring high number of degrees of freedom for computation. There have been some advances with hybridizable discontinuous Galerkin approximations but essentially in the time-harmonic regime, because they require implicit schemes for time integration (see [4] and the references therein).

Another possibility to explore seems to be Trefftz methods. They are now widely used with time-harmonic formulations [1], [2], while the studies are still limited for reproducing temporal phenomena [3]. Trefftz-type methods distinguish themselves by the choice of basis functions: they are local solutions of initial equation. Thus, in case of time-dependent problems, space-time meshes are required.

Classical Trefftz-type approximation uses the exact solutions of the acoustic and elastic systems taken with different frequencies in order to obtain better numerical error. We have computed a polynomial basis using the Taylor expansions of generating exponential functions which are the exact solutions of the initial acoustic and elastodynamic systems. This basis, compared to the classical one based on trigonometric functions, requires less degrees of freedom for the same level of accuracy.

In the present work, we develop the theory for coupled elasto-acoustic system. We show the existence and the uniqueness of solution for acoustic, elastic and coupled elasto-acoustic wave propagation systems, and the unconditional numerical stability of the scheme. The method requires less degrees of freedom, compared to the classical DG method, in order to achieve the same accuracy.

Wave simulations in 2D media show a high sensitivity to the handling of transmission conditions. The numerical results have been validated by comparison with analytical solution in 2D. The obtained convergence order is higher than the one of polynomial basis used for computation.

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Error analysis of an ADI splitting for discontinuous Galerkin discretizations of linear Maxwell's equations

Marlis Hochbruck[1], **Jonas Köhler**[2]

[1] *Karlsruhe Institute of Technology (KIT), Germany* marlis.hochbruck@kit.edu
[2] *Karlsruhe Institute of Technology (KIT), Germany* jonas.koehler@kit.edu

In this talk we investigate the convergence of an alternating direction implicit (ADI) method for discontinuous Galerkin discretizations of Maxwell's equations on product domains. This method is both unconditionally stable and computationally cheap (each time step is of linear complexity).

We prove that the scheme converges with optimal order in time and space with constants which are independent of the spatial mesh widths and thus are robust under mesh refinements. The proof is based on our earlier work on the ADI scheme applied to the continuous Maxwell's equations considered as an abstract Cauchy problem [1] and techniques established for the full discretization of a locally implicit scheme comprising the Crank–Nicolson and the Verlet scheme in [2]. The results for the Crank–Nicolson and for the Verlet scheme on the full grid are special cases of this analysis which are detailed in [3]. In fact we show that similar to the Verlet scheme, the ADI scheme under consideration can be interpreted and analyzed as a perturbation of the Crank–Nicolson scheme.

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Locally implicit time integration for linear Maxwell's equations

Marlis Hochbruck[1], **Andreas Sturm**[2]

[1] *Karlsruhe Institute of Technology (KIT), Germany* marlis.hochbruck@kit.edu
[2] *Karlsruhe Institute of Technology (KIT), Germany* andreas.sturm@kit.edu

An attractive feature of discontinuous Galerkin (dG) spatial discretizations of Maxwell's equations is their ability to handle complex geometries by using unstructured, possibly locally-refined meshes. Furthermore, dG methods lead to block diagonal mass matrices which in combination with an explicit time integration method allow for a fully explicit scheme. However, such explicit approaches require a constraint on the time step size related to the diameter of the smallest mesh element to ensure stability, the well-known CFL condition. This makes the simulation inefficient, in particular if the number of tiny mesh elements is small compared to the total number of elements. A natural way to overcome this restriction is using implicit time integrators but these come with the expense of having to solve a large linear system in each time step.

A more suitable approach consists in treating only the tiny mesh elements implicitly while retaining an explicit time integration for the remaining coarse elements. This results in so-called locally implicit methods. In this talk we consider a second order locally implicit method proposed by [1] and its analysis in [2]. Both the efficiency and the error analysis of this method strongly rely on the skew-adjointness of the Maxwell-operator and its (central fluxes) dG discretization. Unfortunately, this skew-adjointness does not hold for stabilized (upwind fluxes) dG discretizations. However, upwind fluxes dG methods exhibit many advantages such as a superior stability behavior and higher accuracy.

In this talk we present how the locally implicit method can be adapted to treat the upwind fluxes dG discretizations. We show that the new method preserves the efficiency of the underlying locally implicit scheme. Moreover, we give an error analysis for the full discretization based on a variational formulation and energy techniques. We prove that the new method is again of second order in time and that it exhibits the higher spatial accuracy of an upwind fluxes dG method [3].

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Convergence Analysis of Energy Conserving Explicit Local Time-stepping Methods for the Wave Equation

Marcus J. Grote[1], **Michaela Mehlin**[2], **Stefan Sauter**[3]

[1] *Institute of Mathematics, University of Basel, Switzerland* marcus.grote@unibas.ch
[2] *Institute of Applied and Numerical Analysis, KIT, Germany* michaela.mehlin@kit.edu
[3] *Institute for Mathematics, University of Zurich, Switzerland* stas@math.uzh.ch

Local adaptivity and mesh refinement are key to the efficient simulation of wave phenomena in heterogeneous media or complex geometry. Locally refined meshes, however, dictate a small time-step everywhere with a crippling effect on any explicit time-marching method. In [1, 2, 3] a leap-frog (LF) based explicit local time-stepping (LTS) method was proposed, which overcomes the severe bottleneck due to a few small elements by taking p small time-steps in the locally refined region for every larger (global) time-step Δt used elsewhere.

Despite the many different explicit LTS methods that were proposed and successfully used for wave propagation in recent years – see [4] for references –, a rigorous space-time convergence theory is still lacking. Here we consider the classical wave equation and prove convergence of the LTS-LF method when combined with a standard conforming finite element method (FEM) in space.

Let u denote the solution of the classical wave equation and u_h denote the fully discrete Galerkin solution with continuous piecewise polynomial finite elements of order ℓ. Under standard smoothness assumptions on u, we rigorously prove that for $\Delta t, h \to 0$:

$$\|u - u_h\|_{L^\infty([0,T];L^2(\Omega))} \leq C(1+T)(h^{\ell+1} + \Delta t^2),$$

where the constant C depends only on u but neither on h, Δt, p nor on T.

Numerical results further illustrate the usefulness of the LTS-LF Galerkin FEM in the presence of corner singularities.

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High order local time discretization for wave equations based on domain decomposition methods.

J. Chabassier[1], **S. Imperiale**[2]

[1] *Inria - University of Pau and Pays de l'Adour,* juliette.chabassier@inria.fr
[2] *Inria - LMS, Ecole Polytechnique, CNRS - Université Paris-Saclay*
sebastien.imperiale@inria.fr

In this talk we present a time discretization strategy for linear wave propagation that aims at using locally the most adapted time discretization among a family of implicit (see [1]) or explicit (see [2]) fourth order schemes. The domain of interest being decomposed into several regions, different fourth order time discretization can be chosen depending on the local properties of the spatial discretization (mesh size and quality, order of the finite elements) or the physical parameters (high wave speed, low density). The objective of this strategy is to be able to choose the highest time-step Δt possible for efficiency while obtaining a given accuracy. Although in our strategy only one time-step is defined for the simulation it achieves the same goal as local time-stepping strategy (where multiple time-steps are defined locally) and can be proven to be equivalent in some configurations.

Assuming that the wave propagation problem is solved in a domain Ω decomposed into a region Ω_c and Ω_f, the solution's approximations U_c^n and U_f^n at time $n\Delta t$ are given by the following algebraic scheme (we denote $\Gamma = \partial\Omega_f \cap \partial\Omega_c$)

$$\begin{cases} \mathbb{P}_c(A_c)\,[U_c^n]_{\Delta t^2} + \mathbb{Q}_c(A_c) M_c^{-1}(K_c\,\{U_c^n\}_{1/4} + C_c\,\Lambda^n) = 0, & \textit{(wave equation in } \Omega_c\textit{)} \\ \mathbb{P}_f(A_f)\,[U_f^n]_{\Delta t^2} + \mathbb{Q}_f(A_f) M_f^{-1}(K_f\,\{U_f^n\}_{1/4} - C_f\,\Lambda^n) = 0, & \textit{(wave equation in } \Omega_f\textit{)} \\ C_c^T U_c^n - C_f^T U_f^n = 0, & \textit{(solution's continuity on } \Gamma\textit{)} \end{cases}$$

where $A_{c/f} = \Delta t^2 M_c^{-1} K_c$, the mass matrices $M_{c/f}$ are lumped or black diagonal, $K_{c/f}$ are stiffness matrices, Λ^n corresponds to an approximation of the flux of the solution at time $n\Delta t$ on Γ, the polynomial $\mathbb{P}_{c/f}$ and $\mathbb{Q}_{c/f}$ are given by the type of scheme chosen (for explicit schemes $\mathbb{P}_{c/f}(x) = 1 - x\,\mathbb{Q}_{c/f}(x)/4$), $C_{c/f}$ are coupling matrices computed using mortar finite elements along Γ and

$$[V^n]_{\Delta t^2} = (V^{n+1} - 2V^n + V^{n-1})/\Delta t^2, \quad \{V^n\}_{1/4} = (V^{n+1} + 2V^n + V^{n-1})/4.$$

Together with stability results (based upon energy preservation) some theoretical and numerical space/time convergence results will be presented.

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MS21 – Unfitted Finite Element Methods: Analysis and Applications

(Erik Burman, Mats Larson, Maxim Olshanskii, Arnold Reusken)

Wednesday, 13:30 – 15:10, Hotel Fleischers Sivle

Silvia Bertoluzza – *The Fat Boundary Method: new results and perspectives*

Sara Zahedi – *A Space-Time Cut Finite Element Method*

Alexey Chernyshenko – *A hybrid finite volume - finite element method for bulk-surface coupled problems*

Christian Engwer – *Mass conservation for a cut-cell dG discretization for PDEs on manifolds*

Thursday, 15:30 – 17:10, Hotel Fleischers Sivle

Alexandre Ern – *A Cut Hybrid High-Order Method for Elliptic Interface Problems*

Peter Hansbo – *Finite elements for bulk problems with embedded lower-dimensional structures*

Christoph Lehrenfeld – *Higher order isoparametric unfitted space-time finite element methods for problems involving moving domains*

Robert Eymard – *Compactness properties of non-conforming finite elements spaces*

Friday, 08:30 – 10:10, Hotel Fleischers Sivle

Maxim Olshanskii – *New unfitted FEM for PDEs on evolving surfaces*

Arnold Reusken – *Space-time unfitted Finite Element Methods for PDEs with moving discontinuities*

Erik Burman – *Cut finite element methods with boundary value correction*

Carl Lundholm – *A space-time cut finite element method for the heat equation*

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The Fat Boundary Method: new results and perspectives

Silvia Bertoluzza[1], **Vincent Chabannes**[2], **Mourad Ismail**[3], **C. Prud'homme**[2]

[1] *CNR-IMATI, Italy* silvia.bertoluzza@imati.cnr.it
[2] *Université de Strasbourg, France* {chabannes,prudhomm}@unistra.fr
[3] *Université Grenoble Alpes, France* Mourad.Ismail@univ-grenoble-alpes.fr

The Fat Boundary Method (FBM), introduced in [2], is a fictitious domain method for solving partial differential equations in a domain with holes. The typical situation, which is met for instance in the context of fluid particle flows, is that of a perforated domain, $\Omega = \square \setminus \overline{B}$, where $\square$ is a simple shaped domain, say a cube, and B is a collection of (possibly many) smooth open subsets (the holes). The method consists in splitting the initial equations into two problems to be coupled via Schwartz type iterations: the solution of a global problem set in $\square$, for which we assume that fast solvers can be used, and the solution, fully in parallel, of a collection of independent local problems defined on an auxiliary domain ω composed by narrow strips around the connected components of B (the so called *fat boundary*). The coupling between the global problem and the local ones is based on the one hand on the interpolation of a globally defined field on the artificial boundary γ' which together with ∂B delimits the auxiliary domain ω, and on the other hand on the prescription of a jump in the normal derivative across the boundary of B. While most fictitious domain methods result in a degradation in the accuracy in comparison with boundary fitted methods, under suitable assumptions the FBM retains optimality, even when using high order discretizations. More precisely it is possible to show that *if the solution u is sufficiently smooth in Ω, domain of definition of the original problem*, then the FBM achieves the best order of approximation allowed by the chosen approximation spaces ([1]).

For the class of applications that we have in mind (such as the simulation of blood flow, where the holes are given by the red blood cells) it is however fundamental to consider a wider class of equations (in particular the Navier-Stokes equation) and to take into account, in the analysis, the effect of the approximate computation of the integrals involved in the coupling between the local and the global problem. The aim of this talk is on the one hand to present the extension of the above method to the Stokes problem (a crucial step for the solution of the Navier-Stokes equation) and to present some preliminary results related with the effect of numerical quadrature on stability and convergence.

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A Space-Time Cut Finite Element Method

Mats G. Larson[1], **Sara Zahedi**[2]

[1] *Department of Mathematics and Mathematical Statistics, Umeå University, SE–901 87 Umeå, Sweden* mats.larson@math.umu.se
[2] *Department of Mathematics, KTH Royal Institute of Technology, SE–100 44 Stockholm, Sweden* sara.zahedi@math.kth.se

We present a space-time cut finite element method for a time-dependent convection-diffusion equation modeling the evolution of insoluble surfactants on the interface separating two immiscible fluids.

The finite element method is based on a space-time approach with continuous elements in space and discontinuous elements in time. The interface can be arbitrarily located with respect to a fixed background mesh. The strategy is to embed the time-dependent domain where the PDE has to be solved, in a fixed background grid equipped with a standard finite element space and then take the restriction of the finite element functions to this domain. In [1] we proposed a space-time cut finite element method for coupled bulk-surface problems in time-dependent domains using linear elements in space and time. We now extend our method and solve PDEs on evolving surfaces using higher order elements. A new stabilization term is introduced which ensures that the method leads to linear systems with bounded condition number also when higher order elements are used.

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A hybrid finite volume - finite element method for bulk-surface coupled problems

Alexey Y. Chernyshenko[1], **Maxim A. Olshanskii**[2]

[1] *Institute of Numerical Mathematics, Moscow 119333, Russia* chernyshenko.a@gmail.com
[2] *University of Houston, Houston, Texas 77204-3008, USA* molshan@math.uh.edu

We develop a hybrid method for solving a system of advection-diffusion equations in a bulk domain coupled to advection-diffusion equations on an embedded surface. A monotone nonlinear finite volume method [1] for equations posed in the bulk is combined with a octree trace finite element method for equations posed on the surface [2]. In the octree TraceFEM one considers the bulk finite element space of piecewise trilinear globally continuous functions and further uses the restrictions (traces) of these functions to the surface. In our approach, the surface is not fitted by the mesh and is allowed to cut through the background mesh in an arbitrary way. Moreover, the surface is not triangulated in the common sense. The background mesh is an octree grid with cubic cells. The octree mesh can be easily refined or coarsened locally based on different adaptivity criteria. However, an octree grid provides only the first order (staircase) approximation of a general geometry. Allowing the surface to cut through the octree grid in an arbitrary way overcomes this issue, but challenges us with the problem of building efficient bulk–surface discretizations. We demonstrate that the hybrid TraceFEM –non-linear FV method complements the advantages of using octree grids by delivering the higher order accuracy for both bulk and surface numerical solutions.

Systems of coupled bulk–surface partial differential equations arise in many engineering and natural science applications. As an example of an application, we consider the modeling of contaminant transport in fractured porous media. One standard model leads to a coupled system of advection–diffusion equations in a bulk (matrix) and along a surface (fracture). A series of numerical experiments with both steady and unsteady problems and different embedded geometries illustrate the numerical properties of the hybrid approach. The method demonstrates great flexibility in handling curvilinear or branching lower dimensional embedded structures.

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ENUMATH 2017
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Massconservation for a cut-cell dG discretization for PDEs on manifolds

Christian Engwer[1], **Sebastian Westerheide**[2]

[1] *University of Münster, Germany* christian.engwer@uni-muenster.de
[2] *University of Münster, Germany* sebastian.westerheide@uni-muenster.de

Cut-Cell methods are an attractive class of numerical schemes for solving PDEs on complex-shaped domains. They allow to handle implicitly described domains, e.g. via a level-set and can cope with strong deformations or topological changes.

We discuss extensions to the unfitted DG scheme to solve a class of coupled PDEs on complex-shaped domains, as it can be found in many biological applications. These applications characterize as PDEs on time-dependent domains and their surfaces, which possibly undergo strong deformations and changes in topology.

Surface PDEs are handles in a consistent extension, inspired by the Eulerian surface FEM. A particular issue for such eulerian methods for evolving domains is mass conservation. We introduce the general approach of handling surface PDEs via cut-cell methods and discuss modifications to ensure mass conservation in the stationary case and for evolving domains.

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A Cut Hybrid High-Order Method for Elliptic Interface Problems

Erik N. Burman[1], **Alexandre Ern**[2]

[1] *Department of Mathematics, University College London, London, UK–WC1E 6BT, UK*
e.burman@ucl.ac.uk

[2] *Université Paris-Est, CERMICS (ENPC) and INRIA, 77455 Marne-la-Vallée cedex 2, France*
alexandre.ern@enpc.fr

We devise and analyze an unfitted finite element method for elliptic interface problems where the space approximation is performed using the Hybrid High-Order (HHO) method. HHO methods have been recently introduced in the context of linear elasticity [1] and scalar diffusion [2]. HHO methods are based on discrete unknowns that are discontinuous polynomials on the mesh skeleton. Such methods several attractive features: The construction is dimension-independent, it can be deployed for arbitrary polynomial orders, and general grids, including non-matching interfaces or polyhedral cell shapes, can be used. Positioning unknowns at mesh faces is also a natural way to express at the discrete level fundamental continuum properties such as local mass or force balance. The cornerstone of the construction are fully local, problem-dependent, reconstruction operators. This approach can offer reduced computational costs by organizing simulations into (fully parallelizable) local solves and a global transmission problem. HHO methods are nonconforming finite element methods that can, in particular, be linked to the Hybridizable Discontinuous Galerkin (HDG) setting [3]. In the present work, we investigate how the HHO method can be extended to approximate elliptic interface problems using uniftted meshes. Following the general Cut-FEM methodology [4], discrete unknowns attached to mesh faces cut by the interface are doubled. The local interface problem uses Nitsche's method, designed to be robust with respect to the contrast in the diffusion coefficient. The associated degrees of freedom may be eliminated through the local solves.

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MS21 – Unfitted Finite Element Methods: Analysis and Applications

Finite elements for bulk problems with embedded lower-dimensional structures

Erik Burman[1], **Peter Hansbo**[2], **Mats G. Larson**[3]

[1] *Department of Mathematics, University College London, United Kingdom*
e.burman@ucl.ac.uk
[2] *Department of Mechanical Engineering, Jönköping University, Sweden* peter.hansbo@ju.se
[3] *Department of Mathematics and Mathematical Statistics, Umeå University, Sweden*
mats.larson@math.umu.se

We present a new approach, presented in [1, 2], for adding lower–dimensional reinforcements (trusses, membranes, beams, plates) to elastic structures, as well as beam reinforcement of Kirchhoff plates. The elastic structure is discretised using standard C^0 finite elements, and the lower–dimensional reinforcements are discretised by the CutFEM technique of letting the basis functions of the elastic body represent also the reinforcements, which are allowed to pass through the elements. This allows for a fast and easy way of assessing where the elastic body should be supported, e.g., in an optimisation loop. We also reinforce Kirchhoff plates using the same concept, with the plate discretised using C^0 elements and a continuous/discontinuous Galerkin method.

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MS21 – Unfitted Finite Element Methods: Analysis and Applications

Higher order isoparametric unfitted space-time finite element methods for problems involving moving domains

C. Lehrenfeld[1], **J. Preuß**[1]

[1] *Institute for Numerical and Applied Mathematics, University of Göttingen, Lotzestr. 16-18, 37083 Göttingen, Germany,* lehrenfeld@math.uni-goettingen.de

In physics, biology, chemistry and engineering many applications of simulation science involve complex and evolving geometrical shapes. In many important problems these geometrical shapes exhibit topology changes or strong deformation which makes the numerical treatment very challenging. 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. 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 level set domains. We present an approach which allows for a higher order accurate and robust numerical treatment of domains that are prescribed by level set functions [1, 2]. The approach is based on isoparametric mappings that are specifically tailored. We combine this approach with a space-time discretization [3, 4] to obtain *robust* higher order methods in space and time.

Implementational aspects of the space-time method, the isoparametric mapping and the necessity of stabilization mechanisms will be discussed. Further, we outline the most important ingredients in the analysis to obtain provable high order a priori error bounds and demonstrate the practical feasibility of the method on numerical examples for moving fictitous domain and moving interface problems.

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Compactness properties of non-conforming finite elements spaces

R. Eymard[1]

[1] *Laboratoire d'Analyse et de Mathématiques Appliquées, CNRS, UPEM, UPEC, 5 boulevard Descartes, Champs-sur-Marne 77454 Marne-la-Vallée Cedex 2, France.*
Robert.Eymard@u-pem.fr

The non-conforming finite elements are the keystone of the Crouzeix-Raviart scheme [1] for the approximation of the Stokes and Navier-Stokes equations, since they allow the approximation of the velocity at the faces of the mesh. The analysis of their use for the Navier-Stokes equations cannot be completed without a compactness property. We show that it is possible to write a general framework for all the families of non-conforming finite elements on any kind of polytopal mesh.

Considering the case of homogeneous Dirichlet boundary conditions on a domain $\Omega \subset \mathbb{R}^d$, let $\mathfrak{T} = (\mathcal{M}, \mathcal{F})$ be a polytopal mesh of Ω, where $\mathcal{M}$ is the set of the cells and $\mathcal{F}$ is a the set of the faces of the mesh. We then define, for any $p \in (1, +\infty)$, the non-conforming $W_0^{1,p}(\Omega)$ space on $\mathfrak{T}$, denoted by $W_{\mathfrak{T},0}^{1,p}$, as the space of all functions $w \in L^p(\Omega)$ such that:

1. *[$W^{1,p}$-regularity in each cell]* for all $K \in \mathcal{M}$, the restriction $w_{|K}$ of w to K belongs to $W^{1,p}(K)$. We then denote by $w_{|K,\sigma}$ the trace of $w_{|K}$ on any face σ of K, and $\nabla_{\mathfrak{T}} w$ is the "broken gradient" equal to $\nabla(w_{|K})$ in K, for all $K \in \mathcal{M}$.

2. *[Continuity of averages on internal faces]* for all internal face σ common to the cells K and L, $\displaystyle\int_\sigma w_{|K,\sigma}(\mathbf{y})\mathrm{d}\gamma(\mathbf{y}) = \int_\sigma w_{|L,\sigma}(\mathbf{y})\mathrm{d}\gamma(\mathbf{y})$.

3. *[Homogeneous Dirichlet BC for averages on external faces]* for all external face σ of a cell K, $\displaystyle\int_\sigma w_{|K,\sigma}(\mathbf{y})\mathrm{d}\gamma(\mathbf{y}) = 0$.

We then show a series of properties for this space $W_{\mathfrak{T},0}^{1,p}$, including a compactness property enabling the convergence proof in the case of non-linear problems.

It is then noticeable that, in the case $p = 2$, all the standard non-conforming finite element approximations of an elliptic problem with diffusion matrix Λ can be defined by a finite dimensional space $V \subset W_{\mathfrak{T},0}^{1,p}$, and by the following scheme:

Find $u \in V$ such that, for all $w \in V$, $\int_\Omega \Lambda(\mathbf{x})\nabla_{\mathfrak{T}} u(\mathbf{x}) \cdot \nabla_{\mathfrak{T}} w(\mathbf{x})\mathrm{d}\mathbf{x} = \int_\Omega f(\mathbf{x})w(\mathbf{x})\mathrm{d}\mathbf{x}$.

Then the convergence properties are directly issued from the general framework considered above.

This work has been completed within the study of "Gradient Discretisation Methods", by J. Droniou, R. Eymard, T. Gallouët, R. Herbin and C. Guichard.

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ENUMATH 2017
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MS21 – Unfitted Finite Element Methods: Analysis and Applications

New unfitted FEM for PDEs on evolving surfaces

Maxim Olshanskii[1], **Xianmin Xu**[2]

[1] *University of Houston, Houston, Texas, USA* molshan@math.uh.edu
[2] *Institute of Computational Mathematics and Scientific Computing, Chinese Academy of Sciences, Beijing, China* xmxu@lsec.cc.ac.cn

In this talk we discuss a new approach for solving PDEs on evolving surfaces using a combination of the trace finite element method [1] and an extension procedure for a function from a manifold to an ambient domain. The numerical approach is based on a Eulerian description of the surface problem and employs a time-independent background mesh that is not fitted to the surface. The surface and its evolution may be given implicitly, for example, by the level set method. The presented approach applies simple finite difference approximations of time derivatives and trace FEM to a problem posed on a fixed steady surface at each time step. We avoid a space-time problem formulation, and hence a reconstruction of the surface–time manifold or time integration at quadrature nodes is not involved.

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Space-time unfitted Finite Element Methods for PDEs with moving discontinuities

Arnold Reusken[1], **Christoph Lehrenfeld**[2], **Igor Voulis**[3]

[1] *RWTH Aachen University, Germany* reusken@igpm.rwth-aachen.de
[2] *University Göttingen, Germany* lehrenfeld@math.uni-goettingen.de
[3] *RWTH Aachen University, Germany* voulis@igpm.rwth-aachen.de

We present a particular class of space-time unfitted finite element methods (or CutFEM) that are very suitable for problems with moving discontinuities. As two prototype problem classes we consider a mass transport equation that arises in two phase incompressible flows and a time-dependent Stokes interface problem. In the former class the PDE consists of a convection-diffusion equation with a so-called Henry condition imposed at an evolving interface. This condition enforces a discontinuity in the solution. In the time-dependent Stokes equation there are discontinuities in density, viscosity, pressure and the derivative of the velocity across an evolving interface. For these two classes of problems we present well-posed space-time weak formulations. Based on these formulations we introduce discontinuous Galerkin (DG only in time) space-time finite element discretizations. These finite element methods use fixed grids, which are unstructured in space and have a tensor product structure in space-time. The grids are not fitted to the evolving interface. To obtain optimal discretization accuracy we use the CutFEM technique in space-time. This technique will be explained and results of error analyses briefly addressed. Results of numerical experiments with these methods will be presented.

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Cut finite element methods with boundary value correction

E. Burman[1], **T. Boiveau**[2], **S. Claus**[3], **P. Hansbo**[4], **M. Larson**[5]

[1] *Department of Mathematics, University College London, Gower Street, London, UK-WC1E 6BT, United Kingdom* e.burman@ucl.ac.uk
[2] *Université Paris-Est, CERMICS , ENPC* thomas.boiveau.12@ucl.ac.uk
[3] *Cardiff School of Engineering, Cardiff University,* ClausS2@cardiff.ac.uk
[4] *Department of Mechanical Engineering, Jönköping University* Peter.Hansbo@ju.se
[5] *Department of Mathematics, Umeå University* mats.larson@umu.se

Recently there has been an increased interest in so called cut finite element methods [2]. This is a class of geometrically unfitted finite element methods where typically interface or boundary conditions are imposed using Lagrange multipliers or some variant of Nitsche's method. The advantage of such methods is that complex geometries do not need to be meshed, but the geometry data can be built into the variational formulation.

In this talk we will consider a cut finite element ficitious domain method for the Poisson problem in the spirit of [4]. We use continuous finite element spaces of polynomial order k for the approximation of the solution in the bulk, while the (smooth) boundary is approximated by a piecewise polygonal discrete geometry that may cut through elements. Such a discrete geometry can for instance be obtained taking the nodal interpolant of the distance function of the boundary on the space of piecewise affine continuous functions. Dirichlet boundary conditions are imposed on the discrete geometry using either the symmetric or the non-symmetric Nitsche method. To get robustness of stabilization parameters and condition number with respect to the interface position we stabilize the formulation on the boundary using a ghost penalty term [1]. We correct for the low order approximation of the geometry using a boundary value correction in the Nitsche formulation. This technique uses a local correction based on a Taylor series extrapolating the solution from the discrete geometry to the physical geometry. We present stability and error estimates for both the symmetric and non-symmetric versions [3, 5]. The theoretical development is illustrated with some numerical examples.

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A space-time cut finite element method for the heat equation

A. Logg[1], **C. Lundholm**[2], **M. Nordaas**[3]

[1] *Chalmers University of Technology, Sweden* logg@chalmers.se
[2] *Chalmers University of Technology, Sweden* carlun@chalmers.se
[3] *Chalmers University of Technology, Sweden* magne@chalmers.se

Finite element methods for overlapping meshes (see e.g. [2]) may provide a more computationally efficient alternative to traditional methods for complex geometries. In particular, for complex time-dependent geometries such techniques may eliminate the need for costly remeshing. Here, the concept of overlapping meshes means that the discretised geometry consists of a hierarchy of meshes, ordered from bottom (background) mesh to top, with each mesh having a prescribed time-dependent movement. For each mesh a finite element space is constructed, and the composite finite element space for the overlapping meshes is obtained by at each point taking functions from the finite element space corresponding to the uppermost mesh intersecting that point.

The present work further studies the space-time formulation introduced in [1] for two and three spatial dimensions. The method is based on a consistent space-time formulation of the parabolic problem, with a Nitsche-type handling of the interfaces between meshes. We consider $\mathrm{cG}(p)$ elements in space and $\mathrm{dG}(q)$ elements in time, and we demonstrate optimal order convergence of the method. The method is implemented using the multimesh functionality of the freely available open-source project FEniCS [3].

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MS22 – Advances in numerical linear algebra methods and applications to PDEs

(Valeria Simoncini, Mattia Tani)

Tuesday, 15:30 – 17:10, Hotel Fleischers Tarald

Zdenek Strakoš – *Preconditioning and discretization*

Maya Neytcheva – *Analysis and experience in preconditioning of discrete PDE-constrained optimization problems*

Mattia Tani – *Preconditioning for linear systems arising from isogeometric analysis*

Jarle Sogn – *Robust preconditioners for optimality systems – an infinite-dimensional perspective*

Wednesday, 13:30 - 15:35, Hotel Fleischers Tarald

Marco Verani – *hp-AFEM and angles between polynomial subspaces*

Mariarosa Mazza – *Spectral analysis and spectral symbol for the 2D curl-curl (stabilized) operator with applications to the related iterative solutions*

Elias Jarlebring – *Disguised and new quasi-Newton methods for nonlinear eigenproblems*

Valeria Simoncini – *Matrix-equation-based strategies for certain structured algebraic linear systems*

Uwe Köcher – *Solver and preconditioning technology for fully coupled poroelasticity models*

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Preconditioning and discretization

Zdeněk Strakoš[1], **Tomáš Gergelits**[2], **Jan Papež**[3]

[1] *Charles University, Czech Republic* strakos@karlin.mff.cuni.cz
[2] *Czech Academy of Sciences, Czech Republic* gergelits@cs.cas.cz
[3] *Inria Paris, France* jan.papez@inria.fr

Preconditioners efficiently using coarse space information (such as, e.g., multilevel preconditioners or domain decomposition techniques with coarse space components) seem to offer the only way towards iterative solvers of the discretized problems with a linear cost. Algebraically constructed preconditioners (see, e.g., [1]) are based on an approximate solution of (a part of) the problem. One may ask in which way they provide a global exchange of information in function spaces associated with the underlying mathematical model. This leads to investigating interconnections between preconditioning and discretization.

A step in this direction has been made in the context of linear elliptic partial differential equations and operator preconditioning in [2]. Among other results it shows that algebraic preconditioning of a symmetric positive definite algebraic system $Ax = b$ can be equivalently seen as transformation of the discretization basis as well as of the associated inner product. Numerical experiments illustrate how some of the original basis functions with local support are in this way transformed into functions supported over the whole discretization domain.

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Analysis and experience in preconditioning of discrete PDE-constrained optimization problems

Maya Neytcheva[1], **Owe Axelsson**[1,2], **Anders Ström**[1], **Zhao-Zheng Liang**[1]

[1] *Department of Information Technology, Uppsala University, Sweden*
maya.neytcheva@it.uu.se

[2] *Institute of Geonics, Czech Academy of Sciences, Ostrava, Czech Republic*
owe.axelsson@it.uu.se, abstrm@gmail.com, zhao-zheng.liang@it.uu.se

Many inverse and parameter estimation problems can be formulated as PDE-constrained optimization problems, where the constraint is determined by a scalar or vector partial differential equation. Very often, when discretized, such problems are large scale and require fast, efficient and robust iterative solution methods.

In recent years much research effort has been devoted to constructing efficient preconditioners for solving the discrete algebraic systems arising from various constrained optimization problems. The matrices in the so-obtained linear systems of equations possess a specific block structure and, depending on the target problem, can be definite or indefinite. Various authors have worked on how to precondition these matrices, applying the existing knowledge and the experience of general block-preconditioners for definite and indefinite systems, arising from the discretization of scalar or vector (systems of) PDEs.

We consider problems with box constraints and report some approaches to precondition the arising matrices. We present some spectral analysis of the resulting preconditioned matrices and address the computational aspects when implementing the preconditioners in an efficient manner. Numerical experiments, illustrating the performance of the preconditioners will also be shown.

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Preconditioning for linear systems arising from isogeometric analysis

Giancarlo Sangalli[1], **Mattia Tani**[2]

[1] *Università di Pavia, Italy* giancarlo.sangalli@unipv.it
[2] *Università di Pavia, Italy* mattia.tani@unipv.it

Isogeometric analysis (IGA) is a method to numerically solve partial differential equations (PDEs). It is based on the idea of using B-splines (and their generalizations) both for the parametrization of the domain, as it is typically done by computer aided design software, and for the representation of the unknown solution. IGA can also be seen as an extension of the classical finite element method, where the basis functions are allowed to have a higher regularity [1].

One of the main computational efforts in isogeometric software is the solution of the linear system arising from the discretization. It is known that many approaches that are popular in the context of C^0 finite elements, both direct and iterative, tend to perform poorly when applied to isogeometric linear systems. In particular, their effectiveness deteriorates as the spline degree p is increased.

In [2], an effective preconditioning strategy for was proposed. In this approach, the preconditioning step is the solution of a discretized differential problem analogous to the original one, but with constant coefficients and trivial domain geometry. This new problem can be efficiently solved using a well-established direct solver that fully exploits the tensor structure of the basis functions.

In this talk, we describe this approach and discuss some recent advances. In particular, we explore the possibility of using the FFT to reduce the cost of the application of the preconditioner.

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Robust preconditioners for optimality systems - an infinite-dimensional perspective

Jarle Sogn[1], **Walter Zulehner**[2]

[1] *Johannes Kepler University Linz* jarle.sogn@gmail.com
[2] *Johannes Kepler University Linz* zulehner@numa.uni-linz.ac.at

In this talk we consider optimization problems in function space with objective functionals of tracking type and elliptic partial differential equations (PDEs) as constraints, like inverse problems for elliptic PDEs or optimal control problems with elliptic state equations. Such problems typically involve an additional regularization/cost term depending on a regularization/cost parameter.

The discretized optimality systems of such problems are typically ill-conditioned due to high-dimensional approximation spaces and/or small regularization/cost parameters. Preconditioners for these discretized optimality systems based on the concept of Schur complements have been frequently proposed in literature leading to robust convergence properties of associated preconditioned Krylov subspace methods.

We will show how to exploit this strategy already for the formulation of the optimality systems in function space, which naturally leads to alternative formulations of the elliptic PDE-constraint. Besides the usual weak form also the strong and the very weak form come into play. We discuss possible implications of this approach for preconditioning the discretized optimality systems.

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hp-AFEM and angles between polynomial subspaces

Claudio Canuto[1], **Ricardo H. Nochetto**[2], **Rob Stevenson**[3] **Marco Verani**[4],

[1] *Politecnico di Torino, Italy* claudio.canuto@polito.it
[2] *University of Maryland, USA* rhn@math.umd.edu
[3] *University of Amsterdam, The Netherlands* r.p.stevenson@uva.nl
[4] *Politecnico di Milano, Italy* marco.verani@polimi.it

In [1] for the Poisson problem in two dimensions, it has been considered the standard adaptive finite element loop solve, estimate, mark, refine, with estimate being implemented using the p-robust equilibrated flux estimator, and, mark being Dörfler marking. As a refinement strategy it has been employed p-refinement. In particular, under the validity of a "saturation-type" conjecture, it has been obtained a precise result on the amount by which the local polynomial degree on any marked patch has to be increased in order to achieve a p-independent error reduction. Furthermore, hinging upon [2], the algorithm can be turned into an instance optimal hp-adaptive method by the addition of a coarsening routine. In this talk we prove the above conjecture in the case of a square domain by resorting to a careful estimate of the angle between suitable polynomial subspaces.

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Spectral analysis and spectral symbol for the 2D curl-curl (stabilized) operator with applications to the related iterative solutions

Mariarosa Mazza[1], **Ahmed Ratnani**[2], **Stefano Serra-Capizzano**[3]

[1] *Max-Planck Institut für Plasmaphysik, Garching, Germany* mariarosa.mazza@ipp.mpg.de
[2] *Max-Planck Institut für Plasmaphysik, Garching, Germany* ahmed.ratnani@ipp.mpg.de
[3] *University of Insubria, Como, Italy* stefano.serrac@uninsubria.it

In this work, we focus on large and highly ill-conditioned linear systems of equations arising from different formulations of the Maxwell equations appearing, e.g., in Time Harmonic Maxwell as well as in the MagnetoHydroDynamics, a combination of Maxwell and Navier-Stokes equations used to describe the dynamics of the plasma.

First, we consider a compatible B-Spline discretization based on a discrete De Rham sequence [1] of the 2D curl-curl operator stabilized with zero-order term, and study the structure of the resulting coefficient matrices A_n. It turns out that A_n is a principal submatrix of a two-by-two block matrix where each block is, up to low-rank perturbations, a two-level banded Toeplitz matrix and where the bandwidths grow linearly with the degree of the B-splines.

Moreover, looking at the coefficients of A_n, we identify the so-called *symbol* of $\{A_n\}_n$, a function which compactly describes its asymptotic spectral behaviour. From the knowledge of the symbol and using the theory of the Generalized Locally Toeplitz sequences (see [3]) we show that the matrices A_n are affected by three severe sources of ill-conditioning related to the relevant parameters: the matrix size, the spline degree and the stabilization parameter. As a consequence, when used for solving the associated linear systems, classical methods like the Conjugate Gradient (CG) are extremely slow and their convergence speed is not robust with respect to the parameters.

On this basis, we replace the zero-order stabilization with a divergence-type one and we compute the symbol of the corresponding B-spline discretization matrix-sequence. We use then the retrieved spectral information to design a strategy made up of different basic iterative solvers able to satisfactory deal with the sources of ill-conditioning. In detail, we use a 2D vector extension of the multi-iterative approach proposed in [2] as preconditioner for the CG and as a result we obtain a computationally attractive and robust solver. Finally, a variety of numerical tests and some open problems are discussed.

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Disguised and new quasi-Newton methods for nonlinear eigenproblems

E. Jarlebring[1], **A. Koskela**[2], **G. Mele**[3]

[1] *KTH Royal Institute of Technology, Stockholm, Sweden* eliasj@kth.se
[2] *KTH Royal Institute of Technology, Stockholm, Sweden* akoskela@kth.se
[3] *KTH Royal Institute of Technology, Stockholm, Sweden* gmele@kth.se

We are concerned with nonlinear eigenvalue problems (NEPs) of the type $M(\lambda)v = 0$, where $M : \mathbb{C} \to \mathbb{C}^{n\times n}$ is a holomorphic function. This class of problem arise frequently in the context of PDE-eigenvalue problems, when absorbing boundary are constructed in a frequency dependent way, e.g., with Dirichlet-to-Neumann maps. In this work we take a quasi-Newton approach to NEPs of this type, with particular attention given to applications in wave probagation. We investigate which types of approximations of the Jacobian matrix lead to competitive algorithms, and provide convergence theory. The convergence analysis is based on theory for quasi-Newton methods and Keldysh's theorem for NEPs. We derive new algorithms and also show that several well-established methods for NEPs can be interpreted as quasi-Newton methods, and thereby provide insight to their convergence behavior. In particular, we establish quasi-Newton interpretations of Neumaier's residual inverse iteration and Ruhe's method of successive linear problems, which form the basis of some of the most efficient methods for NEPs. The algorithms and improvements of the algorithms are applied to large-scale nonlinear eigenvalue problems arising in the study of wave propagation. For reproducability and replicability our software is provided freely available online: https://arxiv.org/pdf/1702.08492.pdf.

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Matrix-equation-based strategies for certain structured algebraic linear systems

Valeria Simoncini[1]

[1] *Dipartimento di Matematica, Alma Mater Studiorum Università di Bologna, and IMAT-CNR, Pavia, Italy.* valeria.simoncini@unibo.it

The mathematical formulation of various application problems naturally gives rise to *systems* of linear matrix equations. This is the case for instance in regulator equations in robust control, in mixed finite element formulations of certain stochastic Galerkin diffusion problems, and in discretized Stokes and Navier-Stokes equations. We describe some numerical strategies for solving these systems, both in the small and large scale cases. Numerical experiments illustrate the performance of the new methods.

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Solver and preconditioning technology for fully coupled poroelasticity models

Uwe Köcher[1]

[1] *Helmut-Schmidt-University, Univ. of the German Federal Armed Forces Hamburg, Germany.*
koecher@hsu-hamburg.de

In this contribution a high-order variational space-time discretisation and linear system solver technology including preconditioning for the multi-physics problem of coupled flow and deformation of a fluid-saturated porous media described by Biot's model of poroelasticity is presented.

For the discretisation in time a discontinuous Galerkin method is applied. For the discretisation in space a mixed finite element method is applied. The quasi-static elasticity problem is discretised with a standard conforming method in space. The flow problem is discretised with a Raviart-Thomas finite element method for the flux and a discontinuous Galerkin method for the pressure in space.

The arising coupled linear block systems are solved with different iterative and operator splitting approaches. The solver technology and preconditioning strategy for higher-order discontinuous time discretisations is under strong development and the latest results are presented. The solver technology is further used for efficient poroelastic wave propagation simulations.

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MS23 – Numerical Methods in Biophysics

(Fred Vermolen, Etelvina Javierre)

Monday, 15:50 – 17:30, Hotel Fleischers Bergslien

Etelvina Javierre – *A poroelastic growth model to study fluid-mechano-chemical interactions in avascular tumors*

Chandrasekhar Venkataraman – *Modelling and simulation of intratumor phenotypic heterogeneity*

Madzvamuse – *A robust and efficient adaptive multigrid solver for the optimal control of phase field formulations of geometric evolution laws*

Fred Vermolen – *Mathematical Models for the Simulation of Burns Injuries*

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A poroelastic growth model to study fluid-mechano-chemical interactions in avascular tumors

E. Javierre[1], **C. Rodrigo**[2], **F.J. Gaspar**[2]

[1] *Centro Universitario de la Defensa, Academia General Militar, Ctra. Huesca s/n, Zaragoza 50090, Spain* etelvina@unizar.es
[2] *Departamento de Matemática Aplicada, Universidad de Zaragoza, Zaragoza, Spain* carmenr@unizar.es, fjgaspar@unizar.es

The development and growth of tumor tissues are primarily caused by altered cellular proliferation and death kinetics triggered by a wide variety of factors that include hereditary and environmental conditions. The enhanced proliferation kinetics creates a growing amorphous tissue stiffer than the host tissue that, when growing in a confined space, creates physical forces and stress that compress the blood and lymphatic vessels and produce hypoxia and lack of nutrients. This work focuses on this early stage of cancer progression, corresponding to the so-called avascular tumor growth, that evolves until the proliferation of active cells at the tumor rim is balanced by the death of cells at the necrotic core.

In this framework, we consider the tumor tissue as a biphasic poroelastic material consisting of a solid phase (cells and extracellular matrix) and a fluid phase (interstitial fluid) in line with Rosse et al. [1]. Oxygen primarily, but also other biochemical species [2, 3], will be considered to close the mechano-chemical coupling. Hence, the governing equations consist of the momentum conservation of the solid phase -taking into account both interstitial fluid pressure and tissue growth-, the mass conservation equations for the solid and fluid phases, Darcy's law and mass conservation of the considered biochemical species. Our focus in this work is on the efficient solution of the resulting multi-physics problem. We propose a solution algorithm based on the finite volume discretization of the problem on a staggered grid. Numerical simulations of a reference model problem are presented.

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Modelling and simulation of intratumor phenotypic heterogeneity

Chandrasekhar Venkataraman[1]

[1] *University of St Andrews, UK* cv28@st-andrews.ac.uk

A growing body of evidence suggests that the emergence of phenotypic heterogeneity and drug resistance in tumours is due to a process of adaption or evolution. Specifically, it is hypothesised that spatial variations in the concentration of abiotic factors within the tumour environment may create local niches driving natural selection. In this talk we investigate the validity of such a hypothesis by developing a mathematical model linking the dynamics of a phenotypically structured tumour cell population with the concentrations of abiotic factors in the microenvironment. For biological relevance we use parameters in the model that are obtained from experimental data and we pose the system on real 3D tumour geometries obtained from image data. We compare numerical simulations of the full model using a finite element approximation with semi-analytical results on the asymptotically selected trait and observe good agreement between the two approaches.

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A robust and efficient adaptive multigrid solver for the optimal control of phase field formulations of geometric evolution laws

A. Madzvamuse[1], **FW. Yang**[1], **C. Venkataraman**[2], **V. Styles**[1]

[1] *University of Sussex, School of Mathematical and Physical Sciences, Department of Mathematics, Pevensey III, Brighton, BN1 9QH, UK* a.madzvamuse@sussex.ac.uk
[2] *School of Mathematics & Statistics, University of St Andrews, UK*

In this talk, I will present a novel solution strategy to efficiently and accurately compute approximate solutions to semilinear optimal control problems, focusing on the optimal control of phase field formulations of geometric evolution laws. The optimal control of geometric evolution laws arises in a number of applications in fields including material science, image processing, tumour growth and cell motility. Despite this, many open problems remain in the analysis and approximation of such problems. In the current work we focus on a phase field formulation of the optimal control problem, hence exploiting the well developed mathematical theory for the optimal control of semilinear parabolic partial differential equations. Approximation of the resulting optimal control problem is computationally challenging, requiring massive amounts of computational time and memory storage. The main focus of this work is to propose, derive, implement and test an efficient solution method for such problems. The solver for the discretised partial differential equations is based upon a geometric multigrid method incorporating advanced techniques to deal with the nonlinearities in the problem and utilising adaptive mesh refinement. An in-house two-grid solution strategy for the forward and adjoint problems, that significantly reduces memory requirements and CPU time, is proposed and investigated computationally. Furthermore, parallelisation as well as an adaptive-step gradient update for the control are employed to further improve efficiency. A number of computational results that demonstrate and evaluate our algorithms with respect to accuracy and efficiency are presented. A highlight of the present work is simulation results on the optimal control of phase field formulations of geometric evolution laws in 3-D which would be computationally infeasible without the solution strategies proposed in the present work.

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Mathematical Models for the Simulation of Burns Injuries

Fred J. Vermolen[1], **Daniel C. Koppenol**[2]

[1] *Delft Institute of Applied Mathematics, Delft University of Technology, The Netherlands*
F.J.Vermolen@tudelft.nl

[2] *Delft Institute of Applied Mathematics, Delft University of Technology, The Netherlands*
D.C.Koppenol@tudelft.nl

Every year millions of people around the globe are subject to accidents that lead to burn injuries. High degree burns and severe cutaneous wounds will give complications in many cases. These complications are excessive contraction or hypertrophic scarring. Hypertrophic scarring is an altered topology of the skin which gives aesthetic problems to the patients. Contraction of the wound, which is an evolutionary mechanism, limits the mobility of the patient. In this talk several models and numerical methods for modeling the contraction and formation of hypertrophic scars will be discussed. The models involve systems of partial differential equations which are based on reaction-transport equations, as well as on mechanical balance. These equations are solved by the use of the finite-element method. These models are useful to model large areas of skin. A set-back of the models is the large number of parameters that are unknown. To this extent, parameter sensitivity analysis will be presented, where the analysis is based on stochastic principles. Mechanical models based on the Neo-Hookean, as well as morphoelasticity will be presented.

Next to these continuum-scale models, we will present some cell-based models, which are based on stochastic principles for migration, cell proliferation (division), differentiation and cell death. These models are applicable on small areas, however, these models are useful in the sense that the input parameters are often close to what can be measured experimentally on the cellular scale.

MS24 – Structure preserving discretizations and high order finite elements for differential forms

(Snorre H. Christiansen, Ragnar Winther, Ana Alonso Rodrıguez, Francesca Rapetti)

Monday, 15:50 – 17:55, Hotel Fleischers Sivle

Richard Falk – *A New Approach to Numerical Computation of the Hausdorff Dimension of Invariant Sets of Iterated Function Systems*

Andrew Gillette – *Decompositions of (Trimmed) Serendipity Spaces*

Kaibo Hu – *Well-Conditioned Frames for Finite Element Methods*

Francesca Rapetti – *The discrete relations between fields and potentials*

Claire Scheid – *A structure preserving numerical discretization framework for the Maxwell Klein Gordon equations in 2D.*

Tuesday, 08:30 – 10:10, Hotel Fleischers Sivle

Roberta Tittarelli – *A residual a posteriori error estimator for the Hybrid High-Order Method*

Wietse Boon – *Mixed-Dimensional Approach to Flows in Fractured, Deformable Media*

Ashish Bhatt – *Structure-preserving ERK Methods for Non-autonomous DEs*

Miroslav Kolář – *Numerical Solution of Area-Preserving Geodesic Curvature Flow*

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MS24 – Structure preserving discretizations and high order finite elements for differential forms

A New Approach to Numerical Computation of the Hausdorff Dimension of Invariant Sets of Iterated Function Systems

Richard S. Falk[1], **Roger D. Nussbaum**[2]

[1] *Department of Mathematics, Rutgers University, USA* falk@math.rutgers.edu
[2] *Department of Mathematics, Rutgers University, USA* nussbaum@math.rutgers.edu

We present a new approach to the computation of the Hausdorff dimension of the invariant set of an iterated function system (IFS) by combining finite element approximation theory with theoretical results about the properties of the eigenfunctions of a class of positive, linear Perron-Frobenius operators L_s. Under appropriate assumptions on the IFS, the Hausdorff dimension of the invariant set of an IFS is the value $s = s_*$ for which the spectral radius λ_s of L_s is equal to one. To approximate this eigenvalue, we first use a collocation method employing continuous piecewise linear or bilinear functions to reduce the infinite dimensional eigenvalue problem to a finite dimensional one. The key property of the approximation scheme is that it preserves the positive structure of the operator L_s. Using the theory of positive linear operators and explicit a priori bounds on the derivatives of the strictly positive eigenfunction v_s corresponding to λ_s, we can modify the matrix produced by the collocation scheme to produce matrices A_s and B_s whose spectral radii bracket λ_s. These spectral radii are easily found by a standard variant of the power method, since the spectral radius of A_s (and of B_s) is the only eigenvalue with that modulus. In this way, we obtain rigorous upper and lower bounds on the Hausdorff dimension s_*, and these bounds converge to s_* as the mesh size approaches zero. Although the present theory is not applicable when higher order piecewise polynomials are used, we demonstrate by numerical examples the promise of this approach. Applications to the computation of the Hausdorff dimension of invariant sets arising from classical continued fraction expansions in one dimension and also to complex continued fractions are described.

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Decompositions of (Trimmed) Serendipity Spaces

Andrew Gillette[1], **Tyler Kloefkorn**[2]

[1] *Department of Mathematics, University of Arizona, USA* agillette@math.arizona.edu
[2] *Department of Mathematics, University of Arizona, USA* tkloefkorn@math.arizona.edu

We recently introduced the family of trimmed serendipity finite element differential form spaces, defined on cubical meshes in any number of dimensions, for any polynomial degree, and for any form order in [2]. The relation between the trimmed serendipity and (non-trimmed) serendipity family developed by Arnold and Awanou in [1] is analogous to the relation between the trimmed and (non-trimmed) polynomial finite element differential form families on simplicial meshes from finite element exterior calculus. The first part of this talk will present key definitions and results regarding trimmed and non-trimmed serendipity spaces. The second part of the talk will examine different ways to decompose these spaces into direct sums and how these decompositions inform basis function construction.

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Well-Conditioned Frames for Finite Element Methods

Kaibo Hu[1], **Ragnar Winther**[2]

[1] *Beijing International Center for Mathematical Research, Peking University, 100871 Beijing, China.* kaibo@pku.edu.cn
[2] *Department of Mathematics, University of Oslo, P.O. Box 1053 Blindern, NO-0316 Oslo, Norway.* rwinther@math.uio.no

We discuss representations of high order C^0 finite element spaces on simplicial meshes in any dimension. For high order methods the conditioning of the basis is likely to be important. However, so far there seems to be no generally accepted concept of "a well-conditioned bases", or a general strategy for how to obtain such representations. In the talk we will argue that the L^2 condition number is a proper measure of the conditioning of the basis. This condition number is independent of the elliptic problem to be solved by the method, and it will lead to constructions which balance desired properties of the stiffness matrix and the preconditioner. In fact, we will not restrict the discussion to representations by bases, but instead allow representations by frames. In particular, we will construct frames for the finite element spaces that lead to L^2 condition numbers which are bounded independently of the polynomial degree. A key tool to obtain this result is the properties of the bubble transform, introduced previously in [1].

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The discrete relations between fields and potentials with high order Whitney forms

Ana Alonso Rodriguez[1], **Francesca Rapetti**[2]

[1] *Math. Dept., Università degli Studi di Trento, Italy* alonso@science.unitn.it
[2] *Math. Dept., Université Côte d'Azur, Nice, France* frapetti@unice.fr

Besides the list of nodes and of their positions, the mesh data structure also contains incidence matrices, saying which node belongs to which edge, which edge bounds which face, etc., and there is a notion of (inner) orientation of the simplices to consider. In short, an edge, face, etc. is not only a two-node, three-node, etc. sub- set of the set of nodes, but such a set plus an orientation of the simplex it subtends. These matrices are very meaningfull. Besides containing all the information about the topology of the domain, for the lowest approximation polynomial degree, they help connecting the dofs describing potentials to dofs describing fields. As an example, the relation $\mathbf{E} = -\mathrm{grad}\, V$ at the continuous level becomes $\mathbf{e} = -G\,\mathbf{v}$ where G coincides with the node-to-edge incidence matrix and $\mathbf{e}$ (resp. $\mathbf{v}$) is the vector of edge circulations (resp. values at nodes) of the electric field $\mathbf{E}$ (resp. the scalar electric potential V). When fields and potentials are approximated by forms of higher polynomial degree, the discrete equivalent of the field/potential relation is more structured. The involved matrices present a structure by blocks, each block taking into account of the transmission of dofs associated to a geometrical dimension. We wish to investigate the block-structure of these matrices, when fields and potentials are approximated by high order Whitney forms [4], with dofs given either by the well-known moments [3, 1] or by the more recent weights on the small simplices [4, 2].

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A structure preserving numerical discretization framework for the Maxwell Klein Gordon equations in 2D.

S. H. Christiansen[1], **T. G. Halvorsen**[1], **C. Scheid**[2]

[1] *Department of Mathematics, University of Oslo, Norway.* snorrec@math.uio.no
[2] *Côte d'Azur University, J. A. Dieudonné Laboratory, Nice, France.*
Claire.Scheid@unice.fr

As an attempt to develop structure preserving numerical schemes for some non linear wave equations arising in theoretical physics, we focus on the case of the Maxwell Klein Gordon (MKG) equations in dimension 2. The equations are derived from a Lagrangian through a variational principle. The Lagrangian is invariant through some gauge transformations. As a consequence, Euler-Lagrange equations contain constraint equations that are preserved by the solutions making the theory consistent. One should thus strive to preserve this symmetry at the discrete level.

The coupling between the electromagnetic field and the complex Klein Gordon scalar field arises through a covariant derivative involving two parts: the gradient of the electromagnetic field and a product of the electromagnetic and the Klein Gordon fields. Classical discretization methods, such as standard Finite Difference methods or Finite Element methods, usually approximate these two parts separately. By doing this, the gauge symmetry is broken. To recover gauge symmetry at the discrete level, we propose to take advantage from Lattice Gauge Theory introduced in [1]. It approximates the covariant derivative in a consistent way and at the same time preserves the local gauge symmetry and as a result, preserves the constraint. This approach has been already successfully applied in e.g. [2, 3].

We propose to continue the analysis of this type of method for MKG and investigate the possibility of including time discretization. Hence, we develop a fully discrete scheme for the MKG equations and prove its convergence. The strategy of proof, based on a discrete energy principle, is developed in the more general context of mechanical Lagrangian and is next applied to the particular case of MKG equations.

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A residual a posteriori error estimator for the Hybrid High-Order Method

Daniele A. Di Pietro[1], **Roberta Tittarelli**[2]

[1,2]*Institut Montpelliérain Alexander Grothendieck, Université de Montpellier, Montpellier, France,*
[1]daniele.di-pietro@umontpellier.fr
[2]roberta.tittarelli@umontpellier.fr

A residual-type error estimator for the Hybrid High-Order discretizations is presented. It is devised such that the upper bound of the energy-norm of the error is guaranteed and the lower bound is local. Numerical tests confirm theorical predicitions and show its efficiency for adaptive mesh refinement.

We study residual-type error estimators for Hybrid High-Order (HHO) discretizations of diffusive problems. The HHO method, recently introduced in [1, 3], has several advantageous features: it supports fairly general meshes including polyhedral elements and nonmatching interfaces, it allows arbitrary approximation orders, and it has a moderate computational cost thanks to hybridization and static condensation. When diffusive problems with sufficiently smooth solutions are considered, the HHO method corresponding to a polynomial degree $k \geq 0$ displays an optimal order of convergence of $(k+1)$ in the energy norm and a superconvergence in $(k+2)$ in the L^2-norm. For non-smooth solutions, on the other hand, achieving optimal convergence requires the use of a posteriori-driven mesh adaptivity.

We present here residual-based a posteriori error estimates for the energy-norm of the error, and we prove upper and (local) lower bounds. The construction relies on the residual-based approach of [2], where an upper bound without undetermined constants is proved. The error estimators are used to drive an adaptive algorithm including local mesh refinement. Two mesh adaptation strategies are presented. The first strategy classically consists in regenerating a locally refined standard mesh based on the error distribution predicted by the a posteriori error estimators. The second strategy, on the other hand, exploits the possibility to use polyhedral elements: the computation is performed on a polyedral mesh obtained by adaptive agglomeration from a fine mesh composed of standard elements. This approach has the advantage of avoiding remeshing, thus waiving a sizeable contribution to the computational cost in industrial applications. Numerical tests are presented to confirm theorical predicitions and show the efficiency of the estimator for physical applications.

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Mixed-Dimensional Approach to Flows in Fractured, Deformable Media

Wietse M. Boon[1], **Jan M. Nordbotten**[1]

[1] *University of Bergen, Norway* wietse.boon@uib.no

The mixed-dimensional representation of a fractured medium is a flexible strategy which handles a wide variety of fracture networks in a robust manner. In such a representation, the fractures and intersections are considered as lower-dimensional manifolds and the associated, governing equations are fully coupled.

In this work, a mixed-dimensional model is formed by combining Darcy flow with linear elasticity in a fractured medium. Keeping later purposes such as transport problems and fracture propagation in mind, the main interest is to obtain accurate flux fields and stress states which possess physical conservation properties. For this purpose, mixed finite elements are employed in the dimensionally hierarchical setting. The symmetry of the stress tensor is then imposed in a weak sense, which allows for the use of familiar, conforming, finite elements with relatively few degrees of freedom.

We present theoretical results including well-posedness of the variational formulation, as well as stability and convergence of the mixed finite element discretization scheme. These results are supported by numerical examples in two and three dimensions.

Structure-preserving ERK Methods for Non-autonomous DEs

Ashish Bhatt[1], **Brian E. Moore**[2]

[1] *Universität Stuttgart, Germany* ashish.bhatt@mathematik.uni-stuttgart.de
[2] *University of Central Florida, USA* brian.moore@ucf.edu

In this talk, we consider structure-preserving discretizations for a non-autonomous differential equation (DE) of the form

$$\dot{z}(t) = f(t,z) = N(z(t)) - \gamma(t)z(t), \quad z : \mathbb{R} \to \mathbb{R}^d. \tag{12}$$

A non-constant function $\mathcal{I} : \mathbb{R}^d \to \mathbb{R}$ is a conformal property of this DE if it satisfies the equation

$$\frac{d}{dt}\mathcal{I}(z) = -2\gamma(t)\mathcal{I}(z) \tag{13}$$

for all $z = z(t, z_0)$, all initial values $z_0 \in \mathbb{R}^d$, and all $t \in \mathbb{R}$. Exponentially decaying momentum, 2-norm of the solution, symplecticness, and Casimir are some examples of conformal properties of a differential equation. Structure-preserving integrators preserve conformal properties of an equation up to the machine precision. It is widely recognized that structure-preserving integrators are advantageous compared to non-structure-preserving integrators for DEs, especially for long time integration.

Conformal property $\mathcal{I}$ is referred to as a first integral when $\gamma = 0$ in (12),(13). Integrators preserving first integrals have been studied extensively in earlier works. The purpose of this talk is to present integrators which preserve conformal properties instead. It was shown in [1, 2] that such integrators can be obtained by imposing restrictions on coefficients of exponential Runge-Kutta methods for a DE having the conformal properties. In this talk, we present these restrictions and illustrate advantages of structure-preserving integrators using numerical experiments.

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Numerical Solution of Area-Preserving Geodesic Curvature Flow

Miroslav Kolář[1], **Michal Beneš**[1], **Daniel Ševčovič**[2]

[1] *Department of Mathematics, Faculty of Nuclear Science and Physical Engineering, Czech Technical University in Prague, Trojanova 13, 120 00, Praha, Czech Republic*
kolarmir@fjfi.cvut.cz
michal.benes@fjfi.cvut.cz

[2] *Department of Applied Mathematics and Statistics, Faculty of Mathematics, Physics and Informatics, Comenius University, Mlynská Dolina, 842 48, Bratislava, Slovakia*
sevcovic@fmph.uniba.sk

We investigate the numerical solution of the evolution law for a constrained non-local geometric flow for closed curves on a surface [1]. Our model reads as

$$\mathcal{V}_{\mathcal{G}} = -\mathcal{K}_{\mathcal{G}} + \mathcal{F},$$

where $\mathcal{V}_{\mathcal{G}}$ is the normal velocity and $\mathcal{K}_{\mathcal{G}}$ is the geodesic curvature of a closed, nonselfintersecting curve $\mathcal{G}_t$ evolving on a surface given by a graph of a smooth 2-dimensional function φ. The force term $\mathcal{F}$ is given as

$$\mathcal{F} = \frac{1}{|\mathcal{G}_t|} \int_{\mathcal{G}_t} \mathcal{K}_{\mathcal{G}} \mathrm{d}\mathcal{S}.$$

This flow is a generalization of a motion law which originates in the physical theory of phase transitions [2] for crystalline materials and describes the evolution of closed embedded curves with constant enclosed area.

It can be proved this motion conserves the area of the enclosed surface. We show how such a surface flow can be projected into a flow of planar curve Γ_t with the non-local normal velocity. The motion law for the curve Γ_t is treated by means of the parametric method [2, 3] resulting in a system of degenerate parabolic partial differential equations.

For the numerical solution of the parametric equations we propose the method of flowing finite volume for the spatial discretization in combination with the Runge-Kutta time integration. Several computational results demonstrating the qualitative and quantitative behavior of the solution will be presented.

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MS25 – PDE Software Frameworks

(Robert Klöfkorn, David Ham)

Thursday, 13:30 – 15:10, Hotel Fleischers Tarald

Robert Klöfkorn – *DunePy: Combining Dune and Python*

Jørgen S. Dokken – *Shape Optimization with Multiple Meshes*

David Ham – *Firedrake: a symbolic numerical mathematics approach to the finite element method.*

Eirik Keilegavlen – *Discretization of mixed-dimensional problems using legacy codes*

Thursday, 15:30 – 17:10, Hotel Fleischers Tarald

Daniele Prada – *Advances in Feel++ : an Open-Source C++ Framework for solving Martin Kronbichler – High-order infrastructure in the* `deal.II` *finite element libray*

Steffen Müthing – PDELab, HPC and code generation: How to tune a discretization framework for performance

PDEs with applications in Health, Physics and Industry.

Antonello Gerbi – *The LifeV Finite Elements library: recent developments and cardiovascular applications*

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DunePy: Combining Dune and Python

Andreas Dedner[1] **and Robert Klöfkorn**[2]

[1] *Mathematics Institute, University of Warwick, Coventry CV4 7AL, UK*
a.s.dedner@warwick.ac.uk
[2] *International Research Institute of Stavanger (Bergen office), Thormøhlensgt. 55, 5006 Bergen, Norway*
Robert.Kloefkorn@iris.no

The Distributed and Unified Numerics Environment *Dune* is a modular toolbox for solving partial differential equations using grid-based methods, e.g., finite element or finite volume schmes. It is written in C++ using static polymorphism (templates) to achieve high efficiency. Interfaces are provided for all the main building blocks: the tessellation of the domain, the discrete function space used for ansatz and trial functions, operators (linear and non linear), and inverse operator based on Newton methods for non linear operators and direct or iterative solvers for linear operators. These interfaces provide the basis for the user code and during compile time a range of realizations of these interfaces can be combined to allow for the development of a wide range of numerical schemes for solving very complex systems of PDEs. This flexibility comes at the cost of in some parts quite high demands on the C++ knowledge of the user.

Recently there has been some efforts to add a scripting layer to *Dune*. In this talk I will present the concepts used to make the high level program structure of a simulation package easier to modify and maintain using the Python language without loosing the efficiency and flexibility provided by the Dune framework. This requires mechanisms for exporting C++ code to Python for which we use the *pybind11* package.

Flexibility is maintained by providing tools for generating the templated C++ class for the required interface realization at run time and using just in time compilation of the required Python modules. With this approach the full flexibility of combining different building blocks provided by Dune is still available within the new Python framework. High level control (pre and post processing, time loops etc.) can now be done within the Python layer while time critical parts of the code (assembly, solving etc.) is taken care of by the original *Dune* structures.

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Shape Optimization with Multiple Meshes

Jørgen S. Dokken[1], **Simon Funke**[1], **August Johansson**[1], **Stephan Schmidt**[2]

[1] *Simula Research Laboratory, Martin Linges vei 25, 1364 Fornebu, Norway* dokken@simula.no
[2] *Institut für Mathematik Universität Würzburg Campus Hubland Nord Emil-Fischer-Straße 40, 97074 Würzburg, Germany* stephan.schmidt@mathematik.uni-wuerzburg.de

For shape optimization problems, the computational domain is the design variable. Changing the shape of an airfoil in a channel to minimize drag is such a problem. The evolving domains complicate the numerical solution of shape optimization problems, and typically require large mesh deformations with quality checks and a re-meshing software as a fallback. We propose an approach for solving shape optimization problems on multiple overlapping meshes. In this approach, each mesh can be moved freely and hence the multi-mesh approach allows larger deformation of the domain than standard single-mesh approaches. The approach has been implemented in FEniCS and dolfin-adjoint, by employing the already tested environment for multi-mesh [1]. We give examples of derivation of the shape-optimization problem for a Stokes flow and present implementation of this in FEniCS.

Consider a general PDE constrained shape optimization problem

$$\min_{\Omega,u} \quad J(u(\Omega),\Omega) \qquad \text{subject to } F(u(\Omega),\Omega)=0, \tag{14}$$

where J is the goal functional, $F(u,\Omega)$ is the state equations, u is the solution of the state equation, Ω is the domain of state equations.

We choose to divide the domain Ω into two non-overlapping domains by creating an artificial interface Γ, s.t. $\Omega=\Omega_0\cup\Omega_1$ and $\Gamma=\Omega_0\cap\Omega_1$. The meshes used to represent Ω is created by meshing the original domain Ω and new domain Ω_1. Therefore there the meshes will not be aligned at the boundary Γ. Extension to an arbitrary number of overlapping domains is possible. A modified weak formulation of the state equations are formulated where the continuity over the artificial boundary is enforced by using Nitsches method.

For minimization, we choose a gradient based scheme and using the adjoint method. By employing the Hadamard formulas for Volume and Surface objective functions[2] we get the functional sensitivities as a function of the moving boundary. For deformation of the mesh, a Laplacian smoothing and a set of Eikonal convection equations[3] is used. We conclude that with a multi-mesh-approach, the meshes are preserved better than with a single-mesh approach.

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Firedrake: a symbolic numerical mathematics approach to the finite element method.

David A. Ham[1]
Thomas Gibson[1] **Miklós Homolya**[2] **Lawrence Mitchell**[1,2], **Paul H.J. Kelly**[2]

[1] *Department of Mathematics, Imperial College London* David.Ham@imperial.ac.uk
[2] *Department of Computing, Imperial College London*

Firedrake is an automated system for the solution of PDEs using the finite element method. The high level interface uses the Unified Form Language (UFL) of the FEniCS project to allow expression of complex variational forms in a language that is close to that of the underlying mathematics. However Firedrake takes this symbolic approach further, employing symbolic reasoning at the finite element, tensor contraction and low-level optimisation levels to produce a composible series of abstractions for the various stages from equation down to high performance code. The result is a flexible, capable and high performance system for the creation of finite element models. Firedrake enables domain scientists and engineers, numericists and computer scientists to benefit from a high productivity environment which they can exploit to advance their fields of expertise, while simultaneously benefitting from the advances of others.

In addition to introducing the core concepts of Firedrake, this presentation will present recent advances in Firedrake's capabilities, such as programmable hybridised solvers, and automated sum factorisation for high order elements.

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Discretization of mixed-dimensional problems using legacy codes.

Eirik Keilegavlen[1], **Alessio Fumagalli**[2], **Runar Berge**[3], **Ivar Stefansson**[4], **Inga Berre**[5]

[1] *Department of Mathematics, University of Bergen, Norway* Eirik.Keilegavlen@uib.no
[2] *Department of Mathematics, University of Bergen, Norway* Alessio.Fumagalli@uib.no
[3] *Department of Mathematics, University of Bergen, Norway* Runar.Berge@uib.no
[4] *Department of Mathematics, University of Bergen, Norway* Ivar.Stefansson@uib.no
[5] *Department of Mathematics, University of Bergen, Norway* Inga.Berre@uib.no

Simulations that involve coupling of domains with different dimensions are relevant for several applications. As an example, in porous media simulations, fractures may act as an important conduit for fluid flow that should be incorporated in the simulation model. One popular approach is to treat the fracture as a lower-dimensional manifold embedded in the simulation domain, effectively defining a mixed-dimensional problem. However, existing simulators tend to aim for mono-dimensional problems, and the inclusion of lower-dimensional features is commonly done on an ad hoc basis.

Here, we present an open source software framework, termed PorePy, that is designed for mixed-dimensional simulations. The software allows mono-dimensional sub-problems to be treated with a wide range of numerical approaches. Inter-dimensional couplings, both discretization and matrix assembly, are handled by PorePy. We show application of the framework to flow and transport problems in fractured porous media.

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Advances in Feel++ : an Open-Source C++ Framework for solving PDEs with applications in Health, Physics and Industry.

Silvia Bertoluzza[3], Vincent Chabannes[1], Guillaume Dollé[1], Giovanna Guidoboni[1], Romain Hild[1], Mourad Ismail [6], Thibaut Metivet [1,6], Daniele Prada[2,3], Christophe Prud'homme[1], Riccardo Sacco[4], Lorenzo Sala[1], Marcela Szopos[1] Christophe Trophime[5] and Jean-Baptiste Wahl[1]

[1]*Université de Strasbourg, CNRS, IRMA UMR 7501, Cemosis, F-67000 Strasbourg, France;* [2] prada@imati.cnr.it
[3]*CNR-IMATI Pavia, Italy;* [4]*Politecnico di Milano, Italy;* [5]*CNRS, LNCMI, France,* [6]*Université de Grenoble-Alpes, CNRS, LIPHY UMR 5588, France*

The library Feel++ (Finite Element method Embedded Language in C++, http://www.feelpp.org) offers a domain specific language to partial differential equations embedded in C++. We have been developing the Feel++ framework to the point where it allows to use a very wide range of Galerkin methods and advanced numerical methods such as Hybridized Discontinuous Galerkin (HDG) methods, domain decomposition methods including mortar and three fields methods, fictitious domain methods or certified reduced basis (CRB). Feel++ has been used in a wide range of applications in health and physics as well as industrial applications.

We start the session by a general presentation of Feel++ and some recent advances. We then focus on our recent work on HDG methods [1]. In particular we will address multiscale coupling in terms of spatial dimensions, where a three dimensional model needs to be coupled with a zero dimensional model, leading to the coupling between partial and ordinary differential equations. We enforce the coupling via integral boundary conditions (IBCs). This kind of conditions arises in a variety of different fields. In ocular biomechanics, for example, an IBC arises when a model for the perfusion of the lamina cribrosa in the optic nerve head is coupled with a lumped model for the retrobulbar circulation. Another example is high field magnet (more than 24T) engineering, where a target current is imposed on a terminal part of the magnet. We present a novel Hybridized Discontinuous Galerkin (HDG) method for the numerical treatment of problems involving IBCs. The HDG method has several attractive features: i) it provides optimal approximation of both primal and flux variables; ii) it requires less globally coupled degrees of freedom than DG methods of comparable accuracy; iii) it allows local element-by-element postprocessing to obtain new approximations with enhanced accuracy and conservation properties. We will show our novel HDG method and discuss some aspects of its implementation in Feel++. Finally, some numerical results in ocular biomechanics and high field magnet engineering will be presented.

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High-order infrastructure in the `deal.II` finite element libray

Martin Kronbichler[1]

[1] *Institute for Computational Mechanics, Technical University of Munich, Boltzmannstr. 15, 85748 Garching, Germany* kronbichler@lnm.mw.tum.de

This talk presents recent developments for efficient high-order computations in the `deal.II` finite element library [1]. The library comes with a flexible matrix-free evaluation infrastructure based on fast quadrature with sum factorization techniques [2] whose design has been guided by high performance computing principles that fit upcoming exascale architectures. A focus on memory bandwidth and efficient arithmetics by explicit vectorization enable the approach to clearly outperform algorithms based on sparse matrices for quadratic and higher-degree shape functions. Experiments show that the implementation is close to the underlying hardware limits for both continuous and discontinuous elements [3]. For example, our implementation for continuous elements reaches the performance of finite difference stencils on Cartesian meshes, limited by the access to the global result vectors on Intel CPUs and the KNL Xeon Phi. Despite efficiency, the `deal.II` implementation is accessible to the programmer with the full flexibility of the C++ programming language.

The matrix-free kernels are embedded into the versatile solver facilities of `deal.II`, in particular a newly developed geometric multigrid method for adaptively refined meshes for a massively parallel context. The solver has shown excellent parallel scaling to at least 147 456 cores [3], even when combined with matrix-free evaluation whose fast intra-node performance would magnify possible communication bottlenecks.

The high-order infrastructure in `deal.II` also includes various methods to represent curved computational domains. Exact mathematical manifold descriptions can be applied to either the boundaries or the full volume as appropriate [1] and used for the finite element mapping directly or through high-order polynomial approximations. Since using a curved description of the boundary only can affect convergence rates beyond order three, transfinite interpolation techniques for extending a curved boundary, e.g. given by a CAD description, in a smooth way into the domain are available.

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PDELab, HPC and code generation: How to tune a discretization framework for performance

Peter Bastian[1], **René Heß**[2], **Dominic Kempf**[3], **Steffen Müthing**[4]

[1] *IWR, Heidelberg University* peter.bastian@iwr.uni-heidelberg.de
[2] *IWR, Heidelberg University* dominic.kempf@iwr.uni-heidelberg.de
[3] *IWR, Heidelberg University* rene.hess@iwr.uni-heidelberg.de
[4] *IWR, Heidelberg University* steffen.muething@iwr.uni-heidelberg.de

PDELab is a discretization framework built on top of the well-known DUNE libraries[1] that is well-suited to systems of PDEs and supports a wide range of discretization techniques. In this talk we give an introduction to some of the core abstractions of the framework and present some of the underlying design decisions.

As part of the continuing development of PDELab, we have recently focused on the performance of matrix-free methods for DG discretizations. In this context, we will present our current approach to sum-factorized matrix-free operator application and discuss the required changes to the framework to actually achieve good performance within a general framework like PDELab.

As writing the highly tuned integration kernels for sum-factorized DG is not feasible for people who are interested in method or application research, we have also started to employ code generation for this purpose, driven by the well-known UFL language[2]. We will demonstrate how to integrate code generation into the workflow of PDELab and show some performance results.

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The LifeV Finite Elements library: recent developments and cardiovascular applications

A. Gerbi[1], **L. Dede'**[2], **S. Deparis**[3], **D. Forti**[4], **A. Quarteroni**[5]

[1] *CMCS, EPFL, Lausanne, Switzerland* antonello.gerbi@epfl.ch
[2] *MOX, Politecnico di Milano, Milan, Italy* luca.dede@polimi.it
[3] *CMCS, EPFL, Lausanne, Switzerland* simone.deparis@epfl.ch
[4] *CMCS, EPFL, Lausanne, Switzerland* davide.forti@epfl.ch
[5] *CMCS, EPFL, Lausanne, Switzerland* alfio.quarteroni@epfl.ch

In this contribution we present recent advancements in the development of the parallel C++ library LifeV[3] [1] and its use in different patient-specific applications for cardiovascular simulations.

In the first part of the talk, we describe LifeV's main features for developers such as the Expression Templates Assembly, which allows to assemble a FEM matrix by simply writing the weak form of the associated PDE, and advanced block linear algebra tools for the definition and solution of integrated multiphysics problems. We moreover illustrate the latest implementation improvements in terms of mathematical models and computational efficiency; these include a monolithic Fluid-Structure Interaction (FSI) solver for non-conforming grids exploiting the internodes method [2] and the FaCSI preconditioner [3], the variational multiscale method for the Navier-Stokes equations, and a new framework for integrated Electro-Mechanics (EM) and Electro-Mechano-Fluid (EMF) cardiac simulations [4].

In the second part of the talk, we show the most recent results obtained with LifeV by approximating and solving the FSI, EM and EMF problems on large scale patient-specific geometries, in the context of High Performance Computing.

References

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MS26 – Approximation of multi-scale nonlinear PDEs

(Adrian Muntean, Omar Lakkis, Chankdrasekhar Venkataraman, Martin Lind)

Monday, 15:50 – 17:55, Kulturhus

Peter Binev – *Optimal Recovery from Data in a Multispace Setup*

Charlie Dounla Lontsi – *High order Rush-Larsen time-stepping methods for cardiac electrophysiology*

Anne Reinarz – *Multiscale modelling of aerospace composites with lamination defects*

Mariya Ptashnyk – *Homogenization of multiscale models for plant tissue biomechanics*

Tristan Pryer – *Variational problems in L^∞ and applications*

Tuesday, 08:30 – 10:10, Kulturhus

Martin Lind – *Two-scale pressure model: weak solvability*

Omar Richardson – *Two-scale pressure model: finite element approximation*

Arthur Vromans – *Homogenization of coupled PDEs describing chemical corrosion of sewer systems in the presence of mechanical stresses*

Sergey Alyaev – *A robust control volume heterogeneous multiscale method for non-linear flows in porous media*

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Optimal Recovery from Data in a Multispace Setup

Peter Binev[1], **Albert Cohen**[2], **Wolfgang Dahmen**[3], **Ronald DeVore**[4], **Guergana Petrova**[5], **Przemyslaw Wojtaszczyk**[6]

[1] *Department of Mathematics, University of South Carolina, Columbia, SC 29208, USA* binev@math.sc.edu

[2] *Laboratoire Jacques-Louis Lions, Université Pierre et Marie Curie, 75005, Paris, France* cohen@ann.jussieu.fr

[3] *Institut für Geometrie und Praktische Mathematik, RWTH Aachen, Templergraben 55, D-52056 Aachen, Germany* dahmen@igpm.rwth-aachen.de

[4] *Department of Mathematics, Texas A&M University, College Station, TX 77840, USA* rdevore@math.tamu.edu

[5] *Department of Mathematics, Texas A&M University, College Station, TX 77840, USA* gpetrova@math.tamu.edu

[6] *Interdisciplinary Center for Mathematical and Computational Modelling, University of Warsaw, 00-838 Warsaw, ul. Prosta 69, Poland* wojtaszczyk@icm.edu.pl

Let $\mathcal{M}$ be a compact subset of a Hilbert space $\mathcal{H}$ obtain as the manifold of the solutions of $\mathcal{D}_p(u) = 0$, where $\mathcal{D}_p$ is a differential operator depending on the parameters $p \in \mathcal{P}$ taken from some compact set $\mathcal{P}$. The problem of optimal recovery [3] is to find an element $u \in \mathcal{M}$ from measurements of the form $\ell_j(u)$, $j = 1, \dots, m$, where the ℓ_j are known linear functionals on $\mathcal{H}$. Often, the only accessible information about $\mathcal{M}$ is that there is a sequence of (nested) n-dimensional linear subspaces $V_n \subset \mathcal{H}$ such that $\operatorname{dist}(V_n, \mathcal{M}) < \varepsilon_n$ for $n = 0, 1, ..., n$. A recovery algorithm for the single-space formulation was proposed in [2]. Using a different formulation utilizing certain favorable bases chosen to represent V_n and the measurements, we prove their algorithm to be optimal. Our major contribution is to analyze the multi-space case. It is shown that, in this multi-space case, the set of all u that satisfy the given information can be described as the intersection of a family of known ellipsoidal cylinders in $\mathcal{H}$. It follows that a near optimal recovery algorithm in the multi-space problem is provided by identifying any point in this intersection. Evidently, the accuracy of recovery of u in the multi-space setting can be much better than in the single-space problems. The results are reported in [1].

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High order Rush-Larsen time-stepping methods for cardiac electrophysiology

Charlie Douanla Lontsi[1,2,3], **Yves Coudière**[2,1,3], **and Charles Pierre**[4]

[1] *Inria Carmen Team, 33400 Bordeaux, France* charlie.douanla-lontsi@inria.fr
[2] *IMB, UMR5251 CNRS, Univ Bordeaux, Bordeaux-INP, 33400 Bordeaux, France*
[3] *Liryc, Fondation Bordeaux University, 33600 Pessac, France*
[4] *Charles Pierre LMAP, CNRS, Université de Pau, France*

The mathematical models used in cardiac electrophysiology are parabolic PDE, coupled with systems of ODEs called ionic models. These models belong to the class of stiff reaction diffusion equations, where the PDE and ODE both are responsible of the stiffness. One of the most popular model is the so called monodomain and its general form coupled with an ionic model is,

$$\partial_t u = div\,(\sigma \nabla u) + f(u,v), \quad \partial_t v = g(u,v)$$

The PDE displays a diffusion term that is solved implicitely. The reaction term coupled with the ODE system is strongly non linear and we want to solve it explicitely. Therefore, we use IMEX methods. The explicit method for the nonlinear part is an exponential integrator specific to the biophysical context, and coherent with our strong understanding of the time scales (stiffness) of the models.

The reaction term g rewrites as a quasilinear equation $g(u,v) = a(u,v)v + b(u,v)$. In the continuity of the first order Rush-Larsen method, the AB2* method from Perego & Veneziani [2], and the more general framework of exponential integrators [1], a possible scheme for the problem above is

$$\begin{aligned} &\text{PDE}: && \text{any convenient IMEX method of order } k \text{ on } u \\ &\text{ODE}: && v_{n+1} = v_n + \phi_1(\alpha_n h)\left(\alpha_n v_n + \beta_n\right), \end{aligned}$$

with $\phi_1(z) = (\exp(z) - 1)/z$. In order to build an order k approximation of v_{n+1}, we propose to construct α_n and β_n as *nonlinear functions of the k previous values $a(u_{n-i}, v_{n-i})$ and $b(u_{n-i}, v_{n-i})$*. This is not a usual high order exponential method: instead of requiring the computation of several functions ϕ_j, we use the simpler exponential Euler form, but with coefficients α_n and β_n that allows to recover the order k. *This new class of method are called RL_k, for Rush-Larsen of order k.*

For $k = 2$, the choice of α_n and β_n is exactly the one from the AB2* method of Perego & Veneziani [2]. At the order $k = 3$, we find that $\alpha_n = \frac{1}{12}(23a_n - 16a_{n-1} + 5a_{n-2})$ and $\beta_n = \frac{1}{12}(23b_n - 16b_{n-1} + 5b_{n-2}) + \frac{h}{12}(a_n b_{n-1} - a_{n-1}b_n)$. We actually calculated up to the formula of order 4, and can actually prove the convergence of these RL_k scheme. We combined this method with the $S - BDF_k$ formulas for the equation on u. We will present the method, and a numerical study that illustrates its interest for some classical models used in cardiac electrophysiology.

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Multiscale modelling of aerospace composites with lamination defects

Anne Reinarz[1], **T. Dodwell**[2], **T. Fletcher**[3], **L. Seelinger**[4], **R. Butler**[3], **R. Scheichl**[1]

[1] *Department of Mathematical Sciences, University of Bath, UK* akr40@bath.ac.uk
[2] *College of Engineering, Mathematics & Physcial Sciences, University of Exeter, UK*
[3] *Department of Mechanical Engineering, University of Bath, UK*
[4] *Institute for Scientific Computing, University of Heidelberg, Germany*

Due to their very good strength to weight ratio, composite materials make up over 50% of recent aircraft constructions. The materials are manufactured from very thin fibrous layers ($\sim 10^{-4}$m) and even thinner resin interfaces ($\sim 10^{-5}$m). To achieve the required strength, a particular layup sequence of orientations of the fibrous layers is used. Finite element modelling of such materials is extremely challenging due to the huge aspect ratio between layer thickness and the size of the modelled structures (~ 10m), as well as due to the varying anisotropic material properties and the large contrast between fibrous and resin layers.

Modelling an entire airplane wing spar down to the scale of the layer thickness would require about 10^{10} degrees of freedom. Even if only a subsection of the spar is modelled, in manufacturing small localised defects in the form of misaligned fibrous layers can occur, which require an even finer mesh resolution. Current industry standard FE tools, e.g. ABAQUS, are not able to deal with these problem sizes, largely due to the direct linear equation solvers that are employed. This also restricts the parallel scalability; ABAQUS uses shared-memory parallelism and does not scale beyond 120 cores. For this reason, we have implemented a new FE solver in the High Performance Computing library DUNE (Distributed and Unified Numerics Environment) to tackle these problems. To achieve robust scaling, this required the implementation of a new general preconditioning strategy within DUNE.

In this talk, I will describe how we implemented the two-level overlapping Schwarz preconditioner GENEO from [1] in DUNE and how it leads to almost optimal scaling with respect to problem size and number of cores. For the coarse space construction, GENEO computes generalised eigenvectors of the local stiffness matrices on the overlapping subdomains and builds an approximate coarse space by combining the smallest energy eigenvectors on each subdomain via a partition of unity. This preconditioner has been proven to be robust for isotropic problems in [1]. I will show that it gives good results also for anisotropic problems and that it scales well over thousands of cores allowing us to successfully tackle the large problems mentioned above.

The coarse space in GENEO can also be used directly as a multiscale method [2] to reduce the computational cost further. I will show how accurately this multiscale method can model the problem, how the accuracy depends on the number of included eigenvectors and how the construction of the coarse space can be reduced by reusing eigenvector calculations from other subdomains.

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Homogenization of multiscale models for plant tissue biomechanics

Mariya Ptashnyk[1]

[1] *Mathematics, University of Dundee, DD1 4HN Dundee, Scotland, UK*
mptashnyk@maths.dundee.ac.uk

Analysis of interactions between mechanical properties and chemical processes, which influence the elasticity and extensibility of plant tissues, is important for better understanding of plant growth and development. Plant tissues are composed of cells surrounded by cell walls and connected to each other by a cross-linked pectin network of middle lamella. The main feature of plant cells are their walls, which must be strong to resist high internal hydrostatic pressure (turgor pressure) and flexible to permit growth. It is supposed that calcium-pectin cross-linking chemistry is one of the main regulators of plant cell wall elasticity and extension [1].

In the microscopic model for plant cell wall and tissue biomechanics we will consider the influence of the microscopic structure and chemical processes on the mechanical properties of plant tissues. The interplay between the mechanics and the chemistry will be defined by assuming that the elastic properties of the plant cell walls depend on the chemical processes (i.e. on the density of calcium-pectin cross-links) and chemical reactions depend on mechanical stresses within the cell walls, modelling the fact that the stress within the plant cell walls can break the load-bearing cross-links. The microscopic model will constitute a strongly coupled system of reaction-diffusion-convection equations for chemical processes in plant cells, the equations of poroelasticity for elastic deformations of plant cell walls and middle lamella, and Stokes equations for fluid flow inside the cells. To analyse the macroscopic behaviour of plant tissues, the macroscopic models for plant cell wall and tissue biomechanics will be derived using homogenization techniques. In the multiscale analysis we will distinguish between periodic and random distribution of cells in a plant tissue. Numerical solutions for the macroscopic model will demonstrate the patterns in the interactions between mechanical stresses and chemical processes.

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Variational problems in L^∞ and applications

Tristan Pryer[1], **Nikos Katzourakis**[1], **George Papamikos**[1]

[1] *Department of Mathematics and Statistics, University of Reading, Whiteknights, PO Box 220, Reading RG6 6AX, UK.* T.Pryer@reading.ac.uk

In this talk we will present a methodology for the approximation of solutions to problems arising from calculus of variations in L^∞. We are particularly interested in 2nd order minimisation problems that give rise to the ∞-Bilaplacian and ∞-Polylaplacian [1]. We make use of L^p approximations and present a variety of theoretical and numerical results [2, 3, 4].

References

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Two-scale pressure model: weak solvability

M. Lind[1], **A. Muntean**[1], **O.M. Richardson**[1]

[1] *Department of Mathematics and Computer Science, Karlstad University, Sweden*
martin.lind@kau.se
adrian.muntean@kau.se
omar.richardson@kau.se

We consider a coupled micro-macro parabolic-elliptic system modeling the interplay between two pressures in a gas-liquid mixture close to equilibrium that is filling a porous media with distributed microstructures. We establish well-posedness as well as other properties of the system. We also obtain local stability of the inverse micro-macro Robin transfer coefficient.

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Two-scale pressure model: finite element approximation

Martin Lind[1], **Adrian Muntean**[1], **Omar Richardson**[1]

[1] *Karlstad Universitet, Sweden*

martin.lind@kau.se
adrian.muntean@kau.se
omar.richardson@kau.se

We consider the stationary limit of a coupled micro-macro parabolic-elliptic system modelling the interplay between two pressures in a gas-liquid mixture close to equilibrium that is filling a porous medium with distributed microstructures. We obtain error estimates for the discretized problem as well as other properties of the system.

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Homogenization of coupled PDEs describing chemical corrosion of sewer systems in the presence of mechanical stresses

A.J. Vromans[1,2]

[1] *Centre for Analysis and Scientific computing and Applications, Technische Universiteit Eindhoven, Netherland* a.j.vromans@tue.nl
[2] *Institutionen för matematik och datavetenskap, Karlstads Universitet, Sweden*

Sewer corrosion is the degradation of concrete due to sulfuric acid reacting with calcite to form gypsum. In this talk I will apply homogenization techniques to upscale a microscopic system of PDEs combining chemical reactions, diffusion, mechanical displacements and viscoelasticity. This research is done jointly with Adrian Muntean (Karlstad, Sweden), Fons van de Ven (Eindhoven, The Netherlands) and Jan Zeman (Prague, Czech Republic).

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A robust control volume heterogeneous multiscale method for non-linear flows in porous media

Sergey Alyaev[1], **Eirik Keilegavlen**[2], **Jan Martin Nordbotten**[3]

[1] *International Research Institute of Stavanger, Norway* Sergey.Alyaev@iris.no
[2] *Department of Mathematics, University of Bergen, Norway* Eirik.Keilegavlen@uib.no
[3] *Department of Mathematics, University of Bergen, Norway; Department of Civil and Environmental Engineering, Princeton University, USA* Jan.Nordbotten@uib.no

Upscaling of flow from pore to Darcy scale is a long standing research field within flow in porous media. It is well known that non-linearities can occur in near-well regions and high-porosity or fractured media. At the same time, the upscaled non-linear effects associated with high flow rates are hard quantify a priori with single-scale models. Advances in pore-scale imaging, combined with increased computational power has made flow simulations in small pore-scale domain feasible, but computations on domains larger than at most a few centimeters are still elusive.

In this work, we present a multiscale simulation framework that combines local pore scale modelling with a conventional mass-conservative discretization at the Darcy scale. We formulate a control volume heterogeneous multiscale method (CVHMM) by coupling of a Darcy-scale control volume method and a finite element solver for Navier-Stokes equations on the fine-scale pore geometry. This approach yields a coarse scale approximation that adapts to non-linear effects as they arise.

Previous versions of CVHMM are consistent only when the coarse grid is aligned with the upscaled permeability [1]. Herein, we generalize CVHMM by introducing a new coarse solver, thus significantly improving the applicability of the method. The presented method is applied to study flow in near-well regions, as well as media with fractures and irregular grain-shapes. The examples show that the method successfully copes with general grids and pore geometries, and handles flows with varying degree of non-linearities even outside the domain of applicability of classical upscaled models. In terms of computational efficiency, the method seamlessly localizes computations to regions where non-linear effects are important.

References

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MS27 – Numerical methods for simulating processes in porous media

(Iuliu Sorin Pop, Raphael Schulz, Peter Knabner, Barbara Wohlmuth)

Tuesday, 13:30 – 15:10, Hotel Fleischers Osa

Clément Cancès – *Parametrization improving the stability of Newton's method: the case of Richards' equation*

David Seus – *A linear domain decomposition method for partially saturated flow in porous media*

Ping Lin – *A Moving Boundary Computational Model in Cancer Invasion of Tissue*

Mario Putti – *A Monge-Kantorovich based model of plant root dynamics in soils.*

Wednesday, 13:30 – 15:35, Hotel Fleischers Osa

Omar Lakkis – *Well-balanced kinetic schemes for the shallow water equation with bulk recharge and discharge*

Barbara Verfürth – *Multiscale Methods for Waves in Periodic Structures*

Ettore Vidotto – *Operator splitting technique using streamline projection for two-phase flow with gravity in heterogeneous porous media*

Martin Vohralík – *A simple a posteriori estimate on general polytopal meshes with applications to complex porous media flows*

Paul Zegeling – *A moving mesh finite difference method for non-monotone solutions of non-equilibrium equations in porous media*

Thursday, 13:30 – 15:10, Hotel Fleischers Osa

Stefan Turek – *Numerical benchmarking for 3D multiphase flow: New results*

Anibal Coronel – *On the numerical approximation for an inverse problem arising in a two-phase flow in porous media*

Koondanibha Mitra – *A Globally Convergent Scheme for Non-linear Pseudo-parabolic Equations Arising from Non-equilibrium effects in Porous Media*

Anna Kvashchuk – *A two-phase flow simulation method with improved stability*

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Parametrization improving the stability of Newton's method: the case of Richards' equation

Konstantin Brenner[1], **Clément Cancès**[2]

[1] *Université de Nice Sophia Antipolis, 06108 Nice Cedex 02, France.*
konstantin.brenner@unice.fr

[2] *INRIA Lille - Nord Europe, 40, avenue Halley, 59650 Villeneuve d'Ascq, France.*
clement.cances@inria.fr

The choice of a convenient primary variable is a crucial issue when solving numerically partial differential equations. In the case of Richards' equation modeling saturated/unsaturated porous media flows, choosing the pressure as the primary variable is mandatory in saturated region, whereas the saturation has to be chosen in dry regions. This enforces to switch from one variable to another in the simulation of flows with both dry and saturated regions.

We propose a formulation of Richards' equation based on the parametrization of the pressure-saturation relation that allows to recover the variable switching procedure at the continuous level. The equation in its parametrized form is discretized thanks to a monotone Two Point Flux Approximation (TPFA) Finite Volume scheme. Under a simple non-degeneracy assumption on the parametrization —but not on the Richards' equation itself!—, the assumptions of Newton-Kantorovich theorem are fulfilled, hence Newton's method converges locally and quadratically. We provide numerical evidences of the efficiency of our approach.

References

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A linear domain decomposition method for partially saturated flow in porous media

David Seus[1], Koondanibha Mitra[2], Sorin Pop, Florin Radu, Chirstian Rohde

[1] *David Seus*
Institute of Applied Analysis and Numerical Simulation
Chair of Applied Mathematics
Pfaffenwaldring 57
70569 Stuttgart
david.seus@mathematik.uni-stuttgart.de

[2] *Koondanibha Mitra*
Department of Mathematics and Computer Science
Technische Universiteit Eindhoven
PO Box 513
5600 MB Eindhoven
The Netherlands
k.mitra@tue.nl

Multiphase flow processes through porous media appear in a variety of physical situations and applications among which soil remediation, enhanced oil recovery, CO_2 storage, harvesting of geothermal energy, design and building of filters are notable examples. In applications in the subsurface mathematical modelling and simulation are often the only tool available to predict what is happening, since measurements of the subsurface are difficult or not feasible at all. The mathematical and computational challenges then appearing, are manifold. The equations are coupled nonlinear PDEs, that vary in type and involve largely varying physical properties of the soil, like porosity, permeability or soil composition. Moreover, the sheer size and scale of the domains pose computational challenges on their own and make the design of robust discretisation methods a non-trivial task.

We combine a globally convergent L-scheme with a non-overlapping domain decomposition of the Richards equation making use of a linearised Robin type interface condition to decouple both problems and obtain a globally convergent scheme which is robust, compares well even against a Newton iteration, and allows to account for very heterogeneous soil properties (different permeabilities, discontinuous over the interface). In particular, it handles situations well, in which Newton and modified Picard schemes fail. We present an analytical convergence result and discuss in detail numerical experiments and comparisons to different schemes (modified Picard, Newton, non-DD FV scheme).

The work presented is joint work with *Koondanibha Mitra, Florin Radu (University of Bergen), Sorin Pop (Hasselt University) and Christian Rohde (University of Stuttgart)*.

References

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A Moving Boundary Computational Model in Cancer Invasion of Tissue

Ping Lin[1]

[1] *Division of Mathematics, University of Dundee, Dundee DD1 4HN, UK*
plin@maths.dundee.ac.uk

Cancer invasion of tissue is a key aspect of the growth and spread of cancer. Invasion consists in cancer cells secreting various matrix degrading enzymes (MDEs) which destroy the surrounding tissue or extracellular matrix (ECM). Through a combination of proliferation and migration, the cancer cells then actively spread locally into the surrounding tissue. In this talk, we introduce a multiscale model describing the process of cancer invasion of tissue. Our multiscale model is a two-scale model: the macroscopic dynamics of the distributions of cancer cells and of the surrounding extracellular matrix, and the microscale dynamics of the MDEs, produced at the level of the individual cancer cells. These microscale dynamics take place at the interface of the cancer cells and the ECM and give rise to a moving boundary at the macroscale. On the computational side, in order to approximate the newly proposed model, we have developed computational schemes for both the micro scale and the macro scale equations, linking together in a moving boundary formulation of the problem. Further extension of this two-scale numerical method hopefully enables to accurately model all the key processes of cancer invasion. This is a joint work with Dumitru Trucu, Mark Chaplain and Yangfan Wang.

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A Monge-Kantorovich based model of plant root dynamics in soils.

Franco Cardin[1], **Enrico Facca**[1], **Mario Putti**[1], **Paolo Zunino**[2]

[1] *Department of Mathematics, University of Padua, Italy*
facca@math.unipd.it, cardin@math.unipd.it, putti@math.unipd.it
[2] *MOX, Department of Mathematics, Politecnico di Milano, Italy.* paolo.zunino@polimi.it

In this paper we describe the numerical solution of a dynamic model of plant root growth as a function of transpiration demand and soil water availability. The root is simulated using a PDE based Branched Optimal Transportation model that minimizes a lagrangian formed by a nonlinear combination of two terms: a cost proportional to the transport energy and a cost proportional to subsurface biomass allocation. The root model is coupled to a standard optimality based plant transpiration simulator [2] and inserted in a Richards equation solver. We focus our discussion mainly on the numerical solution of the OT based root dynamics model recently proposed by [1]. The OT formulation assumes that the transport potential and density are space and time dependent and satisfy an elliptic PDE with source functions defininig the transported mass distribution. The classical constraint on the gradient norm is replaced by an ODE describing the dynamics of the diffusion coefficient. This ODE contains a power law of the flux magnitude stating that the transport density increases with flux magnitude to maintain minimal energy costs. This ingredient gives rise to a network-like fractal structure of the spatial distribution of the transport density. The source terms contain the plant transpirative demand, localized at the xylem foot, and the water content distribution as given by Richards solver. The numerical solution of the OT problem proceeds as follows. A linear P1 Galerkin is used to approximate the transportation potential, while a piecewise constant P0 Galerkin method on a once-refined triangulation discertizes the transport density. Because of the geometrical complexity of real root trees, a brute force approach aiming at modeling the roots as three-dimensional structures is not feasible. For this reason, we apply a model reduction technique that simplifies interactions of the root root system with the surrounding soil following the work proposed in [3]. We will discuss theoretical and experimental results showing convergence of the scheme as well as the adaptation of the PCG method used in the linear solution of the resulting algebraic systems.

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MS27 – Numerical methods for simulating processes in porous media

Well-balanced kinetic schemes for the shallow water equation with bulk recharge and discharge

Mehmet Ersoy[1], **Omar Lakkis**[2], **Philip Townsend**[3],

[1] *Université de Toulon, France* Mehmet.Ersoy@univ-tln.fr
[2] *Free University of Bolzano–Bozen, Italy and University of Sussex, England UK* lakkis.o.maths@gmail.com
[3] *University of Sussex, England UK* P.J.A.Townsend@sussex.ac.uk

In flood risk assessment modelling, Saint-Venant's shallow water equations (SWEs) must be coupled with other systems describing the interacting meteorological and hydrological phenomena such as rain and groundwater flows. The SWEs must therefore be appropriately modified to accommodate source and sink terms; while modifications of the SWEs in this direction have been recently proposed, e.g., [1, eq.(1.3–4)], we depart from existing literature by proposing a model that is, to the best of our knowledge, novel as a natural extension of the SWEs that is "entropy-consistent" and respects its kinetic formulations connections. Kinetic schemes were developed in the late 1990s and throughout the 2000s [3, 2], and have proved crucial in modelling river flows over long (physical) times.

We call our model a "natural extension" of the standard system as it is approached via matched asymptotic expansions from the Navier–Stokes model. The infiltration-recharge mechanism is treated through boundary conditions similar to the Beavers–Joseph–Saffman conditions appearing in fluid-solid interaction problems, where porous media models for underground flows are coupled with surface flows. This approach also provides the appearance of novel "friction" terms (accounting for the inertial effects of recharge) to ensure moment-conservation consistency. We provide extensive numerical testing to illustrate our findings.

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Multiscale Methods for Waves in Periodic Structures

Barbara Verfürth[1], **Mario Ohlberger**[2]

[1] *Applied Mathematics, University of Münster, Germany* barbara.verfuerth@wwu.de
[2] *Applied Mathematics, University of Münster, Germany* mario.ohlberger@wwu.de

The propagation of electromagnetic fields in periodic materials is considered with growing interest as these media can show unusual behavior, such as frequency band gaps and even negative refraction [3]. To produce such effects, the materials possess some (periodic) *sub-wavelength fine-scale* structures, which nevertheless come into resonance with the incident wave.

The simulation of such problems is quite challenging due to the general wave nature of the problem and the additional fine-scale oscillations from the material inhomogeneities. A direct numerical treatment with standard methods easily exceeds today's available computer resources. Therefore, numerical multiscale methods are used, which extract representative macroscale features by solving only localized fine-scale problems.

One example are time-harmonic Maxwell's equations in a medium with *rapidly oscillating* coefficients, see [1, 2]. Due to the large kernel of the curl-operator, a *homogenized* solution of this problem will give a good approximation (only) in H^{-1}. An additional (fine-scale) corrector allows to improve the homogenized function to yield good approximations in L^2 or $\mathbf{H}(\mathrm{curl})$. This corrector can be computed efficiently by solving only localized fine-scale problems. The associated numerical schemes have optimal convergence rates under mesh refinement, which is confirmed by numerical examples.

Another example is the Helmholtz equation with periodic, *high contrast* coefficients, which leads to an effective permeability with negative real part at certain frequencies in the homogenization limit. In this example again, a (fine-scale) corrector is needed for a good approximation in L^2 and it can be efficiently computed as the solution of local cell problems, see [4]. The corresponding numerical method is used to illustrate the occurrence of frequency band gaps related to negative (effective) permeabilities.

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Operator splitting technique using streamline projection for two-phase flow with gravity in heterogeneous porous media

Ettore Vidotto[1], **Rainer Helmig**[2], **Barbara Wohlmuth**[3]

[1] *Institute for Numerical Mathematics, Technische Universität München, D-85748 Garching b. München, Germany.* (ettore.vidotto@ma.tum.de)
[2] *Institut für Wasser- und Umweltsystemmodellierung, Universität Stuttgart, D-70569 Stuttgart, Germany.* rainer.helmig@iws.uni-stuttgart.de
[3] *Institute for Numerical Mathematics, Technische Universität München, D-85748 Garching b. München, Germany.* barbara.wohlmuth@ma.tum.de

In this talk, we investigate the numerical approximation of two-phase flow in the subsurface in presence of highly heterogeneous media and where capillary effects are neglected. The fractional formulation of the transport equation allows us to choose different methods for each equation, depending on the properties of the problem. Due to the presence of strong discontinuities in the paramentes of the problem, a discontinuous Galerkin method have been employed for solving the pressure equation. The high computational costs of the method are reduced by domain decomposition and algebraic multigrid preconditioner. The transport equation is then solved by means of a fast and stable solver that can handle the advective nature of the equation. A streamline approach combined with the one-dimensional front tracking method represents an efficient choice to solve the advective step, while controlling the overall computational costs. Operator splitting techniques are further employed to split advection with gravity on a non-orthogonal grid spanned by streamlines and gravity lines, respectively. An accurate computation of the streamlines is the most important step in this approach and a new scheme is proposed. The robustness and stability of the method is demonstrated in various tests, where the usage of large time step does not undermine the quality of the solution.

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A simple a posteriori estimate on general polytopal meshes with applications to complex porous media flows

Martin Vohralík[1], **Soleiman Yousef**[2]

[1] *Inria Paris, 2 rue Simone Iff, 75589 Paris, France & Université Paris-Est, CERMICS (ENPC), 77455 Marne-la-Vallée, France* martin.vohralik@inria.fr
[2] *IFP Energies nouvelles, 1 & 4 av. Bois Préau, 92852 Rueil-Malmaison, France* soleiman.yousef@ifpen.fr

We develop an posteriori error estimate for lowest-order locally conservative methods on meshes consisting of very general polytopal elements. We focus on the ease of implementation of the methodology based on H^1-conforming potential reconstruction and $H(\mathrm{div})$-conforming flux reconstruction. In particular, the evaluation of our estimates merely consists in some local matrix-vector multiplications, where, on each mesh element, the matrices are either directly inherited from the given numerical method, or trivially constructed from the element geometry, while the vectors are the degrees of freedom on the given element. We then apply this methodology to unsteady nonlinear coupled degenerate problems describing complex multiphase flows in porous media. Here, on each step of the time-marching scheme, linearization procedure, and linear algebraic solver, we distinguish the corresponding error components. This leads to an easy-to-implement and fast-to-run adaptive algorithm with simultaneously guaranteed overall precision and optimal efficiency ensured through the use of adaptive stopping criteria together with adaptive space and time mesh refinements. Numerous numerical experiments on practical problems in two and three space dimensions illustrate the performance of our methodology.

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A moving mesh finite difference method for non-monotone solutions of non-equilibrium equations in porous media

Paul Andries Zegeling[1], **Hong Zhang**[2]

[1] *Department of Mathematics, Utrecht University, The Netherlands* p.a.zegeling@uu.nl
[2] *Department of Mathematics, Utrecht University, The Netherlands* h.zhang4@uu.nl

An adaptive moving mesh finite difference method is presented to solve two types of equations with a dynamic capillary pressure term from porous media. One is the non-equilibrium Richards Equation and the other is a modified Buckley-Leverett equation. The governing equations are discretized with an adaptive moving mesh finite difference method in the space direction and an implicit-explicit method in the time direction. In order to obtain high quality meshes, an adaptive time-dependent monitor function with directional control is applied to redistribute the mesh grid in every time step, and a diffusive mechanism is used to smooth the monitor function. The behaviour of the central difference flux, the standard local Lax-Friedrich flux and the local Lax-Friedrich flux with reconstruction is investigated by solving a 1D modified Buckley-Leverett equation. With the moving mesh technique, a good mesh quality and a high numerical accuracy are obtained. A collection of one-dimensional and two-dimensional numerical experiments is presented to demonstrate the accuracy and effectiveness of the numerical method.

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Numerical benchmarking for 3D multiphase flow: New results

S. Turek[1], **O. Mierka**[2]

[1] INSTITUTE FOR APPLIED MATHEMATICS (LS3), TU DORTMUND, GERMANY
stefan.turek@math.tu-dortmund.de

[2] *Institute for Applied Mathematics (LS3), TU Dortmund, Germany*
otto.mierka@math.tu-dortmund.de

Based on the reference results in [1] for a 2D rising bubble, we present the extension towards 3D providing test cases with corresponding reference results, including also an axisymmetric configuration which allows 2.5D simulations, for validation and evaluation of numerical multiphase flow components and software tools. Moreover, we provide new (reference) results for Taylor bubble flow configurations. As an outlook, we discuss possible extensions and corresponding problems and challenges towards configurations including topology changes (”breakup”), more complex geometries (”Coiled Flow Inverter”) and additional physical effects (”chemical reactions at the interface”).

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On the numerical approximation for an inverse problem arising in a two-phase flow in porous media

A. Coronel[1],

[1] *Departamento de Ciencias Básicas, Universidad del Bío-Bío, Campus Fdo. May, Chillán, Chile* acoronel@ubiobio.cl

In this paper, we study the inverse problem arising in the model describing vertical equilibrium for two-phase flow in porous media. We consider some physical assumptions such that the mathematical model (direct problem) is an initial boundary value problem for a parabolic degenerate equation. In the case of the inverse problem we consider that we have a set of experimental data for the liquid saturation phase (or for the recovery response) and we want to determine the coefficients (flux and diffusion functions) of the equation. For numerical approach we consider the particular case of the inverse problem: the parameter identification problem. Indeed, we formulate the identification problem as a minimization of a suitable cost function and we derive its numerical gradient by means of the adjoint equation and sensitivity equation method. We start with the discrete Lagrangian formulation and assuming that the direct problem is discretized by the finite volume scheme we obtain the discrete adjoint state and the sensitivity scheme. Then, with the numerical solutions of the direct problem and the discrete adjoint state or the sensitivity scheme we calculate the numerical gradient. The conjugate gradient method allows us to find numerical values of the flux and diffusion parameters. We study the convergence of the numerical schemes and also present some numerical examples.

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A Globally Convergent Scheme for Non-linear Pseudo-parabolic Equations Arising from Non-equilibrium effects in Porous Media

K. Mitra[1], **I.S. Pop**[2], **C.J. van Duijn**[3]

[1] *TU Eindhoven, The Netherlands* k.mitra@tue.nl
[2] *Hasselt University & University of Bergen* sorin.pop@uhasselt.be
[3] *TU Eindhoven & University of Utrecht, The Netherlands* C.J.v.Duijn@TUE.nl

The Richards equation is a commonly used model for unsaturated flow through porous media. Using the Darcy law in the mass balance equation, and bringing the resulting equation to a dimensionless form, for gravity driven flow one gets the equation:

$$\partial_t S(p) = \nabla \cdot \left[k(S) \left(N_c \nabla p - \hat{g} \right) \right]. \tag{15}$$

Here $\hat{g}$ is the unit vector of gravitational acceleration, N_c is the capillary number, and $k(S)$ is a nonlinear function that is determined based on experiments. Two unknowns are involved: S, the water saturation and p, the water pressure. Standard models assume that these are related by a nonlinear relationship determined, again, based on experiments:

$$-p = P_c(S). \tag{16}$$

However (16) does not take into account the hysteresis effects [2] and dynamic effects [1] that are observed from experiments. One of the standard forms that incorporates these effects is:

$$-p = P^+(S) - P^-(S) \cdot \operatorname{sign}(\partial_t S) - \tau f(S) \partial_t S. \tag{17}$$

(15) and (17) constitute a highly non-linear pseudo-parabolic system of equations which is difficult to solve numerically. In this work we consider a linear scheme for these equations, based on L-scheme given in [3, 4] and prove that it is globally convergent. The scheme can be implemented for other models and for hysteresis in permeability. Moreover we propose an improvement over the standard L-scheme that can boost up the time-performance substantially. Finally for one dimensional case we compare the numerical results with travelling wave solutions coming from mathematical analysis and present error characteristics and comparative studies.

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MS27 – Numerical methods for simulating processes in porous media

A two-phase flow simulation method with improved stability

Anna Kvashchuk[1], **Adrian Florin Radu**[2], **Robert Klöfkorn**[3]

[1] *The National IOR Centre of Norway/UiS, Norway* Anna.Kvashchuk@iris.no
[2] *University of Bergen, Norway* Florin.Radu@uib.no
[3] *The National IOR Centre of Norway/IRIS, Norway* Robert.Kloefkorn@iris.no

Efficient numerical modeling of multi-phase flow in porous media is the key to accurate simulation of a wide range of applications.

In this work, we present a new implicit scheme for two-phase flow. The proposed scheme is based on the iterative IMPES (IMplicit Pressure Explicit Saturation) method and, therefore, preserves its efficiency in treatment of nonlinearities, while relaxing the time step condition common for explicit methods. At the same time, it does not involve costly computation of Jacobian matrix required for generic Newton's type methods. In contrast with [1], we are not considering here a global pressure formulation for the two-phase model.

Implicit treatment of capillary pressure term ensures stability and convergence properties of the new scheme. This choice of stabilization is supported by mathematical analysis of the method which also includes rigorous proof of convergence.

Our numerical results indicate that the scheme has superior performance compared with standard IMPES and fully implicit methods on benchmark problems.

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MS28 – Model reduction methods for simulation and (optimal) control

(Peter Benner, Jan Heiland, Martin Stoll, Ralf Zimmermann)

Tuesday, 15:30 – 17:10, Hotel Fleischers Bergslien

Ralf Zimmermann – *Parametrization techniques for reduced-order bases and subspaces*

Christian Himpe – *Cross-Covariance-Based Model Reduction*

Benjamin Peherstorfer – *Online adaptive discrete empirical interpolation for nonlinear model reduction*

Ion Victor Gosea – *Model order reduction of hybrid systems*

Thursday, 13:30 – 15:10, Hotel Fleischers Bergslien

Jan Heiland – *Space-time Galerkin POD for Optimal Control of Nonlinear PDEs*

Carmen Gräßle – *Adaptive trust-region POD for optimal control of the Cahn-Hilliard equation*

Luca Mechelli – *POD-Based Model Predictive Control with control and state constraints*

Kathrin Smetana – *Probabilistic A Posteriori Error Estimates in Model Reduction*

Firday, 08:30 – 10:10, Hotel Fleischers Bergslien

Martin Hess – *Spectral Element Reduced Basis Method in parametric CFD*

Cédric Herzet – *Beyond Galerkin Projection by Using "Multi-space" Priors*

Zoi Tokoutsi – *Real Time Optimization of Thermal Ablation Cancer Treatments – An application of the certified reduced basis method for parametrized optimal control problems*

Julia Brunken – *Model reduction based on space-time variational formulations of transport equations*

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Parametrization techniques for reduced-order bases and subspaces

Ralf Zimmermann[1], **Kristian Debrabant**[1]

[1] *Department of Mathematics and Computer Science, SDU Odense, Danmark*
zimmermann@imada.sdu.dk
debrabant@imada.sdu.dk

The problem of computing one-parameter trajectories of reduced orthogonal bases may be approached via computing one-parameter trajectories in the Stiefel manifold. Likewise, one-parameter trajectories of reduced subspaces (that are, in turn, represented by orthogonal bases) can be obtained via computing one-parameter trajectories in the Grassmann manifold. In [1], a corresponding method was introduced that utilizes sensitivity information on the singular value decomposition in combination with geodesic paths on the respective manifolds. In this talk, we will discuss possibilities for error estimation for this approach and show applications to problems in mathematical finance

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MS28 – Model reduction methods for simulation and (optimal) control

Cross-Covariance-Based Model Reduction

Peter Benner[1], **Sara Grundel**[2], **Christian Himpe**[3]

[1] *Computational Methods in Systems and Control Theory Group at the Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstraße 1, D-39106 Magdeburg, Germany*
benner@mpi-magdeburg.mpg.de

[2] *Computational Methods in Systems and Control Theory Group at the Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstraße 1, D-39106 Magdeburg, Germany*
grundel@mpi-magdeburg.mpg.de

[3] *Computational Methods in Systems and Control Theory Group at the Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstraße 1, D-39106 Magdeburg, Germany*
himpe@mpi-magdeburg.mpg.de

The simulation of input-output systems involves computing an output function based on the solution of a differential equation given an input function. Typically, the input- and output functions are of significant lower order than the intermediary differential equation. It is thus relevant to ask if a lower order mapping from inputs to outputs exists, so that the sought output function can be computed faster.

For nonlinear input-output systems, proper orthogonal decomposition is a popular model reduction method, yet it considers only the differential equation (input-to-state mapping) for the construction of the reduced order model and ignores the output function as the quantity of interest. The presented cross-covariance-based model reduction is a generalization of the cross-Gramian-based reduction, and hence as a balancing-type approach focuses on the input-to-output mapping of the underlying nonlinear system.

To demonstrate the applicability of the investigated model reduction technique, commonly used models of gas transportation networks provide a challenging test subject. This model class consists of square descriptor input-output systems of which the dynamic system's vector field has a hyperbolic linear and a nonlinear component. Hence, gas network models have multiple intricate facets, highlighting the advantages of cross-covariance-based model reduction.

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Online adaptive discrete empirical interpolation for nonlinear model reduction

Benjamin Peherstorfer[1], **Karen Willcox**[2]

[1] *University of Wisconsin-Madison, USA* peherstorfer@wisc.edu
[2] *Massachusetts Institute of Technology, USA* kwillcox@mit.edu

Data-driven model reduction constructs reduced models of large-scale systems by learning the system response characteristics from data. We present a nonlinear model reduction approach for systems of equations stemming from the discretization of partial differential equations with nonlinear terms. Our approach constructs a reduced system with proper orthogonal decomposition and the discrete empirical interpolation method (DEIM); however, whereas classical DEIM derives a linear approximation of the nonlinear terms in a static DEIM space generated in an offline phase, our method adapts the DEIM space as the online calculation proceeds and thus provides a nonlinear approximation. The online adaptation uses new data to produce a reduced system that accurately approximates behavior not anticipated in the offline phase. These online data are obtained by querying the full-order system during the online phase, but only at a few selected components to guarantee a computationally efficient adaptation. Compared to the classical static approach, our online adaptive and nonlinear model reduction approach achieves accuracy improvements of up to three orders of magnitude in our numerical experiments with time-dependent and steady-state nonlinear problems. The examples also demonstrate that through adaptivity, our reduced systems provide valid approximations of the full-order systems outside of the parameter domains for which they were initially built in the offline phase.

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Model order reduction of hybrid systems

Ion Victor Gosea[1], **Athanasios C. Antoulas**[2]

[1] *Data-Driven System Reduction and Identification Group, Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstrasse 1, 39106, Magdeburg, Germany.* gosea@mpi-magdeburg.mpg.de

[2] *Department of Electrical and Computer Engineering, Rice University, 6100 Main Street, MS-366, Houston, TX 77005, USA and Data-Driven System Reduction and Identification Group, Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany.* aca@rice.edu

A *linear hybrid system* (or LHS) is a dynamical system whose discrete dynamics is determined by a finite-state automaton, and whose continuous dynamics at each discrete state (or operational mode) is described by a linear time-invariant differential equation. The so-called finite Moore-automaton is a finite-state deterministic automaton equipped with outputs. The reset maps allow the transition between discrete modes and the discrete events are externally generated inputs.

Linear switched systems (or LSSs) can be viewed as a subclass of LHSs, for which the discrete dynamics is simplified as the discrete events, outputs and states coincide and the reset maps are usually identity maps. Both LHSs and LSS have state-space representations (see [1]), with finitely many state variables, that are used to predict the future behavior of the system.

Hybrid and switched systems offer proper models for distributed embedded systems design where discrete controls are routinely applied to continuous processes. In some cases, the complexity of such systems might be very high. To cope with this issue, introduce *model order reduction* (MOR) techniques specifically tailored for such systems. Most of the approaches developed for LSSs usually generalize well to LHSs.

We propose a data driven MOR method that can be viewed as the extension of the approach in [2], to the class of LHS. Through this new procedure, one can derive state-space models directly from data that is related to the input-output behavior of the original system. Hence, an advantage of the framework is that it does not require the original model, but only frequency domain samples from input-output mappings (or transfer functions) of the original system. We provide a formal definition of such generalized transfer functions for linear hybrid systems. Finally, several numerical examples illustrate the preceding theoretical results.

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Space-time Galerkin POD for Optimal Control of Nonlinear PDEs

Peter Benner[1], **Jan Heiland**[2]

[1] *Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany*
benner@mpi-magdeburg.mpg.de
[2] *Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany*
heiland@mpi-magdeburg.mpg.de

The method of *Proper Orthogonal Decomposition* (POD) is a standard method for the reduction of nonlinear models. In the context of partial differential equations, POD can be seen as the use of snapshots of the solution at certain discrete time points to reveal dominant states which are then used for optimal low-dimensional space discretizations.

If space-time Galerkin discretizations are considered, one can transpose the classical POD to provide also optimal low-dimensional time discretizations; cf. [1].

In this talk, we present the theoretical framework of this POD extension and address its benefits for the use in optimal control. We show applicability of this approach for an optimal control problem for the *Burgers* equation and discuss its efficiency in comparison to established gradient-based methods.

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Adaptive trust-region POD for optimal control of the Cahn-Hilliard equation

Carmen Gräßle[1], **Michael Hinze**[2], **Nicolas Scharmacher**[3]

[1] *Universität Hamburg, Germany* carmen.graessle@uni-hamburg.de
[2] *Universität Hamburg, Germany* michael.hinze@uni-hamburg.de
[3] *Universität Hamburg, Germany* nicolas.scharmacher@uni-hamburg.de

We consider the optimal control of a Cahn-Hilliard system in a trust-region framework. For an efficient numerical solution, the expensive high dimensional PDE systems are replaced by reduced order models utilizing proper orthogonal decomposition (POD-ROM). Within the trust-region POD (TR-POD), the accuracy of the surrogate models is controlled in the course of the optimization. The POD modes are computed corresponding to snapshots of the governing equations which are discretized utilizing adaptive finite elements. In the numerical examples, the smooth as well as the double-obstacle free energy potential are considered.

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POD-Based Model Predictive Control with control and state constraints

L. Mechelli[1], **S. Volkwein**[2]

[1] *University of Konstanz, Germany* luca.mechelli@uni-konstanz.de
[2] *University of Konstanz, Germany* stefan.volkwein@uni-konstanz.de

In the setting of energy efficient building operation, we investigate an optimal boundary control problem governed by linear parabolic convection-diffusion equations with bilateral inequality constraints for the control and the state variables. The aim is to keep the temperature in a room in a certain range with the less possible cost of heating for the heaters for a large time horizon. This leads to model predictive control (MPC) techniques in order to compute the infinite time quadratic cost functional, find the optimal boundary control and approximate the asymptotic behavior of the solution. For the state constraints, in order to gain regular Lagrange multipliers, we utilize a Lavrentiev regularization. After a spatial discretization with finite elements and a time discretization with the implicit Euler method, we solve the problem with a primal-dual active set strategy (PDASS), which has superlinear rate of convergence. To speed up the solution computation, we apply proper orthogonal decomposition (POD) method for model reduction and adjust the PDASS algorithm to the POD-Galerkin reduced problem. For that purpose we apply a-posteriori error estimation.

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Probabilistic A Posteriori Error Estimates in Model Reduction

A. Buhr[1], **A. T. Patera**[2], **and K. Smetana**[3]

[1] *Institute for Computational and Applied Mathematics, University of Münster, Einsteinstr. 62, 48149 Münster, Germany* andreas@andreasbuhr.de
[2] *Department of Mechanical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge MA 02139-4307, USA* patera@mit.edu
[3] *Department of Applied Mathematics, University of Twente, P.O. Box 217, NL-7500 AE Enschede, the Netherlands* kathrin.smetana@wwu.de

In this talk we discuss probabilistic a posteriori error estimates for model reduction procedures for linear Partial Differential Equations (PDEs) that are inf-sup stable.

Starting from results in [2] we present first a probabilistic a posteriori error estimator which estimates the norm of an operator by the norm of the application of the operator to Gaussian random vectors. We employ this a posteriori error estimate within an adaptive algorithm to construct local approximation spaces for local model order reduction procedures. Moreover, we demonstrate that those local approximation spaces yield an approximation that converges with a nearly optimal rate.

Second, we present a probabilistic a posteriori error estimator for the reduced basis (RB) method that does not require the estimation of the inf-sup or coercivity constant of the bilinear form of the considered PDE. One key ingredient of the a posteriori error estimator is the solution of a reduced dual problem with random right-hand side. Here, we extend the approach in [1], where the solution of an adjoint problem with random conditions at the final time is employed to estimate the approximation error for Ordinary Differential Equations. Both the a posteriori error estimator presented in this talk and the one introduced in [1] rely on the small sample statistical method as proposed in [3], which can in particular be used to estimate the norm of a vector by evaluating the inner product of this vector with certain random vectors. By employing the above we show that if the RB approximation error of the dual problem is small the error between the reference finite element solution and the RB primal approximation can be bounded, with high probability, from below and above by the a posteriori error estimator times a constant.

Numerical experiments confirm the theoretical findings.

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Spectral Element Reduced Basis Method in parametric CFD

Martin W. Hess[1], **Gianluigi Rozza**[2]

[1] *SISSA mathLab, International School for Advanced Studies, via Bonomea 265, I-34136 Trieste, Italy* mhess@sissa.it
[2] *SISSA mathLab, International School for Advanced Studies, via Bonomea 265, I-34136 Trieste, Italy* gianluigi.rozza@sissa.it

We consider the incompressible Navier-Stokes equations in a channel, discretized with the spectral element method [1]. With increasing Reynolds number, the incompressible Navier-Stokes system undergoes a bifurcation. We consider a parametrized flow problem with the Reynolds number as a single parameter. Applications of this model are contraction-expansion channels, found in many biological systems, such as the human heart for instance.

The aim of this work is to show the applicability of the reduced basis model reduction [2] to flow problems, discretized with the spectral element method. Depending on the choice of expansion functions of the spectral element method, the Navier-Stokes system matrix forms a block structure of dense and sparse parts. Taking this into account in the model reduction process, can potentially improve on the size and approximation quality of reduced models.

A further aim is to investigate the use of a reduced model approach for bifurcation analysis [3], [4]. Following the different bifurcating branches as well as determining the bifurcation point itself, is a complex computational task. Reduced order models can potentially reduce the computational burden by several orders of magnitude.

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Beyond GALERKIN Projection by Using "Multi-space" Priors

Diallo Mamadou Lamarana[1], **Héas Patrick**[1] **and Herzet Cédric**[1]

[1] *INRIA, Centre Rennes-Bretagne Atlantique, France* mamadou.diallo@inria.fr
cedric.herzet@inria.fr

Let $\mathcal{H}$ be some Hilbert space with induced norm $\|\cdot\|$. We consider the problem of approximating the solutions of a parametric partial differential equation (PPDE), say $\mathcal{M} = \{\boldsymbol{h} : \mathrm{PDE}(\boldsymbol{h}, \theta) = 0 \text{ for some } \theta \in \Theta\}$, within a N-dimensional subspace $V_N \subset \mathcal{H}$. We consider a PPDE whose weak formulation takes the following form:

$$\text{find } \boldsymbol{h} \in \mathcal{H} \text{ such that } \; a_\theta(\boldsymbol{h}, \boldsymbol{h}') = b_\theta(\boldsymbol{h}') \quad \text{for } \boldsymbol{h}' \in \mathcal{H},$$

where $a_\theta(\cdot,\cdot)$ and $b_\theta(\cdot)$ are respectively some bilinear and linear forms.

The orthogonal projection (with respect to $\|\cdot\|$) of the elements of $\mathcal{M}$ onto V_N being usually too computationally-demanding, one standard option is to resort to Galerkin projection:

$$\text{find } \boldsymbol{h} \in V_N \text{ such that } \; a_\theta(\boldsymbol{h}, \boldsymbol{h}') = b_\theta(\boldsymbol{h}') \quad \text{for } \boldsymbol{h}' \in V_N.$$

The "quality" of the Galerkin approximation (its closeness to the true orthogonal projection) depends on the "conditioning" of the operator $a_\theta(\cdot,\cdot)$ and $b_\theta(\cdot)$ (e.g. via their coercivity and continuity constants [1]). In some difficult case, Galerkin projection may thus leads to poor approximation results. In our work, we propose a simple way to improve Galerkin projections.

We consider the setup where V_N corresponds to the N-dimensional subspace computed via a reduced-basis method [1]. Now, while computing the subspace V_N, this type of methodology also generates a sequence of subspaces $\{V_i\}_{i=0}^N$ and some positive scalars $\{\epsilon_i\}_{i=0}^N$ such that

$$V_0 \subset V_1 \subset \ldots \subset V_N,$$

and

$$\sup_{\boldsymbol{h}\in\mathcal{M}} \mathrm{dist}(\boldsymbol{h}, V_i) \leq \epsilon_i.$$

The last inequality provides some information about $\mathcal{M}$ since it implies that the latter is included in the intersection of N (degenerate) ellipsoids, i.e. $\mathcal{M} \subseteq \cap_{i=0}^N \{\boldsymbol{h} : \sup_{\boldsymbol{h}\in\mathcal{M}} \mathrm{dist}(\boldsymbol{h}, V_i) \leq \epsilon_i\}$.

In our work, we propose a new suboptimal projection method exploiting the fact that $\mathcal{M}$ is included in the intersection of a set of *known* ellipsoids. The proposed methodology boils down to the standard Galerkin projection when one single ellipsoid is considered. We provide both theoretical and empirical results showing that the proposed methodology clearly outperforms the standard Galerkin projection in some situations. Our derivations are based on the recent work by Binev et al. [2]

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Real Time Optimization of Thermal Ablation Cancer Treatments
An application of the certified reduced basis method for parametrized optimal control problems

Zoi Tokoutsi[1,2], **Mark Kärcher**[2], **Martin A. Grepl**[3], **Karen Veroy**[2], **Marco Baragona**[1], **Ralph Maessen**[1]

[1] *Philips Research Eindhoven, the Netherlands* tokoutsi@aices.rwth-aachen.de
[2] *Aachen Institute for Advanced Study in Computational Engineering Science (AICES) RWTH Aachen University, Germany* kaercher@aices.rwth-aachen.de
veroy@aices.rwth-aachen.de
[3] *Institut für Geometrie und Praktische Mathematik (IGPM) RWTH Aachen University, Germany* grepl@igpm.rwth-aachen.de

Thermal ablation cancer treatments [1] aim at local thermal dose delivery in the volume surrounding cancerous tissue, which is enough to burn the tumor, while leaving the surrounding healthy tissue and neighboring sensitive risk structures undamaged. Studying the optimal delivery of heat in the tumor and predicting the outcome of the treatment via mathematical models and numerical simulations is part of the ongoing research on thermal ablation treatments, [2], [3]. The heat delivery optimization can be formulated as a parametrized optimal control problem with respect to tissue properties, which vary between patients, the proximity of the tumor to risk structures, and the steering of the heat generating device. In this work we present an optimal control problem motivated by ablative cancer treatments and propose the use of the reduced basis method to create a surrogate model for the optimization, as in [4]. This approach increases the efficiency in solving of the optimal control problem and enables real time updates of the outcome prediction.

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Model reduction based on space-time variational formulations of transport equations

Julia Brunken[1], **Mario Ohlberger**[1], **Kathrin Smetana**[2], **and Karsten Urban**[3]

[1] *Applied Mathematics, University of Münster, Einsteinstr. 62, 48149 Münster, Germany*
julia.brunken@wwu.de, mario.ohlberger@wwu.de
[2] *Department of Applied Mathematics, University of Twente, PO Box 217, 7500 AE Enschede, The Netherlands*
kathrin.smetana@wwu.de
[3] *University of Ulm, Institute for Numerical Mathematics, Helmholtzstr. 20, 89081 Ulm, Germany*
karsten.urban@uni-ulm.de

Motivated by high-dimensional kinetic transport equations we consider in this talk a posteriori error estimation and model reduction techniques for time-dependent transport equations that are based on space-time variational formulations.

Kinetic equations describe densities in phase space consisting of independent space, time, and velocity variables. To tackle the high-dimensionality we employ the Reduced Basis-Hierarchical Model Reduction approach where we use a problem-adapted basis in the velocity variable to arrive at a hyperbolic system in the space-time domain [1].

In this context, efficient error estimators are desirable both for the construction of the reduced basis and the validation of reduced solutions. To derive such estimates it is beneficial to consider space-time variational formulations: these may lead to favorable inf-sup constants, which is important as their inverse enters into error estimates as considered in the Reduced Basis context.

We derive a posteriori error estimators for time-dependent transport equations where the corresponding stationary equation can be described by inf-sup stable variational formulations with possibly different ansatz and test spaces. As a model problem we first consider first order transport [2]. Here, we establish a well-posed space-time variational formulation by using ideas from [3, 4].

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MS29 – Recent advances on polyhedral discretizations

(Paola Antonietti, Stefano Berrone, Daniele Di Pietro, Marco Verani)

Tuesday, 13:30 – 15:10, Hotel Fleischers Kvitanosi

Alessandro Russo – *Serendipity Virtual Element Spaces*

Lorenzo Mascotto – *The hp version of the Virtual Element Method.*

Steffen Weißer – *Anisotropic Polygonal and Polyhedral Finite Elements*

Guiseppe Vacca – *Virtual Elements for the Navier-Stokes problem on polygonal meshes*

Wednesday, 15:55 – 17:35, Hotel Fleischers Kvitanosi

Matteo Cicuttin – *Generic programming tools for Hybrid High-Order methods on arbitrary-dimensional, polytopal meshes*

David Mora – *A Virtual Element Discretization for the Vibration Problem of Thin Plates*

Stefano Scialò – *Flow simulations in poro-fractured media with a VEM-BEM coupled approach*

Ilario Mazzieri – *Stability and dispersion analysis of Discontinuous Galerkin methods for wave propagation problems on polytopic meshes*

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Serendipity Virtual Element Spaces

Lourenço Beirão da Veiga[1], **Franco Brezzi**[2], **Donatella Marini**[3], **Alessandro Russo**[4]

[1] *University of Milano-Bicocca, Italy, and IMATI-CNR, Italy* lourenco.beirao@unimib.it
[2] *IMATI-CNR, Italy* brezzi@imati.cnr.it
[3] *University of Pavia, Italy, and IMATI-CNR, Italy* marini@imati.cnr.it
[4] *University of Milano-Bicocca, Italy, and IMATI-CNR, Italy* alessandro.russo@unimib.it

The Virtual Element Method (in short VEM) is a recently introduced extension of the classical Finite Element Method that allows for much more general element geometry such as polygons in 2D and polyhedra in 3D. The VEM has been applied successfully to several types of partial differential equations, including the Navier-Stokes equations, Elasticity and Electromagnetism.

Serendipity VEM is a general technique that allows to significantly reduce the number of *internal* degrees of freedom in 2D, and the number of *internal and face* degrees of freedom in 3D. The name is borrowed from the classical Serendipity variant of the $\mathbb{Q}_k$ isoparametric finite element for quadrilaterals.

In my talk I will first explain the general ideas behind the serendipity approach for VEM, and then I will present some applications.

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The hp version of the Virtual Element Method.

L. Mascotto[1], **L. Beirão da Veiga**[2], **A. Chernov**[3], **A. Russo**[4]

[1] *Department of Mathematics, Universitá degli Studi di Milano, Italy & Institut für Mathematik, C. von Ossietsky Universität Oldenburg, Germany* lorenzo.mascotto@unimi.it
[2] *Department of Mathematics, Universitá degli Studi di Milano, Italy* lourenco.beirao@unimib.it
[3] *Institut für Mathematik, C. von Ossietsky Universität Oldenburg, Germany* alexey.chernov@uni-oldenburg.de
[4] *Department of Mathematics, Universitá degli Studi di Milano, Italy* alessandro.russo@unimib.it

The Virtual Element Method (VEM) is a recent generalization of the Finite Element Method (FEM), whose main feature is the employment of polygonal/polyhedral decompositions of the computational domain. Virtual Element spaces consists of functions that are polynomials, plus other functions, defined as solution of local PDEs and therefore not known explicitely, which in general guarantee the possibility of having globally continuous approximation spaces.

In the present talk, the hp version of VEM for a 2D Poisson problem is introduced; the basic idea of hp methods is that the convergence of the errors is achieved by means of mesh refinement and by increasing the dimension of local spaces.

After recalling the definition of VEM, we discuss about the approximation properties of VEM in presence of corner singularities. As in hp FEM, it is possible to prove exponential convergence of the errors in terms of the number of degrees of freedom; such an exponential convergence is achieved by geometrically refining the mesh towards the singularity and properly increasing the dimension of local spaces.

We also address the problem of the condition number of the stiffness matrix, which is always a delicate issue in p methods, by introducing new sets of degrees of freedom in the definition of the Virtual Element Space.

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Anisotropic Polygonal and Polyhedral Finite Elements

P. Antonietti[1], **M. Verani**[1], **S. Weißer**[2]

[1] *MOX, Dip. di Matematica, Politecnico di Milano, Italy* paola.antonietti@polimi.it
marco.verani@polimi.it

[2] *Department of Mathematics, Saarland University, Germany* weisser@num.uni-sb.de

In recent years the use of polygonal and polyhedral meshes for the discretization of boundary value problems increased. One of the promising features is the flexibility of the element shapes in the discretization. However, in previous publications the elements usually have to fulfil some kind of isotropy, i.e., they are not allowed to be very thin and elongated. But, such anisotropic elements are of particular interest in the resolution of sharp layers in the solutions of boundary value problems. Internal and boundary layers appear, for instance, in convection dominated diffusion problems and cause additional computational costs due to the need of finer isotropic discretizations or stabilization strategies. Thus, the use of anisotropic elements is desirable in efficient and accurate high performance computations in order to reduce the number of unknowns.

In this talk, anisotropic polygonal and polyhedral elements are characterised in the framework of finite element methods. Their approximation properties are studied with the help of quasi-interpolation operators and their use is demonstrated in polygonal and polyhedral discretization strategies like the BEM-based FEM and the virtual element method (VEM). In particular, the focus lies on the derivation of a posteriori error estimates, which can be applied in adaptive finite element simulations later on.

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Virtual Elements for the Navier-Stokes problem on polygonal meshes

L. Beirão da Veiga[1], **C. Lovadina**[2], **G. Vacca**[1]

[1] *Dipartimento di Matematica e Applicazioni, Università degli Studi di Milano Bicocca, Italy*
lourenco.beirao@unimib.it, giuseppe.vacca@unimib.it
[2] *Dipartimento di Matematica, Università degli Studi di Milano, Italy*
carlo.lovadina@unimi.it

In this talk we propose a family of Virtual Element Methods for the 2D Navier-Stokes. The scheme may be considered as a natural evolution of our recent divergence-free approach developed in [1] for the Stokes problem. However, the non-linear convective term in the Navier-Stokes equations leads to the introduction of suitable projectors. These, in turn, suggest to make use of an enhanced discrete velocity space [3], that is an improvement with respect to that of [1]. Instead, the pressure field is approximated by means of standard locally polynomial functions, without any continuity requirement across the elements. The presented scheme displays the following favourable points.

1. The error components partly decouple: notably, the velocity error does not depend directly on the discrete pressures, but only indirectly through the approximation of the loading and convection terms. This is a consequence of the fact that our methods provide a discrete velocity which is point-wise divergence-free .

2. Another advantage of the method is that, again due to its divergence-free nature, the same Virtual space couple can be used directly also for the approximation of the diffusion problem (in mixed form). This allows for a much easier coupling in Stokes-Darcy problems where different models need to be used in different parts of the domain. This observation adds up with the fact that, thanks to the use of polygons that allow hanging nodes, the gluing of different meshes in different parts of the domain is also much easier.

3. As in [1], the particular choice of degrees of freedom adopted for the velocity space yields a diagonal structure in a large part of the pressure-velocity interaction stiffness matrix.

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Generic programming tools for Hybrid High-Order methods on arbitrary-dimensional, polytopal meshes

Matteo Cicuttin[1], **Daniele Di Pietro**[2], **Alexandre Ern**[1]

[1] *Université Paris-Est, CERMICS (ENPC) and INRIA, 77455 Marne-la-Vallée cedex 2, France*
matteo.cicuttin@enpc.fr, alexandre.ern@enpc.fr
[2] *University of Montpellier, IMAG, 34095 Montpellier, France*
daniele.di-pietro@umontpellier.fr

Hybrid High-Order (HHO) methods have been recently introduced in the context of linear elasticity [1] and scalar diffusion [2] PDEs. HHO methods approximate the solution by using piecewise polynomials attached to mesh faces. Cell-based unknowns, which can be eliminated locally by a Schur complement technique, are also used in the formulation. Some major benefits are that the construction is dimension-independent and the possibility to use general meshes with polytopal cells and non-matching interfaces. In this work, we show how this mathematical flexibility can be efficiently replicated in a numerical software using generic programming. We describe a number of generic algorithms and data structures for HHO methods within a "write once, run on any kind of mesh" framework. Numerical experiments are presented to assess the computational efficiency of the implementation. More details can be found in [3].

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A Virtual Element Discretization for the Vibration Problem of Thin Plates*

D. Mora[1,2], **G. Rivera**[2,3], **I. Velásquez**[2,3]

[1] *GIMNAP, Departamento de Matemática, Universidad del Bío-Bío, Casilla 5-C, Concepción, Chile* dmora@ubiobio.cl
[2] *Centro de Investigación en Ingeniería Matemática (CI²MA), Universidad de Concepción, Concepción, Chile* grivera@ing-mat.udec.cl
[3] *Departamento de Ingeniería Matemática, Universidad de Concepción, Concepción, Chile* ivelasquez@ing-mat.udec.cl

In this talk, we develop a virtual element method (VEM) for the vibration problem of thin plates on polygonal meshes. We consider a variational formulation relying only on the transverse displacement of the plate and propose an $H^2(\Omega)$ conforming discretization by means of the VEM which is simple in terms of degrees of freedom and coding aspects. Under standard assumptions on the computational domain, we establish that the resulting scheme provides a correct approximation of the spectrum and prove optimal order error estimates for the eigenfunctions and a double order for the eigenvalues. The analysis restricts to simply connected polygonal clamped plates, not necessarily convex. Finally, we report several numerical experiments illustrating the behaviour of the proposed scheme and confirming our theoretical results on different families of meshes.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
MS29 – Recent advances on polyhedral discretizations

Flow simulations in poro-fractured media with a VEM-BEM coupled approach

Stefano Scialò[1], **Stefano Berrone**[2], **Sandra Pieraccini**[3]

[1] *Politecnico di Torino – Corso Duca degli Abruzzi, 24 – 10129 Torino, ITALY*
stefano.scialo@polito.it
[2] *Politecnico di Torino – Corso Duca degli Abruzzi, 24 – 10129 Torino, ITALY*
stefano.berrone@polito.it
[3] *Politecnico di Torino – Corso Duca degli Abruzzi, 24 – 10129 Torino, ITALY*
sandra.pieraccini@polito.it

Flow simulations in fractured porous media on large domains are particularly challenging for the intrinsic multi-scale nature of the problem and for its geometrical complexity. Fractures, indeed, have one dimension, the thickness, that is orders of magnitude smaller than the other two, thus making its explicit discretization unpractical. Furthermore, in many cases, the fractures immersed in the porous domain form an intricate network of intersections, thus aggravating the discretization process. According to the Discrete Fracture and Matrix (DFM) model, fractures are represented as planar polygons in a porous three dimensional matrix, and act as interfaces for the solution. An averaged 2D Darcy law governs the flow in the fractures, coupled to a 3D flow model in the porous medium with suitable coupling conditions at matrix-fracture interfaces and at fracture-fracture interfaces.

The proposed numerical scheme is targeted to a dramatic simplification of the meshing burden involved in DFM simulations in highly fractured domains, by exploiting the flexibility of the Virtual Element Method (VEM). Let $\mathcal{D}$ denote the porous matrix, which is split in many sub-domains $\mathcal{D}_k$, $k = 1, \dots, n_{\mathcal{D}}$ by the network of fractures F_i, $i = 1, \dots, I$, such that each of the sub-domains does not cross any of the fractures. Then, the boundary of each sub-domain $\mathcal{D}_k$ is denoted by $\partial\mathcal{D}_k$ and is given by the union of planar faces Γ_ℓ, $\ell \in \mathcal{L}_k$, such that $\partial\mathcal{D}_k = \bigcup_{\ell\in\mathcal{L}_k} \Gamma_\ell$. Each face Γ_ℓ , $\ell \in \mathcal{L} := \bigcup_{k=1}^{n_{\mathcal{D}}} \mathcal{L}_k$ is either part of the boundary of $\mathcal{D}$, either belongs to a fracture plane. Conversely, each fracture F_i, $i = 1, \dots, I$ can be seen as the union of faces Γ_ℓ belonging to the boundary of different matrix blocks $\mathcal{D}_k$, i.e. $F_i = \bigcup_{\ell\in\mathcal{L}_{F_i}} \Gamma_\ell$. For each $i = 1, \dots, I$, the set of polygonal faces Γ_ℓ, $\ell \in \mathcal{L}_{F_i}$ constitutes a mesh suitable for the VEM on fracture F_i, and, in particular, it represents the coarsest possible conforming mesh for the DFM problem. The Boundary Element Method (BEM) is then used to solve problems in the matrix-blocks $\mathcal{D}_k$, $k = 1, \dots, n_{\mathcal{D}}$ coupled to the problems on the fractures on the VEM mesh.

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MS29 – Recent advances on polyhedral discretizations

Stability and dispersion analysis of Discontinuous Galerkin methods for wave propagation problems on polytopic meshes

P. Antonietti[1], **I. Mazzieri**[2]

[1] *MOX-Laboratory for Modeling and Scientific Computing, Department of Mathematics, Politecnico di Milano, P.za Leonardo da Vinci 32, 20133 Milano, Italy* paola.antonietti@polimi.it
[2] *MOX-Laboratory for Modeling and Scientific Computing, Department of Mathematics, Politecnico di Milano, P.za Leonardo da Vinci 32, 20133 Milano, Italy* ilario.mazzieri@polimi.it

In the field of computational seismology the use of accurate and efficient numerical methods is essential for the study of wave propagation phenomena in complex and heterogeneous media.
The main important tools that determine the applicability of a numerical method to the wave propagation problems are the stability and grid dispersion criteria. In this context, the stability criterion determines the largest time step for the explicit time integration scheme such that the numerical solution remains bounded. On the other hand, the grid dispersion criterion determines the smallest number of nodes per wavelength for the spatial discretization such that the numerical solution has a desired accuracy.
In this work we present a two dimensional stability and dispersion analysis for the fully discrete approximation of the elastodynamics equation based on the plane wave method. For space discretization we compare Discontinuous Galerkin methods based on different polytopic grids, while the fully discrete approximation is achieved by employing a leap-frog time integration scheme. Numerical results for DG methods on polytopic grids are compared with those of the classical Spectral Element (SE) method on grids made by standard shaped elements. Finally, we apply the proposed method on benchmark as well as relevant test cases.

CT01 – Finite element techniques

Monday, 15:50 – 17:55, Hotel Fleischers Kvitanosi

Patrick Henning – *Finite Element Approximations of Non- linear Schrödinger Equations*

Robert Schorr – *A non-symmetric finite element and boundary element coupling method for a parabolic-elliptic interface problem*

Piotr Swierczynski – *Higher order energy- correction method for parabolic problems*

Steffen Münzenmaier – *Locally Scaled Least Squares Finite Element Methods for the Transport Equation*

Andreas Hahn – *Stabilized FEM for a Coupled Bulk-Surface Transport Problem*

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT01 – **Finite element techniques**

Finite Element Approximations of Nonlinear Schrödinger Equations

Patrick Henning[1], **Daniel Peterseim**[2]

[1] *Division of Numerical Analysis, KTH Royal Institute of Technology, Stockholm, Sweden*
pathe@kth.se

[2] *Institut für Mathematik, Universität Augsburg, Germany*
daniel.peterseim@math.uni-augsburg.de

In this talk, we discuss numerical and analytical aspects of the finite element method applied to time-dependent nonlinear Schrödinger equations. The usage of finite elements becomes necessary if the equation contains terms that dramatically reduce the overall regularity of the exact solution. Examples of such terms are rough potentials or disorder potentials as appearing in many physical applications. Using finite elements for the space discretization allows for a flexible choice of the time discretization. We will discuss combinations of space and time discretizations including their regularity requirements, what we know about convergence rates and possible coupling conditions between the spatial mesh size and the time step size. At the end we show some numerical experiments.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT01 – **Finite element techniques**

A non-symmetric finite element and boundary element coupling method for a parabolic-elliptic interface problem

Herbert Egger[1], **Christoph Erath**[2], **Robert Schorr**[3]

[1] *TU Darmstadt, Department of Mathematics, Dolivostraße 15, 64293 Darmstadt, Germany*
egger@mathematik.tu-darmstadt.de
[2] *TU Darmstadt, Department of Mathematics, Dolivostraße 15, 64293 Darmstadt, Germany*
erath@mathematik.tu-darmstadt.de
[3] *TU Darmstadt, Graduate School of Computational Engineering, Dolivostraße 15, 64293 Darmstadt, Germany*
schorr@gsc.tu-darmstadt.de

We consider the coupling of a parabolic initial boundary value problem in a bounded interior domain and the Laplace equation on the unbounded exterior domain. For the discretization of this interface problem we consider a classical method of lines approach; the non-symmetric coupling of finite element and boundary element methods in space and a Runge Kutta scheme for time discretization. The non-symmetric discrete systems in space that have to be solved in every time step lead to new challenges in the analysis of this fully discrete system. The convergence rate of the fully discrete system will be investigated in the energy norm of the parabolic system, which allows us to proof the optimal convergence rate of order one for piecewise linear finite elements and piecewise constant boundary elements and the implicit Euler method in time. We conclude with some numerical examples illustrating the theoretical results.

Acknowledgements

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT01 – **Finite element techniques**

Higher order energy-correction method for parabolic problems

Piotr Swierczynski[1], **Barbara Wohlmuth**[2]

[1] *Institute of Numerical Mathematics, Technische Universität München, Germany*
piotr.swierczynski@ma.tum.de
[2] *Institute of Numerical Mathematics, Technische Universität München, Germany*
wohlmuth@ma.tum.de

The presence of re-entrant corners, i.e. corners with angles $\Theta > \pi$, in polygonal domains leads to the loss of regularity of solutions of elliptic problems [1]. This, in turn, means that only a suboptimal order of convergence of their standard piecewise polynomial finite element approximation can be obtained. Recently, an effective method of recovering the full second-order convergence for piecewise linear approximations of elliptic equations on domains with re-entrant corners, when measured in locally modified L_2 and H^1 norms, known as energy-correction, has been proposed [2]. This method is based on a modification of a fixed number of entries in the system's stiffness matrix. The method was further extended to a more general case of higher order polynomial finite element space [3].
Standard discretization approaches such as mesh grading or adaptivity, result in a very restrictive form of a CFL condition. This, in turn, makes the use of explicit time stepping practically impossible. In this talk, we show how the energy-correction method can be applied to regain optimal convergence in weighted norms for parabolic problems and introduce a post-processing strategy yielding optimal convergence order in standard Sobolev norms. Furthermore, the energy-correction can be used on uniform meshes, allowing for application of explicit time stepping schemes with relatively large time steps. In order to use a mass-lumping strategy for higher order finite element discretization, we enrich standard piecewise polynomial spaces with bubble functions and use suitably modified Gauss–Lobatto quadrature rules [4] in the system matrix assembly. This leads to a very efficient discretization of parabolic problems on nonconvex polygonal domains, in which higher order finite element is combined with explicit time stepping. Due to the application of mass-lumping, at each time step, only one vector multiplication with a scaled stiffness matrix needs to be performed.
We confirm all theoretical results with numerical tests and compare the accuracy and computational cost of the proposed method with other existing schemes.

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CT01 – **Finite element techniques**

Locally Scaled Least Squares Finite Element Methods for the Transport Equation

Steffen Münzenmaier[1], **Tom Manteuffel**[2], **Ben Southworth**[3]

[1] *Fakultät für Mathematik, Universität Duisburg-Essen, Germany*
steffen.muenzenmaier@uni-due.de
[2] *Department of Applied Mathematics, University of Colorado at Boulder, United States of America*
tmanteuf@colorado.edu
[3] *Department of Applied Mathematics, University of Colorado at Boulder, United States of America*
ben.southworth@colorado.edu

This talk examines the first-order system least squares method for the transport (or reaction-advection) equation. A general Boltzmann transport equation, which describes the transport of neutral particles through a material media, can be efficiently solved by the the Discrete Ordinates Method (DOM) and Diffusion Synthetic Acceleration (DSA). The dominant computational expense in such a method is performing "transport sweeps", which consist of solving the transport equation for many different angles. These transport sweeps can be solved for example by (lumped) corner balance, SUPG or (upwinded) discontinuous Galerkin methods. Another approach undertaken in the transport community is the so called self-adjoint form, which corresponds to a least-squares finite element method and will be examined in this talk.

The focus of this talk is on problems where the total cross-sections may differ by several orders of magnitude across the spatial domain. When using least squares finite element methods, a naive approach can lead to unphysical behavior, such as unphysical damping, flux-dips, and cross-stream diffusion, requiring excessively fine grids to get a reasonable solution. The first part of this talk examines how these problems can be overcome by applying a proper local scaling to the problem. This can greatly increase the accuracy of the discrete solution without introducing any significant additional computational cost. In the second part of the talk, an efficient AMG-solver for the resulting linear equation systems is presented. The dependence on the scalings introduced earlier with respect to accuracy per cost is closely examined.

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CT01 – **Finite element techniques**

Stabilized FEM for a Coupled Bulk-Surface Transport Problem

Andreas Hahn[1], **Kristin Simon**[2], **Lutz Tobiska**[3]

[1] *Otto-von-Guericke University, Germany* Andreas.Hahn@ovgu.de
[2] *Otto-von-Guericke University, Germany* Kristin.Simon@ovgu.de
[3] *Otto-von-Guericke University, Germany* Lutz.Tobiska@ovgu.de

The presence of surface active agents (surfactants) has a vast influence on the dynamics of flows with interfaces, like drops, bubbles and mixtures of fluids. Such interface flows are an active research area with numerous applications in chemistry, biologie engineering and many more. An inhomogeneous distribution of surfactants results in Marangoni forces which may lead to a destabilization of the interface with essential consequences on the flow structure. This is a complex process whose tailored use in applications requires an understanding of this mutual interplay.

A finite element method based on the Arbitrary Lagrangian Eulerian (ALE) formulation for two-phase flows and transport problems with moving and fixed interfaces is proposed. The full model consist of the Navier-Stokes equations coupled to transport equations in the bulk and on the interface.

We consider the numerical analysis of a finite element method for the sub-problem consisting of the coupled transport of the surfactant. Since standard numerical methods for transport problems suffer from numerical instabilities in the convection dominated case, the Local Projection Stabilization (LPS) methdod is considered for the model:

$$
\begin{aligned}
-\nu_i \Delta u_i + \mathbf{w} \cdot \nabla u_i &= f_i && \text{in } \Omega_i,\ i = 1, 2\ , \\
-\nu_\Gamma \Delta_\Gamma u_\Gamma + \mathbf{w} \cdot \nabla_\Gamma u_\Gamma &= L \sum_{i=1}^{2} S_i(u_i, u_\Gamma) + f_\Gamma && \text{on } \Gamma\ , \\
\nu_2 \frac{\partial u_2}{\partial \mathbf{n}} &= 0 && \text{on } \partial\Omega\ ,
\end{aligned}
$$

where Ω_1 is the *inner* bulk domain and Ω_2 the *outer* bulk domain and $\Gamma = \overline{\Omega}_1 \cap \overline{\Omega}_2$ ist the interface, $u_i : \Omega_i \to \mathbb{R}$ denote the surfactant concentration in the bulk phases Ω_i, $i = 1, 2$, $u_\Gamma : \Gamma \to \mathbb{R}$ is the surfactant concentration on the interface Γ, $\mathbf{w}$ is the velocity field, the positive numbers ν_1, ν_2, ν_Γ are the inverse of the Peclet numbers and L is a scaling factor, $\mathbf{n}$ is the normal to Γ, and $S_i(u_i, u_\Gamma)$ are the source terms modelling the ad- and desorption of surfactant.

CT02 – Finite volume techqniques for hyperbolic models

Tuesday, 17:30 – 19:10, Kulturhus

René Beltman – *Conservative cut-cell discretization for viscous incompressible flow*

Oliver Kolb – *On a third order WENO boundary treatment for networks of hyperbolic conservation laws*

Jan ten Thije Boonkkamp – *Nonlinear Local Boundary Value Problems for the Approximation of Fluxes in the Viscous Burgers Equations*

Emmanuel Franck – *High order implicit relaxation schemes for nonlinear hyperbolic systems*

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT02 – **Finite volume techqniques for hyperbolic models**

Conservative cut-cell discretization for viscous incompressible flow

R. Beltman*, **M.J.H. Anthonissen***, **B. Koren***

* *Eindhoven University of Technology* r.beltman@tue.nl

We consider viscous incompressible flow around an object. This is most accurately modelled by using an object-fitted mesh. However, if multiple asynchronously moving objects are present in the flow the use of object-fitted meshes becomes very expensive because every object needs its own mesh and every time-step requires interpolation between the different meshes.

These excessive computational costs can be circumvented by using only one stationary Cartesian mesh through which the objects move. To accurately take into account the no-slip condition on the boundaries of the objects, the discretization needs to be adjusted in mesh-cells that are intersected by the boundaries of the objects.

In this paper we introduce an extension of the MAC-staggered mesh method [1] to cut-cell meshes. The staggered mesh method is efficient and conserves mass, momentum and energy (in the absence of viscosity), and as such is very suitable for modelling turbulent flows. The staggered positioning of the velocity variables in the mesh makes it hard to extend the method to cut-cells with complicated shapes. We present a new staggered mesh method for cut-cell meshes that gives accurate approximations of the physical fluxes of mass, momentum and energy over the cut-cell boundary. Furthermore, we study the extension of this method to objects moving with respect to the mesh.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT02 – **Finite volume techqniques for hyperbolic models**

On a third order WENO boundary treatment for networks of hyperbolic conservation laws

Oliver Kolb[1], **Alexander Naumann**[1], **Matteo Semplice**[2]

[1] *University of Mannheim, Department of Mathematics, 68131 Mannheim, Germany*
kolb@uni-mannheim.de, anaumann@mail.uni-mannheim.de
[2] *Università di Torino, Dipartmento di Matematica, 20123 Torino, Italy*
matteo.semplice@unito.it

High order numerical methods for networks of hyperbolic conservation laws have recently gained increasing popularity. Here, the crucial part is to treat the boundaries of the single (one-dimensional) computational domains in such a way that the desired convergence rate is achieved in the smooth case but also stability criterions are fulfilled, in particular in the presence of discontinuities. Most of the recently proposed methods rely on a WENO extrapolation technique introduced by Tan and Shu in [*J. Comput. Phys.* 229, pp. 8144–8166 (2010)]. Within the presented work, we refine and in a sense generalize these results for the case of a third order scheme. Numerical evidence for the analytically found parameter bounds is given as well as results for a complete third order scheme based on the proposed boundary treatment.

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CT02 – **Finite volume techqniques for hyperbolic models**

Nonlinear Local Boundary Value Problems for the Approximation of Fluxes in the Viscous Burgers Equations

N. Kumar[1], **J.H.M. ten Thije Boonkkamp**[1], **B. Koren**[1], **A. Linke**[2]

[1] *Eindhoven University of Technology, The Netherlands.* j.h.m.tenthijeboonkkamp@tue.nl
[2] *Weierstrass Institute of Applied Analysis and Stochastics, Germany.*

We present a scheme for computing the numerical fluxes in the semi-discrete viscous Burgers equation. The numerical flux is approximated using a local boundary value problem (BVP), which in this case is the steady Burgers equation. The scheme is inspired by the complete-flux scheme for convection-diffusion-reaction equations, as presented in [1], where the authors use a linear local BVP to derive an integral representation of the flux. Extending the integral representation, to nonlinear local BVP can be cumbersome due to the nonlinearity of the flux function and the local BVP being a singularly perturbed problem.

In the present scheme, the flux is computed from a nonlinear local BVP, which has a monotonic solution and exhibits a boundary layer character for small values of $\epsilon = \nu/\Delta x$, with ν the diffusion coefficient and Δx the grid resolution. Thus, depending on the boundary conditions u_L (left boundary) and u_R (right boundary) the solution of the local BVP is either strictly decreasing ($u_L > u_R$) or increasing ($u_L < u_R$). Further, if $u_L > u_R$, then the numerical flux is always non-negative and in the limit $\epsilon \to 0$, reduces to *Godunov's* flux for the inviscid Burgers equation. For $u_L < u_R$, the flux can be either positive or negative, a classification for identifying the sign of the flux and computing the numerical approximation is presented. Preliminary numerical tests show that the present scheme is more accurate than the linearized local BVP approach presented in [2].

Moreover, the scheme can be combined with WENO construction to have a higher-order approximation of the numerical flux.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT02 – **Finite volume techqniques for hyperbolic models**

High order implicit relaxation schemes for nonlinear hyperbolic systems

E. Franck[1], **D. Coulette**[2], **P. Helluy**[3]

[1] *Inria Grand-Est and IRMA Strasbourg, France* emmanuel.franck@inria.fr
[2] *IRMA Strasbourg, France* coulette@unistra.fr
[3] *Inria Grand-Est and IRMA Strasbourg, France* philippe.helluy@unistra.fr

In this work we consider the time discretization of compressible fluid models which appear in gas dynamics, biology, astrophysics or plasma physics for Tokamaks. In general for the hyperbolic system we use an explicit scheme in time. However, for some applications, the characteristic velocity of the fluid is very small compared to the fastest velocity speed. In this case, to filter the fast scales it is common to use an implicit scheme. The implicit schemes allows to filter the fast scale that we don't want to consider and choose a time step independent of the mesh step and adapted to the characteristic velocity of the fluid. Some typical examples of problems are the low-mach Euler equations or the MHD equations for Tokamaks. The matrices induced by the discretization of the hyperbolic system are ill-conditioned in the regime considered. To treat this problem some preconditioning has been designed (for example [4]). In this work we propose an alternative method based on the relaxation schemes [3]-[2]. This method, coupling with a splitting scheme in time allows to approximate the full nonlinear problem by a set of simpler, linear and independent problems (acoustic equations or transport equations according to the formulation proposed in [2] and [3]) and a local relaxation step. This method can approximate any hyperbolic models and can be generalized to treat models including additional small diffusion terms. Each step of the splitting (relaxation and hyperbolic step) is discretized using a second order implicit scheme and coupling this with a specific splitting we obtain a second order scheme. The high order extension in time is also possible [1]. Performing the resolution solver for the simple hyperbolic systems (Schur complement method coupled with finite element method for the acoustic equation or a matrix-free implicit upwind scheme for the transport equation) and using task-based parallelization we obtain an efficient, robust, scalable and high-order implicit method for nonlinear hyperbolic systems. The kinetic relaxation method and the classical one have been tested on standard fluid equations : compressible Navier-Stokes, isothermal Euler and Burgers equations.

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CT03 – High performance computing and Eigenvalue problems

Tuesday, 17:30 – 19:10, Hotel Fleischers Osa

Emanuel Rubensson – *The Chunks and Tasks model and locality-aware parallel sparse matrix- matrix multiplication*

Pavel Kůs – *GPU Optimisation of Large-Scale Eigenvalue Solver*

Önder Türk – *Chebyshev spectral collocation method approximations of the Stokes eigenvalue problem based on penalty techniques*

Parikshit Upadhyaya – *On the convergence factor of the self-consistent field iteration*

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CT03 – **High performance computing and Eigenvalue problems**

The Chunks and Tasks model and locality-aware parallel sparse matrix-matrix multiplication

Emanuel H. Rubensson[1], **Elias Rudberg**[1]

[1] *Div. of Scientific Computing, Dept. of Information Technology, Uppsala University, Sweden*
emanuel.rubensson@it.uu.se
elias.rudberg@it.uu.se

The Chunks and Tasks model supports implementation of locality-aware communication avoiding algorithms [1]. An example where such algorithms are desirable is sparse matrix-matrix multiplication. When the nonzero patterns of the input matrices are a priori unknown it is, using standard programming models, very difficult to achieve load balance while taking advantage of locality, e.g. clustering of matrix elements in some parts of the matrix. In fact, a common approach is to randomly permute rows and columns of the input matrices to *decrease* data locality and obtain about the same density of nonzero elements everywhere in the matrix, see e.g. [2]. Then, a static distribution of work and data is used in the same way as for dense matrices but with the local block-block multiplies replaced by sparse products. The obvious drawback is that the possibility to exploit the nonzero structure to reduce communication and/or make efficient use of the memory hierarchy is spoiled.

In our implementation of sparse matrix-matrix multiplication using Chunks and Tasks, matrices are instead represented by sparse quaternary trees (quadtrees) of chunks [3]. Matrices are recursively split into four quadrants resulting in a sparse quadtree of chunks. The quadtree representation efficiently exposes parallelism in the matrix-matrix multiplication without destroying data locality. Quadtree representation of sparse matrices is certainly not new [4] and would appear to be a natural way to implement parallel sparse matrix-matrix multiplication. The problem has only been that implementation of this type of dynamic hierarchical algorithms with standard tools such as MPI is an overwhelming task.

We show that our quadtree implementation using Chunks and Tasks takes advantage of data locality resulting in a dramatic reduction of communication and a wall time that is instead dominated by the execution of tasks along the critical path.

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CT03 – **High performance computing and Eigenvalue problems**

GPU Optimisation of Large-Scale Eigenvalue Solver

Pavel Kůs[1], **Hermann Lederer**[2], **Andreas Marek**[3]

[1] *Max Planck Computing and Data Facility, Garching bei München, Germany*
pavel.kus@mpcdf.mpg.de
[2] *Max Planck Computing and Data Facility, Garching bei München, Germany*
hermann.lederer@rzg.mpg.de
[3] *Max Planck Computing and Data Facility, Garching bei München, Germany*
andreas.marek@rzg.mpg.de

Solving large eigenvalue systems is, apart from being a classical problem of linear algebra with broad range of applications, a substantial part of many important problems in material science, computational chemistry, and namely the electronic structure theory, where a key task is the solution of Schrödinger-like eigenproblems [1]. Since the solution of eigenproblem scales as $O(n^3)$, where n is the size of the matrix, it can easily dominate the whole compute-time for large-scale calculations. The ELPA library [2] is a well established eigensolver library used by many computational chemistry codes. It provides efficient implementation in distributed memory with good scaling properties for many thousands of CPU cores as well as optimizations targeting various particular architectures. It also contains specific algorithm advantageous for problems, where only certain part of eigenvalues and eigenvectors are sought.

Since accelerated HPC systems with a high peak performance are expected to play an essential role in the future, their efficient usage will be very important. For this reason, substantial efforts are taken to adapt HPC applications to GPU computing. In this contribution we describe our ongoing effort of improving the performance of the ELPA library on supercomputers with GPU-equipped nodes. We show multiple ways how GPU support can be employed into an already highly optimized parallel MPI-based code and discuss their advantages and drawbacks. We comment on both algorithmic and technical aspects of the problem and show performance comparisons.

Acknowledgement
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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT03 – **High performance computing and Eigenvalue problems**

Chebyshev spectral collocation method approximations of the Stokes eigenvalue problem based on penalty techniques

Önder Türk[1], **Ramon Codina**[2]

[1] *Gebze Technical University, Gebze/Kocaeli, Turkey* onder.turk@yandex.com
[2] *Universitat Politècnica de Catalunya, Barcelona, Spain* ramon.codina@upc.edu

This study aims to investigate numerical solution strategies for the Stokes eigenvalue problem based on the use of penalty formulations. The penalty method is a widely used approach in incompressible Stokes and Navier-Stokes models for relaxing the solenoidal condition. It has some advantages, such as the possibility of condensing discontinuous pressures and write the problem in terms of the velocity only (see, e.g., [1, 4]). The present work extends the application of penalization techniques to the Stokes eigenvalue problem. In general, when the task is to approximate the eigenmodes of the Stokes problem formulated in primitive variables, velocity and pressure, major difficulties arise not only due to the fact that the discretization of the operator leads to a generalized eigenvalue problem, but also due to the existence of zero diagonal entries in the resulting algebraic system. It is shown that the penalty method approach can successfully be adapted for the eigenproblem to rectify associated problems. Two different schemes, namely, the standard penalization with a small penalty parameter, and the iterative penalization that enables relatively large parameters, are implemented. The employment of the latter leads to a so-called inhomogenous generalized eigenvalue problem which requires a special attention. A feasible solution strategy is presented which is adapted from a procedure based on Newton's method proposed for the corresponding standard (inhomogenous) eigenvalue problems in [3]. Concerning the spatial discretization, among other possible options, the Chebyshev spectral collocation method based on expanding the unknown fields in tensor product of Chebyshev polynomials is employed. It is shown that the method constitutes an efficient way of numerically examining the eigensolutions of the Stokes operator with the use of Chebyshev collocation approximation directly (without a decoupling of velocity and pressure, see [2] for details), for the first time to the authors' knowledge.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT03 – **High performance computing and Eigenvalue problems**

On the convergence factor of the self-consistent field iteration

Parikshit Upadhyaya[1], **Elias Jarlebring**[2]

[1] *KTH Stockholm, Sweden* pup@kth.se
[2] *KTH Stockholm, Sweden* eliasj@kth.se

The self-consistent field (SCF) iteration is an iterative algorithm used to solve a class of non-linear eigenvalue problems of the form $H(X)X = X\Lambda, X^TX = I$, where $H : \mathbb{R}^{n\times k} \to \mathbb{R}^{n\times n}, X \in \mathbb{R}^{n\times k}$ and $\Lambda \in \mathbb{R}^{k\times k}$ is a diagonal matrix. These problems arise frequently in the context of quantum chemistry and electronic structure calculations as the discretized Kohn-Sham and Hartree-Fock equations, where we are interested in computing the k smallest eigenvalues. Sufficient conditions for convergence of SCF exist in the current literature, e.g. in, [1], [2] and [3]. In contrast to these results, we provide a convergence theory based on the analysis of SCF as a fixed point iteration with the density matrix XX^T as the state of the algorithm. This allows us to provide necessary and sufficient conditions for local convergence, and an exact formula for the convergence factor. We make several interpretations of the convergence factor formula, e.g., in terms of $|\lambda_k - \lambda_{k+1}|$, also known as the HOMO-LUMO gap. The exact characterization of the Jacobian of the fixed-point iteration to allows us to improve convergence, and low-rank approximations appear to give us competitive improvements of this approach. Our numerical experiments with various problem sizes and different values of k confirm our theoretical predictions for the convergence factor and the acceleration.

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CT04 – Porous media

Tuesday, 17:30 – 19:10, Hotel Fleischers Sivle

Juan Michael Sargado – *A new family of degradation functions for phase-field modeling of brittle fracture and flow in poroelastic materials*

Jakub Solovský – *Investigating vapor intrusion using mathematical model of two-phase compositional flow in porous media*

Ingeborg G. Gjerde – *Mixed methods for hierarchical flow models for non-isothermal wells in porous media*

Menel Rahrah – *Monotonicity analysis and uncertainty quantification in Biot's poro-elasticity model using finite element methods*

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT04 – **Porous media**

A new family of degradation functions for phase-field modeling of brittle fracture and flow in poroelastic materials

Juan Michael Sargado[1], **Eirik Keilegavlen**[2], **Inga Berre**[3,4], **Jan Martin Nordbotten**[5,6]

[1] *Department of Mathematics, University of Bergen, Norway* juan.sargado@uib.no
[2] *Department of Mathematics, University of Bergen, Norway* eirik.keilegavlen@uib.no
[3] *Department of Mathematics, University of Bergen, Norway* inga.berre@uib.no
[4] *Christian Michelsen Research*
[5] *Department of Mathematics, University of Bergen, Norway* jan.nordbotten@uib.no
[6] *Department of Civil and Environmental Engineering, Princeton University, NJ, USA*

In phase-field simulations of fluid-driven fracture in porous media, an important consideration deals with how to properly model fluid flow in the fractures since these are represented as diffuse entities by the phase-field. In particular the flow model must account for the artificial loss of stiffness in material points adjacent to the crack, as a consequence the energy degradation function utilized as part of the phase-field approach. In this work, we make use of a new parametric family of degradation functions having an exponential character. These were originally developed with the aim of achieving high accuracy in the reproduction of critical loads for problems involving solid mechanics, as well as independence of results with respect to the length scale of crack regularization. We study the effect of using different shapes of the degradation function (obtained by altering parameter values) on the simulated deformation response of the poroelastic material, along with the potential of using such knowledge to develop a straightforward definition of effective flow apertures.

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT04 – **Porous media**

Investigating vapor intrusion using mathematical model of two-phase compositional flow in porous media

Jakub Solovský[1], **Radek Fučík**[2], **Tissa H. Illangasekare**[2]

[1] *Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Brehova 7, 115 19 Praha 1, Czech Republic* jakub.solovsky@fjfi.cvut.cz
[2] *Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Brehova 7, 115 19 Praha 1, Czech Republic* radek.fucik@fjfi.cvut.cz
[3] *Colorado School of Mines, Center for the Experimental Study of Subsurface Environmental Processes, 1500 Illinois St., Colorado School of Mines, Golden CO, United States* tissa@mines.edu

This work deals with two phase compositional flow in porous media with kinetic mass transfer. We propose a numerical method based on the mixed hybrid finite element method with several linear solvers (direct and iterative) and parallel implementation using MPI. First, the method is verified on problems with known solutions. Numerical experiments show that the errors are similar for all variations of the method and the experimentally estimated order of convergence is slightly less than one. However, there are significant differences in the computational performance. Then, we use the numerical scheme to investigate non-equilibrium mass transfer in unsaturated porous media using experimental laboratory data and hypothetical field-scale scenarios of vapor intrusion problems. The experiment was focused on evaporation of dissolved TCE in laboratory scale. In the field scale, we examine effects of water table drop or rainfall events on the dynamics of the vapor intrusion into building basements.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT04 – **Porous media**

Mixed methods for hierarchical flow models for non-isothermal wells in porous media

Ingeborg G. Gjerde[1], **Kundan Kumar**[2], **Jan M. Nordbotten**[3]

[1] *University of Bergen, Norway* ingeborg.gjerde@uib.no
[2] *University of Bergen, Norway* kundan.kumar@uib.no
[3] *University of Bergen, Norway* jan.nordbotten@uib.no

Due to the large difference in the spatial scales of a well and the surrounding aquifer, wells are commonly modelled using a lower-dimensional source term. If the dimensional gap is larger than one the solution will not lie in H1, leading to suboptimal convergence rates for finite element solutions. In this work we propose a mixed formulation for the problem in a non-isothermal setting, resulting in a system of coupled elliptic and parabolic equations. We perform numerical analysis of the problem and simulate the scenario of heated water being injected into an aquifer.

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT04 – **Porous media**

Monotonicity analysis and uncertainty quantification in Biot's poro-elasticity model using finite element methods

Menel Rahrah[1], **Fred J. Vermolen**[2]

[1] *Delft Institute of Applied Mathematics, The Netherlands* M.Rahrah@tudelft.nl
[2] *Delft Institute of Applied Mathematics, The Netherlands* F.J.Vermolen@tudelft.nl

Infiltration of large amounts of fresh water into the shallow subsurface would have great value for battling flooding, underground storage of water and reducing the footprint of construction works. A new method to infiltrate high volumes of fresh water has been discovered recently. We refer to this method as Fast, High Volume Infiltration (FHVI). To describe this infiltration method, we consider a model for aquifers in which water is injected. The flow of water induces local deformations of the aquifer, which are described by Biot's poro-elastic formalism. Our aim is to investigate whether large injection rates induce an oscillatory or a pulsating force near the injection point and whether induced displacements and deformations increase the amount of water that can be injected into the aquifer. For this purpose, a finite-element method based on Taylor-Hood elements has been developed to solve the poro-elastic equations. The study contains simulations with oscillatory force boundary conditions as well as pressure pulses. The results are studied for various oscillatory modes over time as well as over the length of the boundary. To quantify the impact of variation of model parameters such as the Young's modulus, the oscillatory modes and the injection pressure pulses, we carry out a probabilistic approach. Since the resulting saddle point problem needs a considerate numerical methodology in terms of possible spurious oscillations, we will also present conditions for a stabilised finite-element method. Furthermore, the numerical schemes used for solving the model of Biot and the heat equation are analysed for monotonicity, positivity and stability.

CT05 – Adaptivity and applications

Tuesday, 17:30 – 18:45, Hotel Fleischers Kvitanosi

Giulio Paolucci – *Adaptive filters for first order Hamilton–Jacobi equations*

Acim Schroll – *An adaptive viscosity scheme for multi–physics PDEs*

Hakan Tarman – *A Spectral Solenoidal-Galerkin Method for Flow Past a Circular Cylinder*

Hynek Řezníček – *Two methods for the numerical modelling of the PM transport and deposition on the vegetation*

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT05 – **Adaptivity and applications**

Adaptive filters for first order Hamilton–Jacobi equations

G. Paolucci[1], **S. Tozza**[2], **M. Falcone**[3]

[1] *Dip. di Matematica - Sapienza Università di Roma, Italy* paolucci@mat.uniroma1.it
[2] *Dip. di Matematica - Sapienza Università di Roma, Italy* tozza@mat.uniroma1.it
[3] *Dip. di Matematica - Sapienza Università di Roma, Italy* falcone@mat.uniroma1.it

The accurate numerical solution of Hamilton-Jacobi equations is a challenging topic of growing importance in many fields of application, e.g. control theory, KAM theory, image processing and material science. Due to the lack of regularity of viscosity solutions, this issue is delicate and the construction of high-order methods can be rather difficult. In recent years a general approach to the construction of high-order methods has been proposed in [3] and further developed in [4].

We consider a class of "filtered" schemes for some first order time dependent Hamilton-Jacobi equations. A typical feature of a filtered schemes S^F is that at the node x_j it is a mixture of a high-order scheme S^A and a monotone scheme S^M according to a filter function F, it can be written as

$$u_j^{n+1} \equiv S^F(u^n)_j := S^M(u^n)_j + \varepsilon \Delta t F\left(\frac{S^A(u^n)_j - S^M(u^n)_j}{\epsilon \Delta t}\right), \quad j \in \mathbb{Z} \tag{19}$$

where $\varepsilon = \varepsilon_{\Delta t, \Delta x} > 0$ is a parameter going to 0 as $(\Delta t, \Delta x)$ is going to 0 and does not depend on n. Filtered schemes are high-order accurate where the solution is smooth, monotone otherwise, and this feature is crucial to prove a convergence result for viscosity solutions as in [1].
Here we improve the scheme (19) introducing an adaptive and automatic choice of the parameter $\varepsilon = \varepsilon^n$ at every iteration. To this end, we use a smoothness indicator in order to select the regions where we can compute the regularity threshold ε^n. Our smoothness indicator is based on the ideas in [2], but other indicators with similar properties can be used. A convergence result and error estimates for the new scheme are given, their proofs are based on the properties of the scheme and of those indicators.

A number of numerical tests confirm that the adaptive filtered scheme works very well and that it can improve the scheme in [1] as well as the WENO schemes in [2].

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT05 – **Adaptivity and applications**

An adaptive viscosity scheme for multi–physics PDEs

E. Adugna[1], **C. V. Hansen**[2], **H. J. Schroll**[3]

[1] *Hawassa University, P.O. Box 5, Hawassa, Ethiopia*
[2,3] *University of Southern Denmark, Campusvej 55, DK-5230 Odense M, Denmark*
[1] *School of Mathematical and Statistical Sciences* adugna@imada.sdu.dk
[2] *Department of Mathematics and Computer Science* cvh@imada.sdu.dk
[3] *Department of Mathematics and Computer Science* achim@imada.sdu.dk

An adaptive viscosity local Lax–Friedrichs scheme is designed for reactive conservation laws with possible degenerate diffusion

$$u_t + f(u)_x = (d(x)u_x)_x + g(u) \ , \quad d(x) \geq 0 \ .$$

The scheme is well suited as "basic–scheme" in high resolution methods. As a central scheme with artificial viscosity it easily applies to systems with degenerate diffusion, for example the compressible Navier–Stokes equations.

Crandall and Majda [1] introduced monotone schemes for hyperbolic conservation laws. Osher [2] developed E–schemes. It is clear that monotone and consistent schemes in conservation form have the E–property. We prove that consistent E–schemes are quasi–monotone and the CFL–condition ensures monotonicity. Thus, the local Lax–Friedrichs scheme as E–scheme is also monotone. In agreement with Tadmor [3], a sufficient condition for the E–property is "enough diffusion". We quantify this statement and design a stable adaptive viscosity method that uses the possibly degenerate, natural viscosity to further reduce numerical diffusion. Stability of the new scheme is proven even in the presence of a nonlinear source term. Using the theory of inverse–monotone matrices, we show stability in L^1 for explicit / implicit ϑ–time stepping. Finally the performance of the adaptive scheme is demonstrated.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT05 – **Adaptivity and applications**

A Spectral Solenoidal-Galerkin Method for Flow Past a Circular Cylinder

Hakan I. Tarman[1]

[1] *Mechanical Engineering Department, Middle East Technical University, Ankara, Turkey*
tarman@metu.edu.tr

Flow past a circular cylinder embodies many interesting features of fluid dynamics as a challenging fluid phenomena. The flow in polar coordinates is governed by N-S equations:

$$\nabla \cdot \mathbf{v} = 0, \quad \partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{u}_0 - \tfrac{1}{\mathrm{Re}} \nabla^2 \mathbf{v} = -\nabla p + \tfrac{1}{\mathrm{Re}} \nabla^2 \mathbf{u}_0 - \mathbf{u}_0 \cdot \nabla \mathbf{u}_0,$$

where Re is the Reynolds number based on the cylinder radius a and the free-stream velocity U_∞ that drives the flow and $\mathbf{v}$ is the flow field superimposed over the basic mode $\mathbf{u}_0$, i.e. $\mathbf{u}(\mathbf{x}, t) = \mathbf{u}_0(\mathbf{x}) + \mathbf{v}(\mathbf{x}, t)$. The basic mode represents the oncoming flow as in [1]. This system is approximated using a Solenoidal-Galerkin projection procedure. The procedure starts with the expansion of the flow field $\mathbf{v}$ in terms of solenoidal expansion functions $\mathbf{U}_\mathbf{q}(\mathbf{x})$ which are generated from a scalar field $\psi_\mathbf{q}(\mathbf{x})$ as follows:

$$\mathbf{U}_\mathbf{q}(\mathbf{x}) = \nabla \times \psi_\mathbf{q} \mathbf{e}_z = \left(\frac{1}{r} \frac{\partial \psi_\mathbf{q}}{\partial \theta}, -\frac{\partial \psi_\mathbf{q}}{\partial r}, 0 \right)$$

with the scalar field in the form

$$\psi(\mathbf{x}) = \sum_\mathbf{q} \hat{\psi}_\mathbf{q} \psi_\mathbf{q}(\mathbf{x}) = \sum_\mathbf{q} \hat{\psi}_\mathbf{q} \mathrm{P}_m(r) S_N(\phi(\theta) - s_n)$$

for the index vector $\mathbf{q} = (m, n)$ and satisfy the boundary conditions. In the expansion, $\mathrm{P}_m(r)$ represents a polynomial with m associated with its degree and $S_N(s - s_n)$ is the cardinal function in the Fourier space of 2π-periodic functions with $\phi(\theta)$ is chosen to concentrate the nodes θ_n in the wake region where $s_n = \phi(\theta_n) = \frac{2n\pi}{N+1}$, $n = 0, 1, \ldots, N$. The procedure proceeds with a weighted inner product

$$\left(\overline{\mathbf{U}}_\mathbf{p}, \mathbf{U}_\mathbf{q} \right)_\omega = \int_0^{2\pi} d\theta \int_1^\infty \overline{\mathbf{U}}_\mathbf{p} \cdot \mathbf{U}_\mathbf{q} \, \omega(r) r dr$$

for projection onto the dual space spanned by $\overline{\mathbf{U}}_\mathbf{p}$. It can be shown that the pressure term ∇p vanishes under the projection provided that dual expansion functions $\overline{\mathbf{U}}_\mathbf{p}$ satisfy $\nabla \cdot \left(\omega \overline{\mathbf{U}}_\mathbf{p} \right) = 0$ and some boundary conditions. In this preliminary study, the infinite domain is truncated at $r = R$ and boundary condition at infinity is approximated by $\mathbf{U}_\mathbf{q}(R, \theta) = \mathbf{0}$. In the expansion, $\mathrm{P}_m(r)$ are selected as Legendre polynomials with $\omega(r) \equiv 1$ and the dual expansion functions $\overline{\mathbf{U}}_\mathbf{p}$ are selected to be the same as the solenoidal expansion functions $\mathbf{U}_\mathbf{q}$.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT05 – **Adaptivity and applications**

Two methods for the numerical modelling of the PM transport and deposition on the vegetation

Luděk Beneš[1], **Hynek Řezníček**[2]

[1] *CTU in Prague, Fac. of Mechanical Engineering, Dept. of Technical Mathematics, Karlovo nam. 13, Prague, 121 35, Czech republic* ludek.benes@fs.cvut.cz
[2] *CTU in Prague, Fac. of Mechanical Engineering, Dept. of Technical Mathematics, Karlovo nam. 13, Prague, 121 35, Czech republic* hynek.reznicek@fs.cvut.cz

Atmospheric particulate matter (PM) is a well known risk factor to human health. Vegetative barriers are one of the most popular ways how to eliminate its effects. Effective and accurate method for modelling influence of the vegetation on the dustines is therefore essential.

We present two different methods for the simulation of transport, dispersion and sedimentation of the particles on the vegetation. The first one is common section model based on the transport equation for particle fraction. If we want to capture wide range of the particle size, large number of PDE's is necessary to solve. The second one is momemtum method, where three equations for evolution of the particle distribution are solved.The method is useful when the behaviour of particles in a wide size range is of concern. Both methods reflect four main processes by which particles depose on the leaves: Brownian diffusion, interception, impaction and gravitational settling.

Both methods are used and compared on two test cases. The first one is the forest in 2D, second one is hedgerow in 3D.

The flow field is computed by the same way in both cases. The Atmospheric Boundary Layer (ABL) is assumed to be incompressible, yet the density is not constant due to the gravity. System of the RANS equations for viscous incompressible flow with variable density is used for description of the flows. The two equations turbulence model is used for the closure of this set of equations. Three effects of the vegetation should be considered: effect on the air flow, i.e. slowdown or deflection of the flow, influence on the turbulence levels inside and near the vegetation, and filtering of the particles present in the flow.

The numerical scheme is based on the finite volume method and artificial compressibility method. For the convective terms the AUSM+up scheme is used. Second order accuracy is achieved via the linear reconstruction, where gradients are calculated using least squares approach. To prevent artificial overshooting, Venkatakrishan limiter is utilized. For the viscous fluxes diamond type scheme is used. Resulting set of ODE equations is integrated using BDF2 method.

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CT06 – New Applications for a posteriori error estimates

Tuesday, 17:30 – 19:10, Hotel Fleischers Bergslien

Birane Kane – *Adaptive Discontinuous Galerkin Methods for flow in porous media*

Korinna Rosin – *A posteriori error estimates for quasi-static thermo-elasticity using fictitious domain methods*

Andreas Rademacher – *Dual weighted residual method based error indicators for the local choice of the finite element*

Rolf Stenberg – *A Posteriori Error Estimates for Kirchhoff Plate Elements*

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT06 – **New Applications for a posteriori error estimates**

Adaptive Discontinuous Galerkin Methods for flow in porous media

Birane Kane[1], **Robert Klöfkorn**[2]

[1] *Institute of Applied Analysis and Numerical Simulation, University of Stuttgart, Germany*
birane.kane@mathematik.uni-stuttgart.de

[2] *International Research Institute of Stavanger, Norway*
Robert.Kloefkorn@iris.no

We present an adaptive Discontinuous Galerkin discretization for the solution of porous media flow problems. We analyze, implement and evaluate numerically interior penalty DG methods for 2d and 3d incompressible, immiscible, two-phase flow. We consider a strongly heterogeneous porous medium and discontinuous capillary pressure functions. We write the system in terms of a phase-pressure/phase-saturation formulation. First and second order Adam-Moulton time discretization are combined with various interior penalty DG discretizations in space such as the Symmetric Interior Penalty Galerkin (SIPG), the Nonsymmetric Interior Penalty Galerkin (NIPG) and the Incomplete Interior Penalty Galerkin (IIPG) [1]. This implicit space time discretization leads to a fully coupled nonlinear system requiring to build a Jacobian matrix at each time step for the Newton-Raphson method. The adaptive approach implemented extends the previous work of [3, 4] by allowing for refinement/coarsening in both the element size, the polynomial degree and the time step size. This adaptive strategy allows to refine the mesh when the solution is estimated to be rough and increase the local polynomial degree when the solution is estimated to be smooth. It also grants more flexibility w.r.t the time step size without hindering the convergence of the method. To our knowledge, this is the first time the concept of local *hp*-adaptivity is incorporated in the study of *2d* and *3d* incompressible, immiscible, two-phase flow problems. The implementation is based on the Open-Source PDE software framework DUNE [2].

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT06 – **New Applications for a posteriori error estimates**

A posteriori error estimates for quasi-static thermo-elasticity using fictitious domain methods

Korinna Rosin[1], **Andreas Rademacher**[1]

[1] *Faculty of Mathematics, LS X, TU Dortmund University, Germany*
Korinna.Rosin@tu-dortmund.de
Andreas.Rademacher@tu-dortmund.de

Industrial processes, such as the deep hole drilling of an engine block, are improved based on numerical simulations. Due to the comparatively long processing time and complex workpiece geometries, the use of efficient simulations is inevitable.

Here we consider quasi-static, decoupled thermo-elastic equations. The drilling tool itself is modeled indirectly by its geometry as well as the surface force and the heat input it induces onto the workpiece, which implies the underlying domain. The material removal is carried out by cell deactivation; a variation of the fictitious domain method. It allows for cutting only parts of a cell, too. We realized this with an adaptation of the quadrature in the semi-removed cells, performed for each time step individually. This approach is also known as finite cell method, cf. [1]. Furthermore, we utilize a massive parallel framework and efficient preconditioning techniques. Numerical experiments reproduce the in-process deformation and heat dissipation, measured in two points on the surface, quite well, [2].

Additionally, we improve the accuracy of the simulation by adaptive methods. A first approach for adaptivity in space and time is based on heuristic residual a posteriori error estimations. However, goal oriented error estimators are favorable for accurate approximations of local quantities, like e.g. the displacements along the bore wall. Hence, we discuss secondly an approach based on the dual weighted residual method, cf. [3, 4]. Numerical examples illustrate the efficient performance of the overall algorithm.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT06 – **New Applications for a posteriori error estimates**

Dual weighted residual method based error indicators for the local choice of the finite element

Andreas Rademacher[1], **Dustin Kumor**[2]

[1] *Institute of Applied Mathematics, TU Dortmund University, Germany*
andreas.rademacher@tu-dortmund.de

[2] *Institute of Applied Mathematics, TU Dortmund University, Germany*
dustin.kumor@tu-dortmund.de

The contribution at hand deals with locking effects within the simulation of problems with local regions of nearly incompressible material behaviour and the possibility to cope with these difficulties by an adaptive choice of the finite element. Here, we consider the problem of linear elasticity, which is discretised with standard d-linear finite elements. It is a well known fact, that this kind of discretisation leads to locking phenomena in the case that Poisson's ratio ν is close to 0.5. The modification of the continuous bilinear form a on the discrete level is one possibility to overcome the drawback of the initial formulation. We discretise the bilinear form a by using a discrete divergence operator div_h leading to the bilinear form a_h, which is realised by applying a one point Gaussian quadrature rule for the corresponding scalar product. This approach is known as selective reduced integration, cf., e.g., [1, Ch. 4].

The aim is a modified assembly of the stiffness matrix. On the element level, we want to choose adaptively one of the bilinear forms a or a_h to compute the element matrix. The adaptive choice of the bilinear form on element level describes a problem with model adaptive character. Therefore we refer to the pioneer approach concerning model adaptivity based on the dual weighted residual (DWR) method described in [2] and modify techniques used therein. The main difference to cope with is the fact that in contrast to the framework in [2] we have two discrete models instead of two continuous ones. So the task is to estimate the difference between these two discretisation errors.

The discretisation error with respect to a user defined quantity of interest can be estimated applying the DWR method. Since the discrete solution is computed by using the bilinear form a in some parts of the domain and the bilinear form a_h in the other parts, the standard approach of the DWR method is not applicable and needs to be modified. We derive an error identity involving some additional terms due to the different bilinear forms and discuss the numerical approximation of it, which has to be handled with special care. Finally, numerical results substantiate the accuracy of the presented error estimator.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT06 – **New Applications for a posteriori error estimates**

A Posteriori Error Estimates for Kirchhoff Plate Elements

Tom Gustafsson[1], **Rolf Stenberg**[2], **Juha Videman**[3]

[1] *Department of Mathematics and Systems Analysis, Aalto University School of Science, Espoo, Finland* tom.gustafsson@aalto.fi
[2] *Department of Mathematics and Systems Analysis, Aalto University School of Science, Espoo, Finland* rolf.stenberg@aalto.fi
[3] *CAMGSD and Mathematics Department, Instituto Superior Técnico Universidade de Lisboa, Lisbon, Portugal* jvideman@math.tecnico.ulisboa.pt

We present a conforming finite element method for the classical Kirchhoff plate bending model and perform an a posteriori error analysis. So far this has not been exhaustively done in the literature. Most papers deal only with clamped or simply supported plates. We will address the combination of clamped, simply supported and free boundaries. Moreover, we consider point and line loads which are both admissible and of great engineering interest.

In addition, we discuss the obstacle problem for the Kirchhoff plate model using C^1 elements with a discontinuous Lagrange multiplier which represents the contact force between the plate and the obstacle. We discretise the arising saddle point problem by a stabilized method which circumvents the Babuska-Brezzi condition.

CT07 – Advanced numerical linear algebra

Tuesday, 17:30 – 19:10, Hotel Fleischers Tarald

Ali Dorostkar – *Using a function representation of structured matrices to construct efficient multigrid methods*

Debora Sesana – *Multigrid methods for block-circulant linear systems*

Sergey Dolgov – *Low-rank tensor decomposition and cross approximation algorithms for parametric PDEs*

Miroslav Kuchta – *Preconditioners for a new generation of cell- based models of cardiac tissue*

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CT07 – **Advanced numerical linear algebra**

Using a function representation of structured matrices to construct efficient multigrid methods

Ali Dorostkar[1], **Maya Neytcheva**[1], **Stefano Serra-Capizzano**[1,2]

[1] *Department of Information Technology, Uppsala University, Sweden*
ali.dorostkar@it.uu.se, maya.neytcheva@it.uu.se
[2] *Department of Science and high Technology, Insubria University, Italy*
stefano.serrac@uninsubria.it

We consider systems of linear algebraic equations with matrices that are large, sparse and possess, up to a permutation, a generalized locally Toeplitz (block) structure. For a matrix of the latter class, using the generalized locally Toeplitz (GLT) theory, we can associate an analytical function, describing its spectrum, the so-called symbol of the matrix.

In earlier works it has been shown that the symbol can be used to construct efficient Multigrid (MG) type methods, cf. [1, 2, 3]. The already developed symbol-based MG methods are applied to matrices arising from two-dimensional partial differential problems, discretized by finite differences, finite elements, and iso-geometric analysis.

In the study, presented here, we develop the technique for three-dimensional problems. Additionally, we provide a smoother based on approximate inverses constructed again with the GLT theory. We test the method numerically for the anisotropic Poisson's problem, discretized using finite elements. Comparison with other established algebraic multigrid techniques is also included.

We note that the symbol-based MG, in particular in three space dimensions, offers not only a very high numerical efficiency but also significant memory savings, particularly important for 3D problems. Furthermore, it allows implementation that increases the amount of computation done locally per degree of freedom, enabling high performance on modern computer architectures.

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ENUMATH 2017
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CT07 – **Advanced numerical linear algebra**

Multigrid methods for block-circulant linear systems

D. Sesana[1]

[1] *Department of Science and High Technology, University of Insubria, Via Valleggio 11, 22100 Como, Italy* debora.sesana@uninsubria.it

Many problems in physics, engineering and applied sciences are governed by functional equations (in differential or integral form) that do not admit closed form solution and, therefore, require numerical discretization techniques which often involve the solution of structured linear systems of large size.
The main novelty contained in the literature treating structured matrices is the use of the symbol, that is a function f that provides a compact description of the asymptotic global behavior of the spectrum of the sequence of matrices $\{A_n\}$ arising from the discretization of a differential or integral problem when the fineness parameter tends to zero.
Among the iterative methods available to solve such systems, in the last 25 years Multigrid methods have gained a remarkable reputation as fast solvers for structured matrices associated to shift invariant operators, where the size n of the problem is large and the system shows a conditioning growing polynomially with n.
The convergence analysis of two particular Multigrid method, the Two-grid and V-cycle, has been handled in a compact and elegant manner by studying few analytical properties of the symbol f associated with the sequence of coefficient matrices (so the study does not involve explicitly the entries of the matrix and, more importantly, the size n of the system (see [3, 1]). In the cases taken into account, especially concerning Toeplitz matrices, this symbol is a (multivariate) scalar-valued function f, while much remains to be done in the case of a matrix-valued symbols, which are obtained for example in the discretization of systems of equations. Regarding the Multigrid method for Toeplitz matrices with matrix-valued symbols, pioneering results were proposed by Huckle and Staudacher [2], although, to our knowledge, when the block symbol is not diagonal no convergence analysis has been performed yet.
In this talk our aim is to fill this gap, generalizing some of the existing proofs for the Two-grid and the V-cycle method for systems with matrix in algebra, such as circulant, Hartley and tao, to the case where the latter have a matrix-valued symbol. The next step will be the extension of such results for matrices not in algebra, such as Toeplitz matrices.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT07 – **Advanced numerical linear algebra**

Low-rank tensor decomposition and cross approximation algorithms for parametric PDEs

Sergey Dolgov[1], **Robert Scheichl**[2]

[1] *University of Bath, Claverton Down, BA2 7AY Bath, United Kingdom* s.dolgov@bath.ac.uk
[2] *University of Bath, Claverton Down, BA2 7AY Bath, United Kingdom* masrs@bath.ac.uk

Partial differential equations with stochastic or parameter-dependent coefficients constitute an important uncertainty quantification task and a challenging high-dimensional problem. It has been approached with many techniques, such as Monte Carlo, Sparse Grids, Reduced Basis and tensor decompositions. The latter two offer potentially a lower complexity by finding a tailored low-rank solution approximation. However, generic low-rank methods, such as Alternating Least Squares (ALS), can disturb the sparsity of the original system. As a result, realistic scenarios with fine unstructured grids and large ranks resisted immediate treatment with these algorithms. We propose to combine the ALS steps for the spatial variables and the cross approximation steps for the other parameters. This scheme respects the sparsity (in fact, block-diagonality) of the system matrix and allows to reuse dedicated solvers for the deterministic problem. We show that the new algorithm can be significantly faster than the Sparse Grids and Quasi Monte Carlo methods for smooth random coefficients. Moreover, the entire solution available in a low-rank representation can be used as a cheap surrogate for accelerating Bayesian inference methods.

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT07 – **Advanced numerical linear algebra**

Preconditioners for a new generation of cell-based models of cardiac tissue

Miroslav Kuchta[1,2], **Aslak Tveito**[2,3], **Karoline Horgmo Jæger**[2], **Kent-Andre Mardal**[1,2], **Marie E. Rognes**[2]

[1] *Department of Mathematics, University of Oslo, Norway* mirok@math.uio.no
[2] *Simula Research Laboratory, Center for Biomedical Computing, Norway* aslak@simula.no, karolihj@simula.no, kent-and@simula.no, meg@simula.no
[3] *Department of Informatics, University of Oslo, Norway*

The classical monodomain and bidomain models of cardiac tissue are based on the modeling assumption of co-existence of extracellular and intracellular spaces and the cell membrane everywhere in the tissue. Due to advances in hardware/numerical methods the averaging volume (size of the computational cell) is nowadays of the same order as the cardiac cell and there is thus a potential for new models which do not use the homogenization strategy. In [1] such model, termed the EMI model, is presented, where the cardiac tissue is represented as a collection of cells with the physics of the extra/intracellular spaces and the membrane described by separate PDEs.

In this talk we focus on efficient algorithms for solving the equations of the EMI model. Two discretizations are considered; solving for electric potentials leads to mortar elements while for electric currents as primary unknowns the $H(\mathrm{div})$ elements are natural. With both approaches the main challenge for efficiency is preconditioning the membrane coupling. The presented preconditoners will be based on fractional Sobolev spaces.

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CT08 – DG methods

Wednesday, 13:30 – 15:35, Hotel Fleischers Kvitanosi

Jonas Köhler – *An ADI-dG method for wave-type equations*

Olga Mula – *A Discontinuous Petrov–Galerkin Method for Radiative Transfer*

Vaclav Kučera – *Analysis of the time growth of the error of the DG method for advective problems*

Dimitrios Zacharenakis – *A posteriori error analysis for a discontinuous Galerkin approximation of the Euler-Korteweg model*

Isabella Furci – *Staggered discontinuous Galerkin methods for the incompressible Navier- Stokes equations: spectral analysis and computational results*

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CT08 – **DG methods**

An ADI-dG method for wave-type equations

Jonas Köhler[1], **Marlis Hochbruck**[2]

[1] *Karlsruhe Institute of Technology, Germany* jonas.koehler@kit.edu
[2] *Karlsruhe Institute of Technology, Germany* marlis.hochbruck@kit.edu

We consider the time integration of homogeneous first order wave-type equations of the form

$$\partial_t u = Lu, \qquad u(0) = u^0,$$

where the first order differential operator $L = A+B$ is split, such that A and B are linear, skew-adjoint operators with decoupled partial derivatives, each acting on one component of u only. This framework includes, e.g., 2D advection and wave equations (splitting analogous to [1]) and 3D Maxwell's equations [2, 3].

An attractive class of time integration schemes making use of such a splitting are alternating direction implicit (ADI) methods. The main feat of these methods is that, on a rectangular domain, they allow for unconditionally stable time integration with linear complexity in each timestep, if spatial discretization is carried out with a suitable method on a tensor structured grid.

In this talk, we consider a method of lines approach using the discontinuous Galerkin (dG) method with maximal element diameter h and polynomial degree k for spatial discretization and the Peaceman–Rachford scheme

$$u^{n+1} = (I - \tfrac{\tau}{2}B)^{-1}(I + \tfrac{\tau}{2}A)(I - \tfrac{\tau}{2}A)^{-1}(I + \tfrac{\tau}{2}B)u^n$$

with timestep size τ to propagate in time. We discuss the efficiency of this full discretization applied to concrete examples included in this framework. Moreover, we show that, under suitable regularity assumptions, the full error of the method after n timesteps satisfies

$$\|u_h^n - u(t^n)\|_{L^2} \leq C(\tau^2 + h^k),$$

where C is a constant depending only on the initial data and the length of the time interval.

More details on the error analysis for the special case of Maxwell's equations in 3D are given in the talk by Marlis Hochbruck in the minisymposium "Advanced discretization methods for computational wave propagation".

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT08 – **DG methods**

A Discontinuous Petrov–Galerkin Method for Radiative Transfer

W. Dahmen[1], **F. Gruber**[1], **O. Mula**[2]

[1] *IGPM, RWTH Aachen, Templergraben 55, 52056 Aachen, Germany*
[2] *Université Paris-Dauphine, PSL Research University, CNRS, UMR 7534, CEREMADE, 75016 Paris, France* mula@ceremade.dauphine.fr

We propose a new approach to the numerical solution of radiative transfer equations with certified a posteriori error bounds. A key ingredient is the formulation of an iteration in a suitable (infinite dimensional) function space that is guaranteed to converge with a fixed error reduction per step. The numerical scheme is based on approximately realizing this *outer* iteration within dynamically updated accuracy tolerances that still ensure convergence to the exact solution. On the one hand, since in the course of this iteration the global scattering operator is only applied, this avoids solving linear systems with densely populated system matrices while only linear transport equations need to be solved. This, in turn, rests on a *Discontinous Petrov–Galerkin* (DPG) scheme which comes with rigorous a posteriori error bounds. These bounds are crucial for guaranteeing the convergence of the outer iteration. Moreover, the application of the global (scattering) operator is accelerated through low-rank approximation and matrix compression techniques. The theoretical findings are illustrated and complemented by numerical experiments with a non-trivial scattering kernel.

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CT08 – **DG methods**

Analysis of the time growth of the error of the DG method for advective problems

Václav Kučera[1], **Chi-Wang Shu**[2]

[1] *Charles University, Prague, Czech Republic* kucera@karlin.mff.cuni.cz
[2] *Brown University, Providence, USA* shu@dam.brown.edu

In this contribution we shall deal with the error analysis of the *discontinuous Galerkin* (DG) finite element method for nonstationary linear advection-reaction problems of the form

$$\frac{\partial u}{\partial t} + a \cdot \nabla u + cu = 0.$$

In standard analysis of such problems, one usually assumes ellipticity of the resulting advection and reaction bilinear forms stated by the well known condition $c - \frac{1}{2}\mathrm{div} a \geq 0$. If one does not assume such an ellipticity condition, the analysis is possible with the use of Gronwall's inequality, which however leads to exponential dependence of constants on time t.

In this talk we shall use a variant of the exponential scaling trick in order to avoid the use of Gronwall's lemma, which results in uniformity of the estimates with respect to time. We introduce a particular exponential scaling function corresponding to elapsed time along individual pathlines. This means that the resulting estimates are exponential not with respect to the final physical time T, but with respect to $\widehat{T}$, the longest time any particle carried by the flow field has spent in the spatial domain Ω. If this quantity is bounded, one obtains time-independent constants in the resulting error estimates. Effectively, the error analysis is carried out in the Lagrangian framework, along individual pathlines the length of which is assumed bounded, instead of the standard Eulerian framework.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT08 – **DG methods**

A posteriori error analysis for a discontinuous Galerkin approximation of the Euler-Korteweg model

Dimitrios Zacharenakis[1], **Jan Giesselmann**[2]

[1,2] *Institute of Applied Analysis and Numerical Simulation, University of Stuttgart, Germany*
zachards@mathematik.uni-stuttgart.de
jgiessel@mathematik.uni-stuttgart.de

Recently, the authors of [1] studied a DG scheme in a multi-phase problem of elastodynamics. They derived a posteriori error estimates for the difference of the numerical and the exact solution. Based on this, our goal is to provide an a posteriori analysis of a DG scheme for the approximation of the one dimensional isothermal Euler-Korteweg (EK) system, which is given by

$$\begin{aligned} \rho_t + (\rho v)_x &= 0 \\ (\rho v)_t + \left(\rho v^2 + p(\rho)\right)_x &= \gamma \rho \rho_{xxx} \end{aligned} \quad \text{in } S^1 \times [0,T), \tag{EK}$$

where S^1 is an interval in $\mathbb{R}$ with periodic boundary conditions. The mass density is denoted by $\rho = \rho(x,t) > 0$, the velocity field by $v = v(x,t)$, $T > 0$ is the time. We model capillarity effects by including density gradients in the energy, leading to the term $\gamma\rho\rho_{xxx}$ in (EK), and $\gamma > 0$ is a capillarity coefficient. The pressure, denoted by p, is a non-monotone function and is related to the Helmholtz free energy $W(\rho)$ by $p(\rho) = \rho W'(\rho) - W(\rho)$. Note that (EK) satisfies the energy balance

$$\frac{d}{dt}\left(\int_{S^1} W(\rho) + \frac{1}{2}\rho v^2 + \frac{\gamma}{2}(\rho_x)^2\right) = 0.$$

We discretize (EK) using a local DG (LDG) formulation. A possible approach to bound the difference between the exact and the numerical solution would be to use the relative entropy technique. However, the energy density has a multi-well shape. Thus, a fundamental component of our analysis is the reduced relative entropy stability framework, and to be able to apply it we introduce sufficiently regular intermediate functions called reconstructions ([3]). Since this involves elliptic reconstructions, part of the a posteriori error estimator resembles the estimator in [2].

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT08 – **DG methods**

Staggered discontinuous Galerkin methods for the incompressible Navier-Stokes equations: spectral analysis and computational results

M. Dumbser[2], F. Fambri[2], I. Furci[1], M. Mazza[1], S. Serra-Capizzano[1], M. Tavelli[2]

[1] *Department of Science and High Technology, University of Insubria, via Valleggio 11, I-22100 Como, Italy*

ifurci@uninsubria.it
mariarosa.mazza@uninsubria.it
stefano.serrac@uninsubria.it

[2] *Laboratory of Applied Mathematics, Department of Civil, Environmental and Mechanical Engineering, University of Trento, Via Mesiano 77, I-38123 Trento, Italy*

michael.dumbser@unitn.it
francesco.fambri@unitn.it
m.tavelli@unitn.it

The goal is to create a fruitful bridge between the numerical methods for approximating partial differential equations (PDEs) in fluid dynamics and the (iterative) numerical methods for dealing with the resulting large linear systems. Among the main objectives are the design of new efficient iterative solvers and a rigorous analysis of their convergence speed. The link we have in mind is either the structure or the hidden structure that the involved coefficient matrices inherit, both from the continuous PDE and from the approximation scheme: in turn, the resulting structure is used for deducing spectral information, crucial for the conditioning and convergence analysis, and for the design of more efficient solvers.

As specific problem we consider the incompressible Navier-Stokes equations, as numerical technique we consider high order accurate Discontinuous Galerkin methods on *staggered* meshes, and as tools we use the theory of Toeplitz matrices generated by a function (in the most general block, multi-level form) and the more recent theory of Generalized Locally Toeplitz matrix-sequences. We arrive at a quite complete picture of the spectral features of the underlying matrices and this information is employed for giving a forecast of the convergence history of the conjugate gradient method, together with a discussion on new more advanced techniques (involving preconditioning, multigrid, multi-iterative solvers). Several numerical tests are provided and critically illustrated in order to show the validity and the potential of our analysis.

References

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[2] S. Serra-Capizzano

Spectral and computational analysis of block Toeplitz matrices with non-negative definite generating functions. BIT (1999) 39, 152 – 175.

CT09 – Kinetics and Maxwell's equations

Thursday, 08:30 – 10:10, Hotel Fleischers Bergslien

Derya Altıntan – *Maximum Entropy Method for Jump-Diffusion Approximations of Chemical Kinetics*

Canan Bozkaya – *Magnetic field and radiation effects on natural convection in a porous enclosure*

Munevver Tezer-Sezgin – *Electrically Driven MHD Flow Between two Parallel Slipping and Partly Conducting Infinite Plates*

Mustafa Gaja – *Splitting Schemes and Compatible Spaces for Incompressible MHD*

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT09 – **Kinetics and Maxwell's equations**

Maximum Entropy Methods for Jump-Diffusion Approximations of Chemical Kinetics

Derya Altıntan[1], **Heinz Koeppl**[2]

[1] *Department of Mathematics, Selçuk University, Turkey* altintan@selcuk.edu.tr
[2] *Department of Electrical Engineering and Information Technology, Technische Universität Darmstadt* heinz.koeppl@bcs.tu-darmstadt.de

Cellular processes consist of biomoleular reactions of very different speeds involving reactants of largely different abundances. In [1], we developed a jump-diffusion approximation of such processes through partitioning reactions into fast and slow subgroups and to approximate fast reactions by a diffusion process while the exact Markov chain representation is retained for the slow group. As a consequence, the state in terms of abundances follows a diffusion process with jumps. By transforming the state representation into purely discrete and purely continuous components we are able to introduce a novel hybrid master equation that defines the probability density over the reaction counting processes. Accordingly, the equation contains terms of the traditional chemical master equation and of the Fokker-Planck equation [2]. In order to solve this equation efficiently we further approximate the diffusion process by its moments dynamics that are then conditioned on the remaining discrete states. An approximate expression of the joint probability densities, solving the hybrid master equation, can then be derived through solving a maximum entropy problem for every of the conditional moments at the time point of interest. The problem can be solved efficiently by relying on semi-definite programming techniques. We assess the approximation quality and the computational complexity of the proposed method by considering a canonical model of gene regulation.

This work is supported by the Scientific and Technological Research Council of Turkey (TÜBİTAK) Program no:3501 Grant, no. 115E252.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT09 – **Kinetics and Maxwell's equations**

Magnetic field and radiation effects on natural convection in a porous enclosure

Canan Bozkaya

Department of Mathematics, Middle East Technical University, 06800, Ankara, Turkey
bcanan@metu.edu.tr

The steady, two-dimensional and laminar magnetohydrodynamic natural convection flow in the presence of radiation and viscous dissipation is considered in a square cavity filled with a porous medium. The flow prediction inside the porous medium follows Darcy's model and is subjected to an inclined uniform magnetic field. The vertical walls of the enclosure are kept at constant temperature while the top and bottom walls are considered thermally insulated. The properties of the fluid and porous medium are homogeneous, isotropic and constant except variation of fluid density with temperature. The fluid and porous medium are in thermal equilibrium and radiative heat flux in y-direction is negligible in comparison to that in the x-direction, and hence the thermo-diffusion velocity is only in the x-direction. The dual reciprocity boundary element method (DRBEM), which is a boundary only discretization technique, is applied for the solution of the non-dimensional governing equations with appropriate boundary conditions for the flow and the temperature. Dual reciprocity BEM aims to transform the differential equations into equivalent boundary integral equations by treating the non-homogeneity through a radial basis function approximation. The stream function equation is solved by DRBEM in the usual way, that is by using the fundamental solution of the Laplace equation. However, in the present study, the diffusion term in the energy equation is modified in the sense that the coefficients of second order derivatives in x- and y-directions are not equal due to higher thermal radiation in x-direction. Thus, the fundamental solution to the modified diffusion term in the energy equation is employed through the application of DRBEM by deriving the corresponding radial basis functions, which is the main contribution of the present study. Numerical calculations are carried out for a wide range of Hartmann and Rayleigh numbers at various magnetic field orientation angles. The numerical results are presented for different values of viscous dissipation and radiation to analyze the effects of them on the flow behavior and the temperature distribution. The flow is significantly affected especially at the core of the cavity and the flow field circulation decelerates with an increase in Hartmann number. Moreover, the core of vortices is converted from the vertical position to the horizontal position as the angle of the external magnetic field increases from zero to $\pi/2$, whereas there is no significant effect of the magnetic field orientation on the isotherms. It is also observed that an increase in radiation results in an increase in the average Nusselt number on the hot wall while it decreases following an increase in the viscous dissipation parameter. The results are compared with the ones given in the literature and a good agreement is observed.

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT09 – **Kinetics and Maxwell's equations**

Electrically Driven MHD Flow Between two Parallel Slipping and Partly Conducting Infinite Plates

M. Tezer-Sezgin[1], **P. Senel**[2]

[1] *Department of Mathematics, Middle East Technical University, Ankara, Turkey*
munt@metu.edu.tr

[2] *Department of Mathematics, Middle East Technical University, Ankara, Turkey*
psenel@metu.edu.tr

This study presents the MHD flow between two parallel conducting plates infinite in length which allow the slip of the fluid and contain at their centers symmetrically placed electrodes of length $2l$, under the effect of vertically applied external magnetic field. The fluid is viscous, incompressible and electrically conducting, and the flow is laminar and steady. The governing dimensionless MHD equations for the velocity $V(x,y)$ and the induced magnetic field $B(x,y)$ are [1]

$$\begin{aligned} \nabla^2 V + Ha\frac{\partial B}{\partial y} &= 0 \\ \nabla^2 B + Ha\frac{\partial V}{\partial y} &= 0 \end{aligned} \qquad -1 < y < 1, \quad -\infty < x < \infty$$

with slip velocity, and partly conducting partly perfectly conducting wall conditions

$$B(x,\pm 1) = 1 \quad x < -l, \qquad B(x,\pm 1) = -1 \quad x > l$$
$$\frac{\partial B}{\partial y}(x,\pm 1) = 0 \quad -l \le x \le -l, \qquad V \mp \alpha\frac{\partial V}{\partial y} = 0 \quad \text{at} \quad y = \mp 1, \quad -\infty < x < \infty$$

where Ha and α are the Hartmann number and the slip length, respectively.

These coupled MHD equations are solved by using the dual reciprocity boundary element method (DRBEM), without an iteration in one stroke and at a small computational expense. The advantage of the DRBEM is made use of obtaining the solution by discretizing only a finite boundary on the plates.

The results show that as Ha increases Hartmann layers of thickness $1/Ha$ for the flow are formed near the conducting parts of the plates, and also shear (parabolic) layers of order of thickness $1/\sqrt{Ha}$ emanating from the end points of the electrodes are observed for both the velocity and the induced magnetic field. When the slip ratio s is increased ($s > 1$), Hartmann layers are diminishing leaving its place to slip phenomena that the slip velocity increases. Increase in the length l of the electrodes causes the fluid to be stagnant in front of the electrodes and it retards the weakening effect of the slip ratio on the Hartmann layers. Obtained solution for the case $l = 0,\ s = 0$ coincides with Hunt and Williams [2] asymptotic solution for large Ha.

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ENUMATH 2017
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CT09 – **Kinetics and Maxwell's equations**

Splitting Schemes and Compatible Spaces for Incompressible MHD

M. Gaja[1], **E. Franck**[2], **A. Ratnani**[1], **J. Lakhlili**[1], **M. Mazza**[1], **E. Sonnendruecker**[1], **S. Serra Capizzano**[3]

[1] *Max Planck Institute for Plasma Physics, Germany* mustafa.gaja@ipp.mpg.de
[2] *Inria Nancy Grand Est and IRMA Strasbourg, France*
[3] *Insubria University, Italy*

We investigate the incompressible Magnetohydrodynamics (MHD) model for the evolution of the perpendicular components of the velocity and the magnetic fields in the context of tokamaks via the novel technique of Isogeometric Analysis (IgA) with high degree B-Splines. The discretization is based on compatible finite element spaces that preserve the natural properties (i.e, divergence-free incompressibility condition) of the resulting operators to avoid spurious modes and related numerical instabilities. The geometry is planar and is written to be easily generalized to a torus case. We present results on the compatible discretization and couple this investigation with a hamiltonian splitting in time which allows to deconstruct the system into 'building-blocks' operators that could be inverted individually. Such operators, Laplacian like and Mass operators (H1 and L2 projectors, respectively) for example, are inverted using a robust and optimal ad-hoc multigrid (MG) designed using the Generalized Locally Toeplitz (GLT) theory. This MG is used as a preconditioner for Krylov-Type solvers where the GLT theory is used to construct an efficient smoother for the MG that eliminates the pathology ensuing from using high order B-Splines discretization.

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CT10 – Gas flows

Thursday, 15:30 – 17:10, Hotel Fleischers Bergslien

Matthias Schlottbom – *An approach for the efficient solution of the time-dependent linear Boltzmann equation*

Daisuke Tagami – *Numerical Analysis of a Generalized Particle-Based Method for Convection-Diffusion Equations and its Application*

Ondrej Pártl – *Numerical Modeling of Non-isothermal Compositional Compressible Gas Flow in Soil and Coupled Atmospheric Boundary Layer*

Ylva Rydin – *High-fidelity sound propagation in a varying 3D atmosphere*

ENUMATH 2017
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CT10 – **Gas flows**

An approach for the efficient solution of the time-dependent linear Boltzmann equation

Matthias Schlottbom[1], **Mike A. Botchev**[2], **Herbert Egger**[3]

[1] *University of Twente, The Netherlands* m.schlottbom@utwente.nl
[2] *University of Twente, The Netherlands* m.a.botchev@utwente.nl
[3] *TU Darmstadt, Germany* egger@mathematik.tu-darmstadt.de

Kinetic equations have proven to be useful models in different applications as, e.g., neutron transport, gas dynamics, semiconductors, photon propagation, opinion dynamics or biological network formation. One of the key challenges in the numerical simulation of kinetic equations is their high-dimensionality. For instance, in neutron transport, the solution depends in general on three spatial, three angular and one temporal variable. Based on the mixed variational formulation analyzed in [1] we will present a strategy for the design of efficient numerical approximation schemes. The formulation of [1] incorporates boundary conditions in a weak sense. Unfortunately, the bilinear form corresponding to the boundary conditions couples spatial and angular variables in a non-smooth way rendering a tensor product approximation not straight-forward. As a remedy we introduce an absorbing layer and consider a perturbed variational problem which leads to matrices with tensor product structure. Hence, even in the full tensor product approximation, the resulting discrete operators can be stored efficiently. We provide corresponding error estimates for our approach.

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CT10 – **Gas flows**

Numerical Analysis of a Generalized Particle-Based Method for Convection-Diffusion Equations and its Application

TAGAMI, Daisuke[1]

[1] *Institute of Mathematics for Industry, Kyushu University*
Motooka 744, Nishi-ku, Fukuoka 819-0395, JAPAN tagami@imi.kyushu-u.ac.jp

Numerical analysis of a generalized particle method is considered for convection-diffusion equations. A generalized particle method have been introduced as a class of particle methods, which can describes widely used particle methods like Smoothed Particle Hydrodynamics (SPH), Moving Particle Semi-implicit (MPS), and others, and truncation error estimates of its interpolants and some approximate differential operators have been established; see Imoto–Tagami [1], [2]. Moreover, error estimates of the generalized particle method for the Poisson equation and the heat equation have been also established; see Imoto–Tagami [3].

This presentation is a next step of series of numerical analysis of generalized particle methods. At this step, the particle motion is considered, which play a key role in practical computational fluid dynamics with particle methods. In general, the particle motion cause particle distributions unevenness and numerical schemes instability. To overcome these difficulties, an implicit characteristic method is introduced into approximatons of material derivative; see, for example, Pironneau [5], Pironneau–Tabata [6], and Notsu–Tabata [4]. Our implicit characteristic method distributes particles again at every time steps, which keeps particle distributions at every time steps regularity conditions. Therefore, energy inequalities and error estimates of the characteristic genelarized particle method are obtained. Finally, some numerical applications show efficiency of our numerical schemes.

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT10 – **Gas flows**

Numerical Modeling of Non-isothermal Compositional Compressible Gas Flow in Soil and Coupled Atmospheric Boundary Layer

Ondřej Pártl[1], **Michal Beneš**[2], **Tissa Illangasekare**[3]

[1] *Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Trojanova 13, 120 00 Prague 2, Czech Republic* ondrej.partl@fjfi.cvut.cz
[2] *Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Trojanova 13, 120 00 Prague 2, Czech Republic* michal.benes@fjfi.cvut.cz
[3] *Center for the Experimental Study of Subsurface Environmental Processes, Division of CEE, Colorado School of Mines, Golden, CO 80401, Colorado, USA* tillanga@mines.edu

We shall present a mathematical and numerical model for non-isothermal compressible flow of a mixture of two ideal gases in a heterogeneous porous medium and in the coupled atmospheric boundary layer above the soil surface.

In our model, the domain in which the flow occurs is divided into the porous medium subdomain and the free flow subdomain. In each subdomain, the flow is described by corresponding balance equations for mass, momentum and energy. On the interface between the subdomains, coupling conditions are prescribed.

In both subdomains, the spacial discretization of the governing equations is carried out via the finite volume method. The time discretization is explicit in the free flow subdomain and semi-implicit in the porous medium subdomain.

In this contribution, we shall also present several computational studies which demonstrate the dynamics of compositional gas flow in land-atmosphere interaction.

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CT10 – **Gas flows**

High-fidelity sound propagation in a varying 3D atmosphere

Ylva Rydin[1], **Ken Mattsson**[2], **Jonatan Werpers**[3]

[1] *Department of Information Technology, Uppsala University, Sweden.*
ylva.rydin@it.uu.se
[2] *Department of Information Technology, Uppsala University, Sweden.*
ken.mattsson@it.uu.se
[3] *Department of Information Technology, Uppsala University, Sweden.*
jonatan.werpers@it.uu.se

The main motivation of the present study is to efficiently model sound propagation in a 3D atmosphere with varying physical properties such as pressure, density and wind speed, in a setting including point sources. An important application of this model is, for example to predict sound propagation from wind turbines. Another application is modelling infra-sound from active volcanoes. The forcing on the atmosphere from both wind turbines and volcanic eruptions is generally modelled as point sources.

It is well known that higher order methods (as compared to first- and second-order accurate methods) capture wave dominated phenomena more efficiently, since they allow a considerable reduction in the degrees of freedom, for a given error tolerance. In particular, high-order finite difference methods are ideally suited for problems of this type. The main difficulty using finite differences is to achieve a stable boundary treatment and accurate treatment of non-smooth features such as point sources. The focus in the present study is to develop a high order finite difference method that can handle these difficulties for the linearised Euler equations, in a 3D varying atmosphere.

In this talk, a provably stable high order finite difference discretisation of the linearised 3D Euler equations on curve linear grids will be presented. Emphasis will be given on accurate representation of point sources in the numerical finite difference approximation. By utilising recently derived upwind Summation-By-Parts (SBP) operators [1], which naturally introduce precise artificial dissipation, we show that some of the conditions on the point source discretisation introduced in [2] can be neglected.

To achieve linear stability the advective terms are discretised upwind SBP operators and the boundary conditions are imposed using a penalty (SAT) technique. The resulting SBP-SAT approximations lead to a fully explicit ODE systems. The usage of upwind SBP operators leads to more accurate numerical approximations, compared with the usage of central-difference first derivative SBP operators, in particular in the presence of point sources.

The novel upwind SBP-SAT discretisation of the 3D Euler equations leads to highly robust and accurate approximations, corroborated through numerical computations in 1D and 3D.

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CT11 – Error estimates for FEM

Thursday, 17:25 – 18:15, Kulturhus

Vladimir Vasilyev – *Error estimates for approximate solutions of some discrete equations*

Max Winkler – *Error estimates for the finite element approximation of normal derivatives and boundary control problems*

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CT11 – **Error estimates for FEM**

Error estimates for approximate solutions of some discrete equations

Vladimir B. Vasilyev

Belgorod National Research University, Belgorod 308007, Russia vbv57@inbox.ru

The main object of the talk is a discrete operator and corresponding equation of the following type

$$(K_d u_d)(\tilde{x}) \equiv \sum_{\tilde{y}\in D_d} K(\tilde{x}, \tilde{x}-\tilde{y}) u_d(\tilde{y}) h^m = v_d(\tilde{x}), \quad \tilde{x} \in D_d, \tag{20}$$

where $D_d = D \cap h\mathbb{Z}^m$, $D \subset \mathbb{R}^m$ is a domain in $\mathbb{R}^m$, u_d is unknown function and v_d is given one of a discrete variable $\tilde{x} \in D_d$, $K(x, y)$ is a kernel defined on $\mathbb{R}^m \times \mathbb{R}^m$, $h > 0$ is enough small.

Such equations usually arise under digitization of corresponding continue equation

$$(Ku)(x) \equiv \int_D K(x, x-y) u(y) dy = v(x), \quad x \in D, \tag{21}$$

these often arise in applications, and these can be treated as pseudo-differential equations in certain sense. As a rule one suggests that a symbol of the operator K has some smoothness property on $\mathbb{R}^m \times (\mathbb{R}^m \setminus \{0\})$.

Key questions under studying the equation (20) are following. First one needs appropriate discrete functional spaces in which the operator K_d is bounded preferably with a norm non-depending on h. Usually such discrete spaces should simulate corresponding spaces for continue operator K. Second one needs to obtain solvability result for the equation (20) from corresponding result for the equation (21) at least for small h. And finally if these are done a comparison between discrete and continue cases and corresponding error estimates for solutions of (20) and (21) are required.

We construct special projectors for studying these operators in dependence on a type of canonical domain D and show how these operators are related to special boundary value problems for holomorphic functions of one and several variables. Also we obtain some comparison results between discrete and continual cases. Some results for Calderon–Zygmund operators K and its discrete analogue K_d are presented in [1, 2], it was done for cases $D = \mathbb{R}^m$ and $D = \{x \in \mathbb{R}^m : x = (x', x_m), x_m > 0\}$, and first steps for more general operators and conical domain $D = \{x \in \mathbb{R}^m : x = (x', x_m), x_m > a|x'|, a > 0\}$ are done in [3].

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ENUMATH 2017
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CT11 – **Error estimates for FEM**

Error estimates for the finite element approximation of normal derivatives and boundary control problems

Max Winkler[1], **Johannes Pfefferer**[2]

[1] *Technische Universität Chemnitz, Germany* max.winkler@unibw.de
[2] *Technische Universität München, Germany* pfefferer@ma.tum.de

In this talk we discuss some new finite element error estimates for the Poisson equation measured on a boundary strip whose width is of order h, the global mesh size. These special estimates have several applications. One example is an error estimate for the normal derivatives of finite-element approximations, also known as surface flux approximation [2]. A further application is the approximation of Dirichlet boundary control problems where such an estimate is required for the Ritz projection of the adjoint state variable [1].

The aim of these investigations is to improve the accuracy of the numerical solutions. This is indeed possible when using special meshes that are refined towards the boundary of the computational domain which leads to even quadratic convergence for both the approximate normal derivative and the approximate control in the $L^2(\Gamma)$-norm, provided that the boundary of the domain is sufficiently smooth. We will see that this remains true for polygonal domains when the opening angles of all corner points are smaller than $120°$. Otherwise, we can exactly specify the convergence rate in dependence of these angles.

In order to prove these results we replace the error on the boundary strip by a weighted $L^2(\Omega)$-norm involving the regularized distance function towards the boundary of the domain as weight function. In this weighted norm one can use the Nitsche trick taking into account a dyadic decomposition towards the boundary to resolve the local refinement, and regularity results in weighted Sobolev spaces to capture corner singularities contained in the solution.

Moreover, we present numerical experiments which confirm that the estimates are sharp.

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CT12 – Homogenization

Thursday, 17:25 – 18:15, Hotel Fleischers Sivle

Mats Brun – *Upscaling of coupled geomechanics, flow and heat in a poro-elastic medium in the quasi-static situation.*

Felix Dietrich – *Derivation of higher-order terms in FFT-based homogenization and their influence on effective properties.*

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September 25 – 29, 2017, Voss, Norway
CT12 – **Homogenization**

Upscaling of coupled geomechanics, flow and heat in a poro-elastic medium in the quasi-static situation.

Mats K. Brun[1], **Florin A. Radu**[2]

[1] *Institute of mathematics, University of Bergen, Norway* mats.brun@uib.no
[2] *Institute of mathematics, University of Bergen, Norway* florin.radu@uib.no

We undertake the formal derivation of Biot's low for a poro-elastic medium completely saturated by a fluid, coupled with heat conduction laws for for both the fluid and solid phase. We assume small displacements of the solid structure (i.e. linear strain), a fully connected void and grain space, that the fluid flow is incompressible, and that the fluid/solid interface coupling conditions may be linearized. We start with the microscale model, and apply the technique of homogenization in order to derive the upscaled model in the case of periodically distributed pores. Assuming the homogenization ansatz holds true, we obtain a fully coupled system of equations on the macro-scale accounting for the effects of geomechanics, heat conduction, and fluid flow within a porous material. The present work relies heavily on previous work done by ([2]) and ([1]).

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ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT12 – **Homogenization**

Derivation of higher-order terms in FFT-based homogenization and their influence on effective properties.

Felix Dietrich[1], **Dennis Merkert**[2],

[1] *University of Kaiserslautern, Paul-Ehrlich-Straße 31, 67663 Kaiserslautern, Germany*
fdietric@rhrk.uni-kl.de

[2] *University of Kaiserslautern, Paul-Ehrlich-Straße 31, 67663 Kaiserslautern, Germany*
dmerkert@mathematik.uni-kl.de

After its introduction by Moulinec and Suquet [1], the so called *Basic Scheme* gained the attention of many researchers and became a topic for further investigation and discussion over the past two decades.

This algorithm can be used to solve the steady-state heat equation or the partial differential equations of quasi-static linear elasticity. It owes its popularity to the straightforward computations in Fourier space, that allow to solve the above mentioned problems on structured grids which arise naturally from e.g. microtomography. An additional mesh generation step as it is required in FE-methods is therefore not necessary.

A method to include the possible effects of higher order derivatives was presented five years ago by Tran, Monchiet and Bonnet [2]. By expanding the physical quantities like the strain or the displacement as asymptotic series, they construct a hierarchical system of *Lippmann Schwinger-type equations* of the form

$$\left[\mathrm{Id} + \Gamma^0 * (C - C^0)\right] \tilde{\epsilon} = -\Gamma^0 * p^\alpha + \theta^\alpha$$

that can be solved for the periodic strain $\tilde{\epsilon}$ iteratively.

Here, Id denotes the identity operator, C is the stiffness distribution containing the elastic coefficients of the material, C^0 represents a constant reference material, and Γ^0 is the Green operator connected to C^0. Furthermore, p^α and θ^α are additional terms depending on the order α of the problem, and the asterisk denotes the convolution.

The derivation of these equations will be presented. Their influence on the effective properties will be discussed and compared to the Basic Scheme of order zero. Further, the incorporation of the extended scheme into a multiscale simulation will be demonstrated.

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A numerical method for computing the overall response of nonlinear composites with complex microstructure. *Computer Methods in Applied Mechanics and Engineering 157 (1998): 69-94*

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CT13 – Ray tracing and optical illumination problems

Thursday, 17:25 – 18:15, Hotel Fleischers Kvitanosi

Carmela Filosa – *An inverse ray mapping method in phase space applied to two-dimensional optical systems.*

Bart van Lith – *Solving inverse illumination problems with Liouville's equation*

ENUMATH 2017
September 25 – 29, 2017, Voss, Norway
CT13 – **Ray tracing and optical illumination problems**

An inverse ray mapping method in phase space applied to two-dimensional optical systems.

Carmela Filosa[1], **Jan ten Thije Boonkkamp**[1], **Wilbert IJzerman**[1,2]

[1] *CASA, Eindhoven University of Technology, PO Box 513 5600 MB Eindhoven, The Netherlands*
c.filosa@tue.nl
j.h.m.tenthijeboonkkamp@tue.nl
[2] *Philips Lighting, High Tech Campus 7, 5656 AE Eindhoven, The Netherlands*
wilbert.ijzerman@philips.com

The computation of the propagation of light through an optical system is a topic of wide interest in illumination optics. In order to improve the design of optical systems the photometric variables at the target need to be calculated very accurately. Existing methods used to this purpose are very slow and computationally expensive. A very common method in non-imaging optics is Monte Carlo (MC) ray tracing which requires tracing millions of rays through the system to obtain the desired accuracy.

In order to improve the classical ray tracing, we provide a new approach to describe the light propagation within non-imaging optical systems. The method employs the phase space (PS) representation of *all* the optical surfaces and it is an extension of the method presented in [1]. Every ray in 2D is identified in the PS of the surface that it hits by two coordinates which are the ray position and the ray direction [2]. As the source can only emit light, the direction of the ray in source PS is given by the direction of the emitted ray. The target can only receive light, therefore the direction of the ray in target PS is given by the direction of the incident ray. Hence, only one phase space is considered for the source and the target. However, every other optical surface receive light at a given position and with a certain direction and emit light at the same position with the direction given by either the law of reflection or the Snell's law. Hence, two different phase spaces are considered for these surfaces: the target PS for the incident rays and the source PS for the emitted rays.

The PS of the source and the target of the optical system show that light is uniformly distributed at the source PS but not the whole target PS is covered by rays. This means that the output luminance is positive in those parts illuminated by the source and equal to 0 in the other parts. In order to compute the target photometric variables we need to know where these jump discontinuities of the luminance occur. To this end, an inverse map from the target to the source is constructed connecting the phase spaces of all the optical surfaces. The method is tested for two-dimensional optical systems where both the reflection and the refraction laws occur. Numerical results prove that the new method gives significant advantages not only in the accuracy but also in the reduction of the number of rays traced compared to MC ray tracing. It is expected that the procedure is suitable also for systems where Fresnel reflection occurs and that it can be extended to three-dimensional systems.

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September 25 – 29, 2017, Voss, Norway
CT13 – **Ray tracing and optical illumination problems**

Solving inverse illumination problems with Liouville's equation

Bart S. van Lith[1], **Jan H. M. ten Thije Boonkkamp**[1], **Wilbert L. IJzerman**[1,2]

[1] *CASA, Eindhoven University of Technology* b.s.v.lith@tue.nl
[2] *Philips Lighting*

In recent years, there has been increased interest in the customisation of lighting systems. Being able to guide light to where it needs to go more effectively allows for light sources that use less energy. With the advent of LED technology and their long lifespans, light sources do not need to be replaceable any more. Without these conventional limits to imagination, designers and engineers are free to create integrated lighting systems. This has also sparked interest in computational methods capable of solving inverse illumination problems.

Much of the research effort is aimed at zero-étendue problems, for instance perfect point sources, producing excellent results [1, 2]. This approach works well if the light source is relatively small compared to the typical size of the optic. In practice, however, all light sources have some spatial extent and therefore have nonzero étendue. Some ad-hoc methods based on zero-étendue methods have been developed to cope with extended sources [3]. There also exists a systematic approach to irradiance tailoring [4]. We propose a method based on the optimal control of Liouville's equation to solve general inverse problems in illumination optics.

In this general framework, any type of optic can be dealt with, be they reflective, refractive or gradient index. The broad theory of optimal control allows for easy constraint handling, for instance shape constraints in production. Moreover, since Liouville's equation acts on phase space, irradiance and intensity customisation are special cases. We demonstrate a proof-of-principle for two-dimensional optics.

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CT14 – Solid mechanics

Thursday, 17:25 – 18:15, Hotel Fleischers Tarald

Vanessa Lleras – *Nitsche-based finite element method for contact with Coulomb friction*

Katharina Rafetseder – *A new approach to mixed methods for Kirchhoff-Love plates and shells*

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Nitsche-based finite element method for contact with Coulomb friction

V. Lleras[1], **F. Chouly**[2], **P. Hild**[3], **Y. Renard**[4]

[1] *University of Montpellier, France* vanessa.lleras@umontpellier.fr
[2] *University of Franche Comté, France* franz.chouly@univ-fcomte.fr
[3] *University of Toulouse, France* phild@math.univ-toulouse.fr
[4] *INSA Lyon, France* Yves.Renard@insa-lyon.fr

In this paper, we consider the unilateral contact problem with Coulomb friction in linear elastostatics. Contact and friction conditions are formulated with a set of inequalities and non linear equations on the boundary with corresponding unknowns that are displacements, velocities and surface stresses.

Various techniques have been devised to enforce contact and friction conditions at the discrete level: penalty methods [1] (the set of inequations associated to contact is replaced with a non linear inequation that approximates them) and mixed methods [2] (a Lagrange multiplier is introduced that stands for the normal stress on the contact boundary and for the tangential stress in case of frictional contact). Here we consider a Nitsche based finite element method (originally proposed in [3]) that aims at treating the boundary or interface conditions in a weak sense, according to the Neumann boundary operator associated to the partial differential equation and in a consistent formulation. It differs in this aspect from standard penalization techniques which are generally non consistent and no additional Lagrange multiplier is needed and no discrete inf sup condition must be fulfilled contrarily to mixed methods.

In [4] a Nitsche-based method was proposed and analyzed for the Signorini's problem. Here we introduce a frictional contact problem and its Nitsche-based finite element approximation. Main results of numerical analysis are detailed: an existence result for discrete solutions based on Brouwer's fixed point theorem, well-posedness of the problem. To show that the problem is well-posed, we use an argument by Brezis for M-type and we define a non linear operator by using the Riesz representation theorem. Some numerical results are presented as well.

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A new approach to mixed methods for Kirchhoff-Love plates and shells

Katharina Rafetseder[1], **Walter Zulehner**[1]

[1] *Johannes Kepler University Linz, Altenberger Straße 69, 4040 Linz, Austria*
rafetseder@numa.uni-linz.ac.at, zulehner@numa.uni-linz.ac.at

In this talk, we present a new procedure to obtain a mixed variational formulation for Kirchhoff plate bending problems with mixed boundary conditions varying from clamped, to simply supported, to free.

The new mixed formulation involves a nonstandard Sobolev space for the auxiliary variable, the bending moments, which are related to the Hessian of the deflection. For the deflection the standard Sobolev space H^1 (with appropriate boundary conditions) is used. Based on a regular decomposition of this nonstandard Sobolev space, a decomposition of the fourth-order problem into three (consecutively to solve) second-order elliptic problems in standard Sobolev spaces is achieved.

On the discrete level this decomposition result can be exploited to derive in a natural way families of finite elements for triangular and quadrilateral meshes and also isogeometric discretizations. The remarkable feature of this method is that it is only based on standard components for second-order problems regarding both the discretization and the solver of the discrete problem.

An extension of this approach to more general fourth-order problems, e.g., Kirchhoff-Love shells, will also be discussed.

CT15 – Parameter estimation and modelling

Friday, 08:30 – 10:10, Hotel Fleischers Osa

Daniel Walter – *A sparse control approach to Optimal Design of Experiments for PDEs*

Clarice Poon – *On the use of total variation minimization of measures – Sampling the Fourier transform along radial lines.*

Aurea Martínez – *Heavy metals phytoremediation: First mathematical modelling results*

Lino J. Alvarez-Vázquez – *Urban heat island effect in metropolitan areas: An optimal control perspective*

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A sparse control approach to Optimal Design of Experiments for PDEs

Ira Neitzel[1], Konstantin Pieper[2] Boris Vexler[3] Daniel Walter[4],

[1] *Rheinische Friedrich-Wilhelms-Universität Bonn, Germany* neitzel.ins.uni-bonn.de
[2] *Florida State University, United States* kpieper@fsu.edu
[3] *TU München, Germany* vexler@ma.tum.de
[4] *TU München, Germany* walter@ma.tum.de

We address the problem of identifying parameters of a physical process, described by a system of elliptic partial differential equations, from previously collected experimental data. In many applications, data is scarcely available and polluted by measurement errors. To obtain reliable estimates of the parameters, this uncertainty in the measurements has to be taken into account in the design of the underlying experiment. To this purpose, we formulate an optimal design problem based on the asymptotic covariance matrix of a least-squares estimator for the parameters, which depends on the number, position, and quality of the measurement sensors. The measurement setup is modeled by a sum of Dirac-delta functions on the spatial experimental domain, which corresponds to a finite number of pointwise measurements of the PDE solutions. We present a function space analysis of the problem formulation and discuss structural properties of optimal measurement designs. For the algorithmic solution, a class of accelerated conditional gradient methods is derived, which exploits the sparsity of the solutions to the design problem.

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CT15 – **Parameter estimation and modelling**

On the use of total variation minimization of measures – Sampling the Fourier transform along radial lines.

Clarice Poon[1], **Charles Dossal**[2], **Vincent Duval**[3]

[1] *University of Cambridge* cmhsp2@cam.ac.uk
[2] *Université de Bordeaux* charles.dossal@math.u-bordeaux.fr
[3] *INRIA Paris / Université Paris-Dauphine* vincent.duval@inria.fr

The problem of parameter estimation for a superposition of point sources is rooted in applications such as astronomy, NMR (nuclear magnetic resonance) spectroscopy and microscopy where the signal of interest can often be modelled as point sources. Methods to tackle this problem include prony methods and finite rate of innovation methods, however, in this talk, we shall focus on the use of total variation minimization (for measures). This convex minimization approach has been a topic of intense research within the mathematical community in recent years, stemming from the seminal paper of Candès and Fernandez-Granda [1]. However, these works have focussed on the case where one samples the Fourier transform at Cartesian grid points. On the other hand, physical constraints can sometimes restrict observations to certain angular directions, and in the case of NMR spectroscopy, one is required to sample along continuous trajectories such as radial lines.

This talk presents an analysis on the use of total variation minimization for the parameter estimation problem when given samples of the Fourier transform along radial lines. On the theoretical level, we provide sufficient conditions on the number of radial lines and the number of samples along these radial lines for which one is guaranteed exact reconstruction. Our main results show that in dimension d, with high probability, one can recover the parameters of a superposition of M point sources by sampling its Fourier transform along $d+1$ radial lines. Furthermore, the number of samples we require along each line is, up to $\log$ factors, linear with M.

Furthermore, as a by-product of our analysis, we present a numerical algorithm for the computation of solutions to this infinite dimensional problem by solving a sequence of univariate problems. This talk is based on the recent preprint [2].

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CT15 – **Parameter estimation and modelling**

Heavy metals phytoremediation: First mathematical modelling results

Aurea Martínez[1], **Lino J. Alvarez-Vázquez**[1], **Carmen Rodríguez**[2], **Miguel E. Vázquez-Méndez**[3]

[1] *E.I. Telecomunicación, Universidade de Vigo, 36310 Vigo, Spain*
aurea@dma.uvigo.es, lino@dma.uvigo.es
[2] *F. Matematicas, Universidade de Santiago de Compostela, 15782 Santiago, Spain*
carmen.rodriguez@usc.es
[3] *E.P.S., Universidade de Santiago de Compostela, 27002 Lugo, Spain*
miguelernesto.vazquez@usc.es

In this work we present the first steps in the mathematical modelling of the processes involved in phytoremediation techniques when applied to heavy metal-contaminated environments. Within the field of water pollution, biosorption is based on the ability of biological materials to remove and accumulate heavy metals from aqueous solutions. This technique has received significant attention in recent years because of its advantages compared to traditional methods: Biosorption uses cheaper materials (in this case, we center our study on the naturally abundant micro- and macro-algae) as biosorbents, since they have shown their ability to take up toxic heavy metals from the environment [1]. The topic has been extensively studied from a biological viewpoint but, as far as we know, the mathematical treatment of the problem has remained unadressed.

In order to analyze this environmental problem, we propose a 2D mathematical model coupling the system of partial differential equations for shallow water hydrodynamics with the system of coupled equations modelling the concentrations of heavy metals, algae and nutrients in large waterbodies. In this first mathematical approach to the problem from the viewpoint of environmental control, we present a numerical algorithm for solving the coupled system, and several preliminary computational examples for a simple realistic case.

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Urban heat island effect in metropolitan areas: An optimal control perspective

Lino J. Alvarez-Vázquez[1], **Francisco Fernández**[2], **Aurea Martínez**[1], **Miguel E. Vázquez-Méndez**[3]

[1] *E.I. Telecomunicación, Universidade de Vigo, 36310 Vigo, Spain*
lino@dma.uvigo.es, aurea@dma.uvigo.es
[2] *C.U.D, Escuela Naval Militar, 36920 Marin, Spain* fjavier.fernandez@cud.uvigo.es
[3] *E.P.S., Universidade de Santiago de Compostela, 27002 Lugo, Spain*
miguelernesto.vazquez@usc.es

This work blends numerical modelling, optimization techniques, and optimal control theory of partial differential equations in order to analyse the mitigation of the urban heat island (UHI) effect, which is a very usual environmental phenomenon where the metropolitan areas present a significantly warmer temperature than their surrounding areas, mainly due to the consequences of human activities. The temperature difference between urban areas and the surrounding suburban or rural areas (that can reach upto 5°C) is larger at night than during the day, and is strongly marked when winds are very weak. At the present time, UHI is considered as one of the major environmental problems in the 21st century (undesired result of urbanization and industrialization) [1].

Mitigation of the UHI effect can be achieved through the use of green roofs/walls or of lighter-coloured surfaces in urban areas, or - as will be addressed in this study - through the setting of new green zones inside the city [2].

In order to study the problem, we introduce a well-posed mathematical formulation of the environmental problem (related to the optimal location of green zones in metropolitan areas), we propose a numerical algorithm for its resolution, and finally we present several numerical results (both for the 2D and the 3D cases).

(This work was supported by funding from project MTM2015-65570-P of Ministerio de Economía y Competitividad (Spain) and FEDER.)

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