Abstracts of talks at the

30 YEARS OF ACTA NUMERICA

Conference, 26 June – 2 July 2022

Plenary talks

Doug **Arnold**: Finite element exterior calculus beyond the de Rham complex

Abstract: The finite element exterior calculus is a leading example of structure-preserving discretization, in that it achieves consistency and stability by preserving at the discrete level key geometric, topological, and algebraic structures of the underlying the partial differential equations . This structure preservation has proved crucial to the development of consistent and stable finite element methods for a variety of problems where standards techniques fail. Specifically, FEEC focuses on differential equations which relate to complexes of differential operators acting on Hilbert function spaces and it requires finite element spaces which form subcomplexes of these complexes, and which can be related to them via commuting projections. The most canonical and most extensively studied such complex is the de Rham complex, which is what is required for application to Darcy flow, Maxwell's equations, the Hodge Laplacian, and numerous other problems. But there are many other important differential complexes as well, arising in elasticity, plate theory, magnetohydrodynamic, incompressible flow, general relativity, and other areas. These complexes are less well known and in many cases their properties and appropriate finite element discretizations have not yet been established. In this talk I will briefly review FEEC, and then discuss a systematic procedure for deriving deriving differential complexes and deriving their crucial properties, illustrated with numerous examples.

Coralia **Cartis**: Dimensionality reduction techniques for nonconvex optimization

Abstract: Modern applications such as machine learning involve the solution of huge scale nonconvex optimization problems, sometimes with special structure. Motivated by these challenges, we investigate more generally, dimensionality reduction techniques in the variable/parameter domain for local and global optimization that rely crucially on random projections. We describe and use sketching results that allow efficient projections to low dimensions while preserving useful properties, as well as other tools from random matrix theory and conic integral geometry. We focus on functions with low effective dimensionality, a common occurrence in applications involving overparameterized models and that can serve as an insightful proxy for the training landscape in neural networks. We obtain algorithms that scale well with problem dimension, allow inaccurate information and biased noise, have adaptive parameters and benefit from high-probability complexity guarantees and almost sure convergence.

Matt **Colbrook**: Numerical analysis in the age of data science through the Solvability Complexity Index hierarchy

Abstract: When can algorithms be trusted? This question is of increasing scientific (and legal) interest as science and society become more reliant on computations. We address this question in two topical areas; verified data-driven dynamical systems, and stability and accuracy guarantees for AI. Building on the work of Turing, Smale, and McMullen, we present a toolkit – the Solvability Complexity Index (SCI) hierarchy – for classifying the difficulty of computational problems and proving the optimality of algorithms.

First, we consider infinite-dimensional operators, Koopman operators, that globally linearise nonlinear dynamical systems. Their growing popularity, dubbed Koopmania, has produced 10,000s of articles over the past decade. Spectral properties of Koopman operators are invaluable for understanding dynamics, but are decidedly difficult to compute, with open problems such as spurious modes and continuous spectra. We introduce Residual Dynamic Mode Decomposition [1], which allows verified, data-driven computation of spectral properties of general Koopman operators for the first time, such as Koopman mode decompositions (including continuous spectra) with error control and without spurious modes. These results form part of a wider programme on the foundations of infinite-dimensional spectral computations through the SCI [2-5].

Second, we consider Smale's 18th problem on the limits of AI. Many current AI methods suffer from "AI hallucinations" and instabilities. Paradoxically, we show well-conditioned problems in scientific computing where stable neural networks with great approximation qualities exist, but can never be trained by an algorithm [6]. This result implies a classification theory that describes when training algorithms exist. We discuss some sufficient conditions for the existence of training algorithms for stable NNs in inverse problems. We introduce FIRENETs, which we prove and numerically verify are stable. FIRENETs only require $O(log(1/eps))$ hidden layers for an eps-accurate solution.

We give numerical examples, demonstrating efficiency and tackling difficult problems in the sciences. The discussed problems are samples of what is likely to be a very rich classification theory - we point to further applications in PDEs, optimization and computer-assisted proofs within the SCI hierarchy.

[1] M.J. Colbrook, A. Townsend, Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems, arXiv, 2021.

[2] M.J. Colbrook, The Foundations of Infinite-Dimensional Spectral Computations, PhD thesis, University of Cambridge, 2020.

[3] M.J. Colbrook, A. Horning, A. Townsend, Computing spectral measures of self-adjoint operators, SIAM Review, 2021.

[4] M.J. Colbrook, B. Roman, A. Hansen, How to compute spectra with error control, Physical Review Letters, 2019.

[5] J. Ben-Artzi, M.J. Colbrook, A. Hansen, O. Nevanlinna, M. Seidel, Computing Spectra – On the solvability complexity index hierarchy and towers of algorithms, arXiv, 2020.

[6] M.J. Colbrook, V. Antun, and A.C. Hansen, The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem, PNAS, 2022.

Ron **DeVore**: Optimal learning from data

Abstract: We consider learning an unknown function f from data observations of f that consist of the value of m linear functionals applied to f . The learning problem is to construct an approximation to f from the data observations. To obtain a quantitative theory, we need a norm in which to measure the error and additional information about f known as model class information. Given the data and the model class information, we describe the smallest possible error of recovery and show how to construct a discrete optimization problem whose solution is near optimal. We discuss variants of this problem when the data is polluted by additive noise. We also discuss how the results presented relate to what is done in Deep Learning. The talk represents joint research with Peter Binev, Andrea Bonito, and Guergana Petrova.

Anders **Hansen**: Generalised hardness of approximation: On new phenomena in numerics and the mathematics of "why things don't work"

Abstract: Alchemists wanted to create gold, Hilbert wanted an algorithm to solve Diophantine equations, researchers want to make deep learning robust in AI, MATLAB wants (but fails) to detect when it provides wrong solutions to linear programs, etc. Why do we fail in so many of these fundamental cases? The reason is typically methodological barriers. The history of science is full of methodological barriers – reasons for why we never succeed in reaching certain goals. In many cases, this is due to barriers in the foundations of mathematics. This talk introduces new such barriers from foundations: the phenomenon of generalised hardness of approximation (GHA). GHA grows out of our solution to the extended 9th problem from Smale's list of mathematical problems for the 21st century. This phenomenon is not a rare issue – but happens on a daily basis in numerical analysis – and causes modern software such as MATLAB to fail on basic problems, and even certify nonsensical solutions as correct.

GHA is close in spirit to hardness of approximation (HA) in computer science. Assuming $P \neq NP$, HA is the phenomenon that one can easily compute an epsilon-approximation to the solution of a discrete computational problem for $\epsilon > \epsilon_0 > 0$, but for $\epsilon < \epsilon_0$ it suddenly becomes intractable. HA was discovered decades ago and has been transformative being the subject of several Goedel, Nevanlinna and ACM prizes. GHA is a similar but distinct mathematical phenomenon that requires a new set of mathematical tools in numerical analysis rather than computer science (NB: GHA is independent of P vs. NP). The GHA phenomenon has so far been detected in optimisation, inverse problems, deep learning and AI, as well as computer-assisted proofs. It is essential in the Solvability Complexity Index (SCI) hierarchy and for understanding "why things don't work", as well as a key tool to understand "why things sometimes work".

Karolina **Kropielnicka**: Split and Conquer

Abstract: Numerical approximation of ODEs and PDEs is often the only way to predict the behavior of a system and mostly it is a challenging task. Various types of equations require distinct approaches and methodologies. Splitting the vector field and working on two or more easier equations often simplifies the calculations and renders numerical approximation more effective. Indeed, we are working with easier vector fields! The payoff, however, is that we lose precision of the calculations while composing the results back together.

Splitting methods are successfully applied to split initial condition from the vector field, in the case of linear and nonlinear equations and also in the case of time dependent right hand side of the problem. We will go through a survey of possibilities and effectiveness in case of numerical analysis of transport equations, wave equations and last but not least Schrödinger-like equations. Moreover we will examine novel splitting methods for a PDE system defined on the entire real line (rather than on a compact interval or a torus).

Gitta **Kutyniok**: The approximation power of deep neural networks: From applied harmonic analysis to numerical analysis of PDEs

Abstract: Despite the outstanding success of deep neural networks in real-world applications, most of the related research is empirically driven and a mathematical foundation is almost completely missing. The main goal of a neural network is to approximate a function, which for instance encodes a classification task. Thus, one theoretical approach to derive a fundamental understanding of deep neural networks focusses on their approximation abilities.

In this talk we will provide an introduction into this research area. After a general overview of mathematics of deep neural networks, we will discuss theoretical results which prove that not only do (memory-optimal) neural networks have as much approximation power as classical systems such as wavelets or shearlets, but they are also able to beat the curse of dimensionality, in particular, in the case of parametric PDEs. We will then provide extensive numerical experiments showing the effectiveness of deep neural networks for the numerical analysis of PDEs. We will conclude the talk by a general discussion of the potential of those new methodologies for the area of numerical analysis.

Caroline **Lasser**: Gaussian beams and their relatives

Abstract: The efficient discretization of highly oscillatory functions is a numerical evergreen. If posed in a high dimensional setting, very few methods are at hand, among them the Gaussian beams. The talk will review the mathematical background of Gaussian beams and their frozen width relatives. The hope is to present at least a partial answer to the question, whether thawed or frozen Gaussian approximations are better.

Yvon **Maday**: A few things I know about mathematical inputs for computational chemistry

*Abstract:*The field of computational chemistry is booming. Until recently indeed very few collaborations have been put forward between quantum chemists and mathematicians (in any case much less in this area than in the context of computational fluid mechanics or structures) especially from the numerical point of view, i.e. how do we solve efficiently the problems the chemist and physicists need to solve.

For the last ten to fifteen years things have been changing and the interactions between the two communities has been significantly growing, with the interesting feature that each community understanding what the other can provide.

The purpose of this talk is to present some of the mathematical models that are of use both at the *ab initio* level and at the molecular simulation one together with a review of existing mathematical contributions that have allowed either to better qualify the level of approximation (contributions on a priori and a posteriori analysis) and propose algorithms to improve the accuracy, and also at the level of the iterative algorithms that are used to solve to relevant problems. We shall also present the current grand challenges and a review of the direction we are focusing on in our Synergy ERC endeavour.

Volker **Mehrmann**: Geometric integration of differential-algebraic equation with symmetries

Abstract: Discretization methods for differential-algebraic equations (DAEs) are considered that are based on the integration of an associated inherent ordinary differential equation (ODE). This allows to make use of any discretization scheme suitable for the numerical integration of ODEs. For DAEs with symmetries it is shown that the inherent ODE can be constructed in such a way that it inherits the symmetry properties of the given DAE and geometric properties of its flow. This in particular allows the use of geometric integration schemes with a numerical flow that has analogous geometric properties.

This is joint work with Peter Kunkel.

Marie **Rognes**: Such stuff as dreams are made on: a finite element tale of optimal transport and brain clearance

Abstract: Your brain has its own waterscape: whether you are reading or sleeping, fluid flows around or through the brain tissue and clears waste in the process. These physiological processes are crucial for the well-being of the brain. In spite of their importance we understand them but little, and mathematical modelling could play a crucial role in gaining new insight. Surprisingly little attention has been paid to the mathematics and numerics of the brain?s waterscape however, and even fundamental knowledge is missing.

In this talk, I will discuss mathematical and numerical aspects relating to the brain's waterscape across scales - from viewing the brain as a multi-network poroelastic

medium at the macroscale, to the intricate mixed-dimensional couplings between the vasculature and brain tissue at the mesoscale, and zooming in to studying electrical, chemical and mechanical interactions between brain cells at the microscale in the form of coupled PDE–ODE problems.

Ari **Stern**: Hybrid finite elements and structure-preserving numerical PDEs

Abstract: Many PDEs contain local symmetries, conservation laws, or other geometric structures that one might wish a numerical method to preserve exactly. We show that hybrid finite element methods, which use discontinuous function spaces and impose continuity and boundary conditions with Lagrange multipliers, are especially well suited to this task. We will discuss various applications of this framework, including to Hamiltonian PDEs, Maxwell's equations, the Yang-Mills equations, and finite element exterior calculus.

Anna Karin **Tornberg**: Integral equation-based numerical methods in microfluidics

Abstract: Integral equation based numerical methods are attractive for the simulations of fluid mechanics at the micro scale such as in droplet-based microfluidics, with tiny water drops dispersed in oil, stabilized by surfactants. We have developed highly accuracte numerical methods for drops with insoluble surfactants, both in two and three dimensions with the latter extended to include also electric fields.

This involves addressing several fundamental challenges that are highly relevant also to other applications: accurate quadrature methods for singular and nearly singular integrals, adaptive time-stepping, and reparameterization of time-dependent surfaces for high quality discretization of the drops throughout the simulations.

30 min Talks

Daniele **Boffi**: On the necessity of the Inf-Sup condition for a mixed formulation

Abstract: We consider a non-conventional mixed approximation of the Poisson problem for which the inf-sup constant is not uniformly bounded as the mesh is refined. The behavior of the inf-sup condition is discussed and the convergence of the finite element approximation is studied. It turns out that, under appropriate hypotheses on the data, the discrete solution is stable and optimally convergent.

José Antonio **Carrillo**: The Landau equation: Particle methods and gradient flow structure

Abstract: The Landau equation introduced by Landau in the 1930?s is an important partial differential equation in kinetic theory. It gives a description of colliding particles in plasma physics, and it can be formally derived as a limit of the Boltzmann equation where grazing collisions are dominant. The purpose of this talk is to propose a new perspective inspired from gradient flows for weak solutions of the Landau equation, which is in analogy with the relationship of the heat equation and the

2-Wasserstein metric gradient flow of the Boltzmann entropy. Moreover, we aim at using this interpretation to derive a deterministic particle method to solve efficiently the Landau equation. Our deterministic particle scheme preserves all the conserved quantities at the semidiscrete level for the regularized Landau equation and that is entropy decreasing. We will illustrate the performance of these schemes with efficient computations using treecode approaches borrowed from multipole expansion methods for the 3D relevant Coulomb case. We will present preliminary results on the spatially inhomogeneous Landau equation. This talk is based on a summary of works in collaboration with R. Bailo, J. Hu, L. Wang, and J. Wu.

Alina **Chertock**: Asymptotic preserving numerical methods for singularly perturbed problems

Abstract: Solutions of many nonlinear PDE systems reveal a multiscale character and thus their numerical resolution present some major difficulties. Such problems are typically characterized by the occurrence of a small parameter representing, say, a low Mach or Fraude number. In the regimes, when the parameter is close to zero, the propagation speeds are very low and therefore the use of explicit numerical methods would require very restrictive time and space discretization steps. This becomes rapidly too costly from a practical point of view and consequently numerical solutions for small values of the parameter may be out of reach. Moreover, standard implicit schemes, which are uniformly stable for any parameter value, may be inconsistent with the limiting problem and therefore may provide a wrong solution in the zero limit. Thus, designing robust numerical algorithms, whose accuracy and efficiency is independent of the size of the small parameter is an important and challenging task. A widely used numerical approach applicable in all-speed regimes is based on asymptotic preserving (AP) numerical methods AP methods guarantee that for a fixed mesh size and time step, the numerical scheme should automatically transform into a consistent and stable discretization of the limit system as the parameter tends to zero.

In this talk, we will presented several AP schemes for Navier–Stokes–Korteweg equation, rotational shallow water equations with Coriolis forces, and for kinetic equations with singular limits, if time permits.

Albert **Cohen**: Optimal sampling in least-squares methods

Abstract: Recovering an unknown function from point samples is an ubiquitous task in various applicative settings: non-parametric regression, machine learning, reduced modeling, response surfaces in computer or physical experiments, data assimilation and inverse problems. In this lecture, I will present recent results that are relevant to the context where the user is allowed to select the measurement points, sometimes referred to as active learning. These results allow us to derive an optimal sampling point distribution when the approximation is searched in a linear space of finite dimension n and computed by weighted-least squares. Here optimal means both that the approximation is comparable to the best possible in this space, and that the sampling budget m barely exceeds n. The main involved tools are Christoffel functions, matrix concentration inequalities, reproducing kernel Hilbert spaces.

Anil **Damle**: Structure in spectral projectors: Algorithms and theory

Abstract: Spectral algorithms are pervasive in modern applications, but the underlying problems rarely start and end with simply computing an invariant subspace. Typically, we use the computed subspace to answer interesting questions. Examples include computing localized basis functions in computational quantum chemistry and clustering the nodes of a graph. In many applications the desired information is present in the appropriate invariant subspace, but it may not be directly revealed by eigenvectors. In this talk we discuss how the important information is often readily extracted from the associated spectral projector. Leveraging this viewpoint, we present a simple algorithmic paradigm that unifies both the aforementioned problems and demonstrate its effectiveness within these applications. In support of these algorithmic developments, we also briefly overview new deterministic bounds on how invariant subspaces change with respect to the two-to-infinity norm as a result of perturbations to the underlying matrix. In contrast to classical theory that often captures changes in invariant subspaces with respect to the spectral or Frobenius norm, our results provide control with respect to "row-wise" norms (directly implying entry-wise bounds on differences between spectral projectors) – making them well suited to the analysis of spectral algorithms in a variety of modern applications.

Patrick **Farrell**: Computing disconnected bifurcation diagrams of partial differential equations

Abstract: Computing the distinct solutions u of an equation $f(u, \lambda) = 0$ as a parameter $\lambda \in \mathbb{R}$ is varied is a central task in applied mathematics and engineering. The solutions are captured in a bifurcation diagram, plotting (some functional of) u as a function of λ. In this talk I will present a new algorithm, deflated continuation, for this task.

Deflated continuation has three advantages. First, it is capable of computing disconnected bifurcation diagrams; previous algorithms only aimed to compute that part of the bifurcation diagram continuously connected to the initial data. Second, its implementation is very simple: it only requires a minor modification to an existing Newton-based solver. Third, it can scale to very large discretisations if a good preconditioner is available; no auxiliary problems must be solved.

We present 3D simulations with over one billion degrees of freedom with robust performance from Reynolds numbers 10 to 5000.

Michael **Feischl**: Optimal adaptive algorithms for time-dependent problems

Abstract: In the recent work [Feischl, Math. Comp., 2022], we prove new optimality results for adaptive mesh refinement algorithms for non-symmetric, indefinite, and time-dependent problems by proposing a generalization of quasi-orthogonality which follows directly from the inf-sup stability of the underlying problem. This completely removes a central technical difficulty in modern proofs of optimal convergence of adaptive mesh refinement algorithms and leads to simple optimality proofs for the Taylor-Hood discretization of the stationary Stokes problem, a finite-element/boundary-element discretization of an unbounded transmission problem, and an adaptive time-stepping

scheme for parabolic equations. The main technical tools are new stability bounds for the LU-factorization of matrices together with a recently established connection between quasi-orthogonality and matrix factorization.

Imre **Fekete**: Local error estimation and step size control in adaptive linear multistep methods

Abstract: In a k-step adaptive linear multistep methods the coefficients depend on the $k-1$ most recent step size ratios. In a similar way, both the actual and the estimated local error will depend on these step ratios.

The classical error model has been the asymptotic model, $ch^{p+1}y^{(p+1)}(t)$, based on the constant step size analysis, where all past step sizes simultaneously go to zero. This does not reflect actual computations with multistep methods, where the step size control selects the next step, based on error information from previously accepted steps and the recent step size history. In variable step size implementations the error model must therefore be dynamic and include past step ratios, even in the asymptotic regime.

In this talk we derive dynamic asymptotic models of the local error and its estimator, and show how to use dynamically compensated step size controllers that keep the asymptotic local error near a prescribed tolerance TOL. The new error models enable the use of controllers with enhanced stability, producing more regular step size sequences. Numerical examples illustrate the impact of dynamically compensated control, and that the proper choice of error estimator affects efficiency.

The talk is based on the recently published open access paper
- C. Arévalo, G. Söderlind, Y. Hadjimichael & I. Fekete: Local error estimation and step size control in adaptive linear multistep methods, *Numerical Algorithms*, 86 (2021), 537–563.

Martin **Gander**: Schwarz methods by domain truncation

Abstract: Schwarz methods use a decomposition of the computational domain into subdomains and need to put boundary conditions on the subdomain boundaries. In domain truncation one restricts the unbounded domain to a bounded computational domain and also needs to put boundary conditions on the computational domain boundaries. In both fields there are vast bodies of literature and research is very active and ongoing. It turns out to be fruitful to think of the domain decomposition in Schwarz methods as truncation of the domain onto subdomains. Seminal precursors of this fundamental idea are by Hagstrom et al. (1988), Desprs (1990) and Lions (1990). The first truly optimal Schwarz method that converges in a finite number of steps was proposed by Nataf (1993) and used precisely transparent boundary conditions as transmission conditions between subdomains. Approximating these transparent boundary conditions for fast convergence of Schwarz methods led to the development of optimized Schwarz methods – a name that has become common for Schwarz methods based on domain truncation. Compared to classical Schwarz methods which use simple Dirichlet transmission conditions and have been successfully used in a wide range of

applications, optimized Schwarz methods are much less well understood, mainly due to their more sophisticated transmission conditions.

A key application of Schwarz methods with such sophisticated transmission conditions are time-harmonic wave propagation problems, because classical Schwarz methods simply do not work then. The last decade has brought many new Schwarz methods based on domain truncation. A review from an algorithmic perspective by Gander and Zhang (2019) showed the equivalence of many of these new methods to optimized Schwarz methods. The analysis of optimized Schwarz methods is however lagging behind their algorithmic development. The general abstract Schwarz framework can not be used for the analysis of these methods, and thus there are many open theoretical questions about their convergence. Like for practical multigrid methods, Fourier analysis has been instrumental for understanding the convergence of optimized Schwarz methods and to tune their transmission conditions. Similar to Local Fourier Mode Analysis in multigrid, the unbounded two subdomain case is used as a model for Fourier analysis of optimized Schwarz methods due to its simplicity. Many aspects of the actual situation, e.g., boundary conditions of the original problem and the number of subdomains, were thus neglected in the unbounded two subdomain analysis. While this gave important insight, new phenomena beyond the unbounded two subdomain models were discovered.

i will give in my presentation a review and precise exploration of convergence behaviors of optimized Schwarz methods based on Fourier analysis taking into account the original boundary conditions, many subdomain decompositions and layered media, both for Helmholtz equations with the good and the bad sign. The transmission conditions used include the lowest order absorbing conditions (Robin), and also more advanced perfectly matched layers (PML), both developed first for domain truncation. I will also show transmission conditions that lead to convergence in a finite number of steps, in the presence of cross points. The work presented here is joint work with Hui Zhang.

Silke **Glas**: Symplectic model reduction of Hamiltonian systems on nonlinear manifolds

Abstract: Classical model reduction techniques project the governing equations onto linear subspaces of the high-dimensional state-space. However, for problems with slowly decaying Kolmogorov n-widths such as certain transport-dominated problems, classical linear-subspace reduced order models (ROMs) of low dimension might yield inaccurate results. Thus, the reduced space needs to be extended to more general nonlinear manifolds. Moreover, as we are dealing with Hamiltonian systems, it is crucial that the underlying symplectic structure is preserved in the reduced model.

To the best of our knowledge, existing literature addresses either model reduction on manifolds or symplectic model reduction for Hamiltonian systems, but not their combination. In this talk, we bridge the two aforementioned approaches by providing a novel projection technique called symplectic manifold Galerkin, which projects the Hamiltonian system onto a nonlinear symplectic trial manifold such that the reduced model is again a Hamiltonian system. We derive analytical results such as stability, energy-preservation and a rigorous a-posteriori error bound. Moreover, we construct a

weakly symplectic convolutional autoencoder in order to computationally approximate the nonlinear symplectic trial manifold. We numerically demonstrate the ability of the method to outperform structure-preserving linear subspace ROMs results for a linear wave equation for which a slow decay of the Kolmogorov n-width can be observed.

Abinand **Gopal**: A fast algorithm for computing quadratures for bandlimited functions

Abstract: Bandlimited functions arise in a wide variety of applications in scientific computing and signal processing. In this talk, we present a fast algorithm for computing quadratures for bandlimited functions, based on recent advances in the numerical treatment of prolate spheroidal wave functions. The resulting quadrature rules are capable of integrating functions with a given bandlimited to high accuracy and can be computed rapidly, with only $O(n)$ operations required to compute an n-point rule with fixed bandlimit.

Carmen **Gräßle**: Residual-based time adaptive discretization in model predictive control

Abstract: We consider time adaptive concepts for the discretization of the prediction and application horizon in model predictive control (MPC). The adaptivity strategy is based on a residual-based a-posteriori error control concept which utilizes a reformulation of the optimality system in each level of the MPC algorithm. By this, we construct not only an adaptive discretization of the prediction horizon, but also an adaptive time discretization of the application horizon, whose length could be chosen adaptively or fixed. The approach is applied to an example of a model predictive control problem for a linear parabolic PDE. Numerical tests illustrate the performance and robustness of the proposed time adaptive concept.

This is joint work with Alessandro Alla and Michael Hinze

Kaibo **Hu**: Finite element diagram chasing

Abstract: The Bernstein–Gelfand–Gelfand (BGG) complexes encode fundamental algebraic and differential structures in continuum mechanics, geometry and relativity. The BGG machinery also provides a constructive tool for deriving numerical schemes. In this talk, we first review the BGG construction and its applications. Then we derive finite elements and splines by diagram chasing. Examples include conforming and compatible discretizations of the Riemannian metric and linearized curvature.

Arieh **Iserles**: On orthogonal systems and stable discretisation of evolution PDEs II

Abstract: In this two-part seminar, we review recent research programme into stable numerical solution of evolution PDEs. When we discretise a PDE, the differential operator becomes a differentiation matrix, and nearly a decade ago it was realised that a spatial discretisation with a skew-Hermitian differentiation matrix yields numerical methods for evolution PDEs that are stable by design. Intuitively, a skew-Hermitian differentiation matrix mimics the anti-self-adjoint nature of the derivative. Thus, we

have undertaken a systematic search of basis functions which give rise to a structured skew-Hermitian differentiation matrix, and in particular when such basis functions are orthogonal. This has led to an overarching theory and to the rediscovery of some bases such as the Malmquist–Takenaka basis and some new ones, such as the Tanh-Jacobi functions.

Part 1, given by Marcus Webb, presents a gentle introduction to this topic, the main characterisation theorem via Fourier analysis, and some basic examples.

Part 2, given by Arieh Iserles, revisits the theory from a high level, and extends the theory to Sobolev orthogonality and beyond.

Annika **Lang**: Simulation of random fields on Riemannian manifolds

Abstract: Random fields are important building blocks in spatial models disturbed by randomness such as solutions to stochastic partial differential equations. The fast simulation of random fields is therefore crucial for efficient algorithms in uncertainty quantification. In this talk I present numerical methods for Gaussian random fields on Riemannian manifolds and discuss their convergence. Simulations illustrate the theoretical findings.

This talk is based on joint work with Erik Jansson, Mihály Kovács, and Mike Pereira.

Tony **Leliévre**: Sampling probability measures on submanifolds

Abstract: Various applications require sampling probability measures restricted to submanifolds. For example, in molecular dynamics, one often considers molecular systems whose configurations are distributed according to the Boltzmann–Gibbs measure with so-called molecular constraints such as fixed bond lengths or fixed bending angles in molecules and/or fixed values of the so-called reaction coordinate function for the computation of free energy differences using thermodynamic integration. Such sampling problems also appear in computational statistics and machine learning.

Probability measures supported on submanifolds can be sampled by adding an extra momentum variable to the state of the system, and discretizing the associated Hamiltonian dynamics with some stochastic perturbation in the extra variable. In order to avoid biases in the invariant probability measures sampled by discretizations of these stochastically perturbed Hamiltonian dynamics, a Metropolis rejection procedure can be considered. The so-obtained scheme belongs to the class of generalized Hybrid Monte Carlo algorithms. A special care should be taken into account in the rejection procedure to avoid biases. We will in particular explain generalizations of a procedure suggested by Goodman, Holmes–Cerfon and Zappa for Metropolis random walks on submanifolds, where a reverse projection check is performed to enforce the reversibility of the algorithm.

References:
- T. Lelivre, M. Rousset and G. Stoltz, Langevin dynamics with constraints and computation of free energy differences, Mathematics of Computation, 81(280), 2071–2125, (2012).

- T. Lelivre, M. Rousset and G. Stoltz, Hybrid Monte Carlo methods for sampling probability measures on submanifolds, Numerische Mathematik, 143(2), 379–421, (2019).
- T. Lelivre, G. Stoltz and W. Zhang, Multiple projection MCMC algorithms on submanifolds, to appear in IMA Journal of Numerical Analysis.

Martin **Licht**: Interpolation and approximation of finite element vector fields

Abstract: We address fundamental aspects in the approximation theory of vector-valued finite element methods, using finite element exterior calculus as a unifying framework. We generalize the Clément interpolant, the Scott–Zhang interpolant, and the Ern–Guermond interpolant to finite element differential forms. Our interpolants respect partial boundary conditions and satisfy a broken Bramble–Hilbert Lemma. This permits us to state local error estimates in terms of the mesh size. Our theoretical results apply to curl-conforming and divergence–onforming finite element methods over simplicial triangulations.

Christian **Lubich**: A large-stepsize integrator for highly oscillatory charged-particle dynamics

Abstract: Computing the motion of charged particles efficiently is a fundamental task in particle methods of plasma physics. The standard integrator is the Boris algorithm, which has the charm of simplicity and good conservation properties. However, in the case of a strong magnetic field it requires small step sizes that resolve the gyrorotations (high-frequency, small-amplitude oscillations) around a slowly moving guiding centre. Xiao and Qin [Computer Physics Comm., 265:107981, 2021] recently proposed a remarkably simple but far from obvious modification of the Boris algorithm to compute the guiding centre of the highly oscillatory motion of a charged parti- cle with step sizes h that are much larger than the quasi-period $\sim \varepsilon$ of gyrorotations. They gave strong numerical evidence but no error analysis. This talk reports on an error analysis of the large-stepsize modified Boris method in a setting that has a strong non-uniform magnetic field and moderately bounded velocities, consid- ered over a fixed finite time interval. The analysis yields an optimal $O(h^2)$ error bound for $h^2 \sim \varepsilon$. It is based on comparing the modulated Fourier expansions with state-dependent frequencies of the exact and numerical solutions, for which the differential equations of the dominant terms are obtained explicitly. The talk is based on joint work with Ernst Hairer and Yanyan Shi.

Georg **Maierhofer**: Structure preserving low-regularity integrators for the Korteweg–De Vries and the nonlinear Schrödinger equations

Abstract: Most classical constructions of time-stepping methods for evolution equations are based on Taylor series expansions. As a result their convergence is dependent on large amount of differentiability (regularity) of the solution, and genuine low-regularity phenomena cannot be resolved reliably. This has led to the recent development of bespoke resonance-based methods which can achieve guaranteed convergence under more lenient requirements on the regularity of initial data. Both the

Korteweg–De Vries (KdV) and the nonlinear Schrödinger (NLS) equations are completely integrable and therefore posses an infinite number of first integrals which are preserved in the exact flow of the equation. Unfortunately, previous derivations of the aforementioned resonance-based methods resulted in poor conservation of this structure in the discrete numerical flow. On the other hand there is a plethora of numerical techniques which can preserve such first integrals, but which require very stringent assumptions on the regularity of solutions to achieve convergence. In this talk, we will consider novel constructions of resonance-based methods which are able to achieve both feats in unison: good convergence in the low-regularity regime and long-time preservation of certain first integrals for both equations. We will demonstrate the advantageous properties of these new methods from a theoretical point of view and in computational experiments and provide an application to the simulation of the evolution of a rough vortex filament in an ideal fluid. This is joint work with Valeria Banica and Katharina Schratz.

Leszek **Marcinkowski**: An adaptive domain decomposition method for DG discretization of a multiscale elliptic problem

Abstract: In this talk, we present an overlapping additive Schwarz method for a discontinuous Galerkin interior penalty discretization of second order elliptic problem in two dimensions, with highly varying coefficients. We propose variants of the adaptively built multiscale coarse space each containing local spaces spanned by functions constructed through solving specially defined eigenvalue problems over the 2D structures related to the interfaces between subdomains.

The methods are easy to construct, inherently parallel, and overall effective. We present a theoretical bound for the condition number of the system, showing it is independent of the contrast in the coefficients when enough local eigenfunctions are added to the coarse space.

Agnieszka **Międlar**: A rational approximation method for large-scale nonlinear eigenvalue problems

Abstract: Eigenvalue problems in which the coefficient matrices depend nonlinearly on the eigenvalues arise in a variety of applications in science and engineering, e.g., dynamic analysis of structures or computational nanoelectronics, to mention just a few. This talk will discuss how the Cauchy integral-based approaches combined with rational approximation offer an attractive framework to develop highly efficient and flexible techniques for solving large-scale nonlinear eigenvalue problems. The main idea is to approximate the functions involved in the eigenvalue problem by rational functions and then apply a linearization. A few different schemes are proposed to solve the resulting linear eigenvalue problem by exploiting the special structure of the underlying linearization.

This is a joint work with M. El-Guide and Y. Saad.

Jean-Marie **Mirebeau**: Numerical methods for the discretization of anisotropic PDEs on Cartesian grids

Abstract: Anisotropy, which refers to the existence of preferred direction in a domain, is a source of difficulty in the discretization of partial differential equations (PDEs). Depending on the application, anisotropy can be due to boundary layers, shocks, or other aspects of the problem structure. Numerous numerical methods have been developed to address the related numerical issues, often based on adaptive representations of the solution via special wavelet bases or elongated finite elements. I will describe Voronoi's first reduction, a tool coming from the field of additive lattice geometry, which turns out to be versatile and efficient for that purpose. This approach will be illustrated with the numerical solution of a Monge–Ampère PDE arising in optics, and with a Finslerian eikonal PDE related to seismic tomography.

Piotr **Mucha**: Burgers' equation on a network

Abstract: I plan to talk the analysis of Burgers' equation on metric graphs. The main goal is to establish the existence of weak solutions in the TV class of regularity. A key point is transmission conditions in vertices obeying the Kirchhoff law. First, we consider positive solutions at arbitrary networks and highlight two kinds of vertices, describing two mechanisms of flow splitting at the vertex. Next we design rules at vertices for solutions of arbitrary sign for any subgraph of hexagonal grid, which leads to a construction of general solutions with TV-regularity for this class of networks. Introduced transmission conditions are motivated by the change of the energy estimation.

The talk is bases on joint research with Aleksandra Puchalska (Warsaw).

Olga **Mula**: Accuracy controlled schemes for the eigenvalue problem of the neutron transport equation

Abstract: In this talk, we present iterative schemes to solve the criticality problem in nuclear reactors with certified a posteriori error bounds of the numerical outputs. Mathematically, the criticality problem consists in solving a generalized eigenvalue problem of an unsymmetric, linear Boltzmann operator. In engineering practice, this problem has classically been addressed at the discrete level and through inverse power iteration methods. There appears to be very little published theory involving infinite-dimensional formulations, with rigorous convergence theory and a posteriori bounds to estimate the distance between the exact, infinite-dimensional solution, and the computed one. In this talk, we present a novel approach based on a Newton-type algorithm formulated first at the continuous L2 level.

Yuji **Nakatsukasa**: Fast and accurate randomized algorithms for linear systems and eigenvalue problems

Abstract: Linear systems and eigenvalue problems are the core problems in numerical linear algebra and ubiquitous in applications. We develop a new class of algorithms for general linear systems and eigenvalue problems. These algorithms apply fast ran-

domized sketching to accelerate subspace projection methods, such as GMRES and Rayleigh-Ritz. This approach offers great flexibility in designing the basis for the approximation subspace, which can improve scalability in many computational environments. The resulting algorithms outperform the classic methods with minimal loss of accuracy. For model problems, numerical experiments show large advantages over MATLAB?s optimized routines, including a 100x speedup over Gmres and a 10 speedup over Eigs. This is joint work with Joel Tropp (Caltech).

Michael **Neilan**: Finite element discretizations on Worsey–Farin splits

Abstract: Worsey–Farin splits were first introduced in 1987 to construct low-order C^1 splines with respect to three-dimensional simplicial triangulations. In this talk, we first summarize how these piecewise polynomial spaces are part of several de Rham complexes consisting of smooth finite element spaces. These discrete complexes lead to two results in the discretization of PDEs. First, we present stable, low-order, and divergence-free finite element schemes for the Stokes problem on Worsey–Farin splits. Second, we show how one of the complexes leads to convergent finite element methods for the 3D Maxwell eigenvalue problem with the use of H^1 Lagrange elements. Implementation aspects of the proposed schemes, amenable to existing finite element software, will also be presented.

Vanni **Noferini**: Nearest Ω-stable matrix via Riemannian optimization

Abstract: Let $A \in \mathbb{C}^{n\times n}$ and let $\Omega \subseteq \mathbb{C}$ be a closed set. Let us endow $\mathbb{C}^{n\times n}$ with the distance induced by the Frobenius norm. In this distance, what is the matrix nearest to A whose eigenvalues are all in Ω? This problem is notoriously very difficult, and algorithms for computing a candidate solution were so far only available for some special choices of Ω. In this talk, I describe an algorithm, based on Riemannian optimization, that attempts to answer the question for a general Ω. For some choices of Ω that are relevant for practical applications, such as Ω being the closed left half plane, the unit circle, or the real line, I will provide some evidence that the new algorithm can perform much better than pre-existing alternatives. The talk is based on joint work with Federico Poloni, published in [V. Noferini and F. Poloni, Numerische Mathematik 148:817-851, 2021].

Alexander **Ostermann**: Exponential integrators: review and recent progress

Abstract: Exponential integrators form a particular class of methods for the numerical integration of stiff initial value problems. They are based on the exact integration of a linear approximation of the vector field; the remainder is then suitably accounted for by the variation of constants formula. The idea of exponential integrators can be traced back to the late 1950s. Their development proceeded in several spurts and was always closely related to the possibility of efficiently calculating the action of the exponential and related matrix functions. This task is not at all independent of which approximation is chosen for the vector field. In my talk I will give a brief overview of the developments to date and discuss some current research questions.

Cecilia **Pagliantini**: Structure-preserving dynamical model order reduction of parametric Hamiltonian systems

Abstract: Abstract: In real-time and many-query simulations of parametric differential equations, computational methods need to face high computational costs to provide sufficiently accurate and stable numerical solutions. To address this issue, model order reduction techniques aim at constructing low-complexity high-fidelity surrogate models that allow rapid and accurate solutions under parameter variation. In this talk, we will consider reduced basis methods (RBM) for the model order reduction of parametric Hamiltonian dynamical systems describing non-dissipative phenomena. The development of RBM for Hamiltonian systems is challenged by two main factors: (i) failing to preserve the geometric structure encoding the physical properties of the dynamics, such as invariants of motion or symmetries, might lead to instabilities and unphysical behaviors of the resulting approximate solutions; (ii) the local low-rank nature of transport-dominated and non-dissipative phenomena demands large reduced spaces to achieve sufficiently accurate approximations. We will discuss how to address these aspects via a structure-preserving nonlinear reduced basis approach based on dynamical low-rank approximation. The gist of the proposed method is to evolve low-dimensional surrogate models on a phase space that adapts in time while being endowed with the geometric structure of the full model.

Benjamin **Peherstorfer**: Neural Galerkin schemes with active learning for high-dimensional evolution equations

Abstract: Fitting parameters of machine learning models such as deep networks typically requires accurately estimating the population loss from training data, which is particularly challenging in science and engineering applications where often few informative training samples are available. This work proposes Neural Galerkin schemes based on deep learning that generate training data samples with active learning for numerically solving high-dimensional partial differential equations. Neural Galerkin schemes fit network parameters by minimizing the residual sequentially over time, which enables adaptively collecting new training data in a self-informed manner that is guided by the dynamics described by the partial differential equations. Our finding is that the active form of gathering training data of the proposed Neural Galerkin schemes is key for numerically realizing the approximation capabilities of networks in high dimensions, especially when features of the solutions evolve locally such as in high-dimensional wave propagation problems and interacting particle systems described by Fokker–Planck and kinetic equations.

This is joint work with Joan Bruna and Eric Vanden-Eijnden.

Leszek **Plaskota**: Adaptive methods for numerical approximation: an asymptotic analysis

Abstract: It is well known that adaptive methods often outperform non-adaptive methods in numerical approximation. Their usefulness is especially visible when the underlying function has singularities. Then adaption can be successfully applied to localize the singular points and help to restore the convergence rate to the one typical

for smooth functions. On the other hand, adaptive methods are also used for approximating smooth problems, and adaptive quadratures for numerical integration are a standard example.

In this talk, we provide an asymptotic analysis of adaptive methods for the problems of numerical L^p approximation, $1 \leq p \leq +\infty$, of functions $f \in C^r([a,b])$, where quantitative results are rather limited in the literature. The allowable methods rely on piecewise polynomial interpolation of degree $r-1$ with adaptive strategy of selecting subintervals. The optimal convergence rate is in this case of order n^{-r}, where n is the number of function evaluations used, and it is already achieved by the uniform (non-adaptive) subdivision of the initial interval; however, the asymptotic constant crucially depends on the chosen strategy. We derive asymptotically best adaptive strategies that give significantly better results that non-adaptive strategy, and show their applicability to automatic L^p approximation with a given accuracy ε.

Corresponding results are derived for adaptive numerical integration, where the addition of adaptive variance reduction leads to a quadrature enjoying the convergence rate $n^{-(r+1/2)}$, and significantly reduces the asymptotic constant.

Jakub **Skrzeczkowski** and Zuzanna **Szymańska**: Convergence of the EBT method for a non-local model of cell proliferation with discontinuous interaction kernel

Abstract: We present a new proliferation model of cells living within a colony that is a non-local equation with a discontinuous interaction kernel. We provide detailed proof of the well-posedness of the problem and we investigate the convergence of the EBT algorithm applied to solve the equation. The main difficulty lies in the low regularity of the kernel which is not Lipschitz continuous, thus preventing the application of standard arguments. Therefore, we use the radial symmetry of the problem instead and transform it using spherical coordinates. The resulting equation has a Lipschitz kernel with only one singularity at zero. We introduce a new weighted flat norm and prove that the particle method converges in this norm. We present numerical simulations confirming the theoretical results. Furthermore, we discuss the range of applicability of the model, select suitable data and apply the Bayesian method to perform parameter estimation. Finally, we prove the stability of posterior distributions in the total variation norm which exploits the theory of spaces of measures equipped with the weighted flat norm.

- Z. Szymańska, J. Skrzeczkowski, B. Miasojedow, P. Gwiazda. (2021) "Bayesian inference of a non-local proliferation model", Royal Society Open Science 8 (11), 211279;
- P. Gwiazda, B. Miasojedow, J. Skrzeczkowski, Z. Szymańska. (2022) "Convergence of the EBT method for a non-local model of cell proliferation with discontinuous interaction kernel", IMA Journal of Numerical Analysis, 00, 1–37;

Aretha **Teckentrup**: Convergence and robustness of Gaussian process regression

Abstract: We are interested in the task of estimating an unknown function from data given as a set of point evaluations. In this context, Gaussian process regression is often used as a Bayesian inference procedure, and we are interested in the convergence as the

number of data points goes to infinity. Hyper-parameters appearing in the mean and covariance structure of the Gaussian process prior, such as smoothness of the function and typical length scales, are often unknown and learnt from the data, along with the posterior mean and covariance. We work in the framework of empirical Bayes', where a point estimate of the hyper-parameters is computed, using the data, and then used within the standard Gaussian process prior to posterior update. Using results from scattered data approximation, we provide a convergence analysis of the method applied to a fixed, unknown function of interest.

[1] A.L. Teckentrup. Convergence of Gaussian process regression with estimated hyper-parameters and applications in Bayesian inverse problems. SIAM/ASA Journal on Uncertainty Quantification, 8(4), p. 1310–1337, 2020.

Nick **Trefethen**: Fooled by optimality

Abstract: An occupational hazard of mathematicians is the investigation of objects that are "optimal" in a mathematically precise sense, yet may be far from optimal in practice. This talk will discuss an extreme example of this effect: Gauss–Hermite quadrature on the real line. For large numbers of quadrature points, Gauss–Hermite quadrature is a very poor method of integration, much less efficient than simply truncating the interval and applying Gauss–Legendre quadrature or the periodic trapezoidal rule. We will present a theorem quantifying this difference and explain where the standard notion of optimality has failed.

Milo **Viviani**: On the infinite dimension limit of invariant measures and solutions of Zeitlin's 2D Euler equations

Abstract: In this talk we consider a finite dimensional approximation for the 2D Euler equations on the sphere, proposed by V. Zeitlin, and show their convergence towards a solution of the Euler equations with marginals distributed as the enstrophy measure. The method relies on nontrivial computations on the structure constants of the Poisson algebra of functions on $\mathbb{S}^2$, that appear to be new. Finally, we discuss the problem of extending our results to Gibbsian measures associated with higher Casimirs, via Zeitlin's model.

Mario **Ulrich**: On the power of function values for L_2-approximation

Abstract: We give an overview of recent developments on the L_2-approximation using function values. In particular, we explain how the famous solution to the Kadison–Singer problem finally leads to a tight comparison between sampling numbers and Kolmogorov width (in L_2) for general classes of functions.

Marcus **Webb**: On orthogonal systems and stable discretisation of evolution PDEs I

Abstract: In this two-part seminar, we review recent research programme into stable numerical solution of evolution PDEs. When we discretise a PDE, the differential operator becomes a differentiation matrix, and nearly a decade ago it was realised that a spatial discretisation with a skew-Hermitian differentiation matrix yields numerical

methods for evolution PDEs that are stable by design. Intuitively, a skew-Hermitian differentiation matrix mimics the anti-self-adjoint nature of the derivative. Thus, we have undertaken a systematic search of basis functions which give rise to a structured skew-Hermitian differentiation matrix, and in particular when such basis functions are orthogonal. This has led to an overarching theory and to the rediscovery of some bases such as the Malmquist–Takenaka basis and some new ones, such as the Tanh-Jacobi functions.

Part 1, given by Marcus Webb, presents a gentle introduction to this topic, the main characterisation theorem via Fourier analysis, and some basic examples.

Part 2, given by Arieh Iserles, revisits the theory from a high level, and extends the theory to Sobolev orthogonality and beyond.

Melanie **Weber**: Constrained optimization on manifolds

Abstract Many applications involve non-Euclidean data, such as graphs, strings, or matrices. In such cases, exploiting Riemannian geometry can deliver algorithms that are computationally superior to standard nonlinear programming approaches. This observation has resulted in an increasing interest in Riemannian methods in the optimization and machine learning community. In this talk, we consider the problem of optimizing a convex function on a (Riemannian) manifold subject to convex constraints. Several classical problems that arise in machine learning applications can be phrased as constrained optimization tasks on manifolds. This includes matrix-valued tasks, such as barycenter problems and the computation of Brascamp–Lieb constants. The latter is of central importance in many areas of mathematics and computer science through connections to maximum likelihood estimators in Gaussian models, Tyler?s M-estimator of scatter matrices and the computation of marginals in quantum information theory. In this talk, we present algorithms for solving constrained optimization problems on manifolds and discuss applications to the two problems described above. Based on joint work with Suvrit Sra.

Ragnar **Winther**: The bubble transform and the de Rham complex

Abstract: We introduced the bubble transform for scalar-valued functions in a paper in FoCM in 2016. The construction relied on a domain and a simplicial mesh, but nospecific finite element space entered into theconstruction.However, a key property of thederived decomposition is that itis invariant with respect to continuous piecewise polynomialspaces, and therefore represents a new tool for understanding finite element spaces of arbitrarypolynomial degree. The purpose of this talk is to discuss a similar construction for differentialforms. The key properties of the decomposition are that it commutes with the exterior derivative,preserves the standard finite element spaces of differential forms, and is bounded in L_2.

Yunan **Yang**: Benefits of weighted training in Machine Learning and PDE-based inverse problems

Abstract: Many models in machine learning and PDE-based inverse problems exhibit

intrinsic spectral properties, which have been used to explain the generalization capacity and their ill-posedness. This talk discusses weighted training for computational learning and inversion with noisy data. The highlight is that we allow weighting in both the parameter and data spaces. The weighting scheme encodes both a priori knowledge of the object to be learned and a strategy to weight the contribution of training data in the loss function. We demonstrate that appropriate weighting from prior knowledge can improve the generalization capability of the learned model in such problems.