Advanced numerical methods for non-local problems

Conference in honour of Prof. Dr. Dr. h.c. Wolfgang Hackbusch

9th-11th January, 2024 at Boğaziçi University, Istanbul

	Conference Program		
	January 9 Tuesday	**January 10 Wednesday**	**January 11 Thursday**
09:30	Jinchao Xu	Wolfgang Hackbusch	Martin J. Gander
10:30	Sabine Le Borne	Steffen Börm	**Coffee break (10:30-11:00)**
11:30	**Coffee break**	**Coffee break**	Fatih Ecevit
12:00	Arnold Reusken	Markus Melenk	
13:00	**Lunch break**	**Lunch break**	**Excursion**
14:00	Ronald Kriemann	Andrea Moiola	
15:00	Alexander Litvinenko	Stefan Sauter	
		Dinner at 19:00 Mükellef Karaköy	

Adaptive arithmetic operations with H^2-matrices

Steffen Börm
Christian-Albrechts-Universität, Kiel

H^2-matrices can be used to approximate matrices corresponding to non-local operator in $\mathcal{O}(nk)$ units of storage, where n is the matrix dimension and k the local rank controlling the accuracy of the approximation. Important algebraic operations like the matrix-vector multiplication or the adaptive recompression can be accomplished in $\mathcal{O}(nk)$ or $\mathcal{O}(nk^2)$ operations, respectively.

For the important matrix-matrix multiplication, however, finding an adaptive algorithm with linear, i.e., optimal, complexity has proven a challenge, since interactions of all levels of the matrix hierarchy have to be taken into account. Previous attempts include a non-adaptive algorithm in optimal complexity $\mathcal{O}(nk^2)$ and an adaptive algorithm in non-optimal complexity $\mathcal{O}(nk^2 \log n)$.

In this task, I present a new algorithm that constructs an adaptive approximation of the product of two H^2-matrices in linear, i.e., optimal complexity $\mathcal{O}(nk^2)$. In a first phase, preliminary cluster bases are computed that can represent parts of the product. In a second phase, the resulting representation is converted into the prescribed matrix format. Numerical experiments indicate that the new algorithm indeed shows the optimal scaling behaviour and compares favourably with existing algorithms.

Ray-stabilized Galerkin BEM and efficient computation of the scattering amplitude

Fatih Ecevit
Boğaziçi Üniversitesi
(Joint work with Yassine Boubendir)

We consider the high-frequency multiple scattering problem in the exterior of several convex obstacles. In this context, we review (1) the single-scattering Galerkin boundary element methods (BEM) for the frequency independent approximation of the solutions, and (2) the Neumann series reformulation of multiple scattering problems along with the extension of single-scattering Galerkin BEM to this case.

These strategies provide the guidelines for the frequency independent approximation of multiple scattering iterations. However, important additional issues arise in connection with the Neumann series as it may converge quite slowly or even diverge depending on the underlying geometrical configuration. In this connection, we present our ongoing work on Ray-stabilized Galerkin BEM which still uses the Neumann series reformulation even if it may diverge. Specifically, our approach is based on the calculation of a sufficiently large (depending on the geometry) partial sum of the Neumann series, and computation of the remaining infinite tail in just one solve through the construction of Ray-stabilized Galerkin BEM. We present a preliminary numerical example involving two scatterers.

Considering the high-frequency scattering amplitude, we also present our ongoing work on its Bayliss-Turkel type approximation based on the method of stationary phase, and discuss the extension of this approach to multiple scattering scenarios in conjunction with the Ray-stabilized Galerkin BEM.

Seven Things I would have liked to know when starting to work on Domain Decomposition

Martin J. Gander
Université de Genève

It is not easy to start working in a new field of research. I will give a personal overview over seven things I would have liked to know when I started working on domain decomposition (DD) methods:

1) Seminal contributions to DD not easy to start with
2) Seminal contributions to DD ideal to start with
3) DD solvers are obtained by discretizing 2)
4) There are better transmission conditions than Dirichlet or Neumann
5) "Optimal" in classical DD means scalable
6) Coarse space components can do more than provide scalability
7) DD methods should always be used as preconditioners

The approximation of Cauchy-Stieltjes and Laplace-Stieltjes functions by exponential sums and rational functions

Wolfgang Hackbusch
Max-Planck-Institut für Mathematik in den Naturwissenschaften
(Joint work with Dietrich Braess)

The Čebyšëv approximation of Cauchy-Stieltjes functions [Laplace-Stieltjes functions] by exponential sums [rational functions] is well behaved. In both cases the study of the approximation error is based on elegant results of the rational approximation of $\sqrt{x}$ with respect of a weighted maximum norm. We prove in particular the approximation error of x^{-a}. It turns out that the derived upper bound is sharp for exponential sums, but not for rational approximation. We give details of the underlying analysis using the arithmetic-geometric mean and the Landen transform. A comparison with the Sinc quadrature method shows that the best approximation is by far better. Finally, we explain how the best approximations are determined numerically.

Reducing the Memory Gap between Hierarchical Lowrank Formats

Ronald Kriemann

Max-Planck-Institut für Mathematik in den Naturwissenschaften

Several hierarchical lowrank formats have been designed in the past, e.g. H, Uniform-H or H^2. Typically, with more data dependencies within such a format, e.g., sharing and nesting of cluster bases, the storage requirements sink but on the other hand the arithmetic gets more complicated.

While the handling of lowrank blocks differs in these matrix formats, the actual low-level storage remains the same: double (or single) precision floating point numbers. However, with typical lowrank approximation errors, the corresponding storage precision is much too high, leaving significant room for further storage optimizations, which have different effects on the above lowrank formats and its arithmetic.

We will look at such optimized storage schemes in the context of typical BEM applications.

A block Householder based QR decomposition of hierarchical matrices

Sabine Le Borne

Technische Universität Hamburg

(Joint work with Vincent Griem)

The efficient computation of an accurate QR factorization of a hierarchical matrix is a challenging task. Several approaches have been proposed in the past, often accompanied by several difficulties such as numerical instability, loss of orthogonality or a (significant) increase of ranks in the resulting factors. Recently, a Householder based block approach has been introduced for HODLR matrices. The approach uses a factored form of the orthogonal Q-factor which allows for a block recursion and is hence suitable for structured H-arithmetic. We will generalize this approach to the more general class of hierarchical matrices. The added flexibility with respect to the hierarchical block structures of the matrix A and its factors Q and R require careful algorithmic adjustments such as splitting and re-agglomerating of admissible low-rank blocks whenever possible. More importantly, we discuss strategies to determine admissibility conditions and hence resulting block structures for the factored representation of Q and the upper triangular matrix R. We will conclude with numerical test comparing the proposed approach to some other approaches from the literature.

Computing f-divergences, probability density and characteristic functions in low-rank tensor format

Alexander Litvinenko

Rheinisch-Westfälische Technische Hochschule Aachen

Very often, in the course of uncertainty quantification tasks or data analysis, one has to deal with high-dimensional random variables. Here the interest is mainly to compute characterisations like the entropy, the Kullback-Leibler divergence, more general f-divergences, or other such characteristics based on the probability density. The density is often not available directly, and it is a computational challenge to just represent it in a numerically feasible fashion in case the dimension is even moderately large. It is an even stronger numerical challenge to then actually compute said characteristics in the high-dimensional case. In this regard it is proposed to approximate the discretised density in a compressed form, in particular by a low-rank tensor. This can alternatively be obtained from the corresponding probability characteristic function, or more general representations of the underlying random variable.

The mentioned characterisations need point-wise functions like the logarithm. This normally rather trivial task becomes computationally difficult when the density is approximated in a compressed resp. low-rank tensor format, as the point values are not directly accessible. The computations become possible by considering the compressed data as an element of an associative, commutative algebra with an inner product, and using matrix algorithms to accomplish the mentioned tasks. The representation as a low-rank element of a high order tensor space allows to reduce the computational complexity and storage cost from exponential in the dimension to almost linear.

hp-FEM for the integral fractional Laplacian in polygons

Markus Melenk

Technische Universität Wien

For the Dirichlet problem of the integral fractional Laplacian in a polygon Ω and analytic right-hand side, we show exponential convergence of the *hp*-FEM based on suitably designed meshes, [Faustmann, Marcati, Melenk, Schwab, 2022]. These meshes are geometrically refined towards the edges and corners of Ω. The geometric refinement towards the edges results in anisotropic meshes away from corners. The use of such anisotropic elements is crucial for the exponential convergence result. These mesh design principles are the same ones as those for *hp*-FEM discretizations of the Dirichlet spectral fractional Laplacian in polygons, for which [Banjai, Melenk, Schwab, Numer. Math. 2023] recently established exponential convergence.

The *hp*-FEM convergence result relies on the recent [Faustmann, Marcati, Melenk, Schwab, SIMA 2023] where weighted analytic regularity of the solution is shown in a way that captures both the analyticity of the solution in Ω and the singular behavior near the boundary. Near the boundary the solution has an anisotropic behavior: near edges but away from the corners, the solution is smooth in tangential direction and higher order derivatives in normal direction are singular at edges. At the corners, also higher order tangential derivatives are singular. This behavior is captured in terms of weights that are products of powers of the distances from edges and corners.

Integral equation methods for acoustic scattering by fractals

Andrea Moiola
Università di Pavia

We study sound-soft time-harmonic acoustic scattering by general scatterers, including fractal scatterers, in 2D and 3D space. For an arbitrary compact scatterer we reformulate the Dirichlet boundary value problem for the Helmholtz equation as a first-kind integral equation (IE) involving the Newton potential. The IE is well-posed, except possibly at a countable set of frequencies, and reduces to existing single-layer boundary IEs when the scatterer is the boundary of a bounded Lipschitz open set, a screen, or a multi-screen. When the scatterer is uniformly of d-dimensional Hausdorff dimension in a sense we make precise (a d-set), the operator in our equation is an integral operator with respect to the d-dimensional Hausdorff measure, with kernel the Helmholtz fundamental solution, and we propose a piecewise-constant Galerkin discretization of the IE, which converges in the limit of vanishing mesh width. When the scatterer is the fractal attractor of an iterated function system of contracting similarities we prove convergence rates, and describe a fully discrete implementation using recently proposed quadrature rules for singular integrals on fractals. We present numerical results for a range of examples and make our software available as a Julia code.

Tangential Navier-Stokes equations on evolving surfaces: Analysis and numerical methods

Arnold Reusken
Rheinisch-Westfälische Technische Hochschule Aachen

In this presentation we treat a system of equations that models a lateral flow of a Boussinesq–Scriven fluid on a passively evolving surface. For the resulting Navier-Stokes type system, posed on a smooth closed time-dependent surface, we introduce a weak formulation in terms of function spaces on a space-time manifold defined by the surface evolution. The weak formulation is shown to be well-posed for any finite final time and without smallness conditions on the data. We further extend an unfitted finite element method, known as TraceFEM, to compute solutions to the fluid system. Results of numerical experiments with this method are presented that illustrate how lateral flows are induced by smooth deformations of a material surface.

An integral equation method for acoustic transmission problems with varying coefficients

Stefan Sauter

Universität Zürich

In our talk we will derive an integral equation method which transforms a three-dimensional acoustic transmission problem with variable coefficients and mixed boundary conditions to a non-local equation on the two-dimensional boundary and skeleton of the domain. For this goal, we introduce and analyze abstract layer potentials as solutions of auxiliary coercive full space variational problems and derive jump conditions across domain interfaces. This allows us to formulate the non-local skeleton equation as a direct method for the unknown Cauchy data of the original partial differential equation. We develop a theory which inherits coercivity and continuity of the auxiliary full space variational problem to the resulting variational form of the skeleton equation without relying on an explicit knowledge of Green's function.

Some concrete examples of full and half space transmission problems with piecewise constant coefficients are presented which illustrate the generality of our integral equation method and its theory.

This talk comprises joint work with Francesco Florian, University of Zurich and Ralf Hiptmair, ETH Zurich.

Nonlocal Properties of ReLU Neural Networks and Training Algorithms

Jinchao Xu

King Abdullah University of Science and Technology

In this talk, I will present some recent findings on the nonlocal properties of ReLU Neural Networks (NNs) used for numerical solutions of Partial Differential Equations (PDEs) and their training algorithms. We will begin by introducing ReLU NNs, highlighting their connections to classical finite element methods. After providing an overview of our convergence analysis for these NN methods, the focus will shift to the training algorithms designed to solve optimization problems associated with these methods. A theoretical result explaining both the successes and challenges of NN-based methods trained with gradient-based methods like SGD and Adam will be discussed. Subsequently, I will introduce a new class of training algorithms theoretically capable of achieving, and numerically observed to reach, the asymptotic rate of the underlying discretization algorithms, a feat gradient-based methods cannot accomplish.