Numerical Analysis and Scientific Computation with Applications

NASCA26

$$Ax = b$$

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix}$$

$$\|Ax - b\|_2 \to min$$

$$u_t - \nabla \cdot (A \nabla u) = f$$

Kalamata, Greece 09–12 June, 2026

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NASCA26

Numerical Analysis and Scientific Computation with Applications

Book of Abstracts

9-12 June 2026,
Kalamata, Greece

Edited by

Mustapha Hached
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Contents

Numerical Analysis and Scientific Computation with Applications
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NASCA26 is the fifth edition of the International Conference on Numerical Analysis and Scientific Computation with Applications, which is organized by the National and Kapodistrian University of Athens (NKUA), and the University of the Littoral - Opal Coast (ULCO), held in Kalamata, Greece, June 9-12, 2026. The present book of abstracts includes 7 invited lectures and 87 contributed talks, presented by 94 participants originating from numerous countries around the world.

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Plenary talks

Preconditioning Strategies for a Nested Primal–Dual Method

Stefano Aleotti[1], Claudia Binda[1], Marco Donatelli[1]

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Abstract

Regularization techniques for image reconstruction problems typically involve a smooth term and a potentially non-smooth convex term. A common approach to solving these problems is the use of proximal gradient methods. To accelerate the convergence of these first-order iterative algorithms, extrapolation strategies have been introduced in the literature. We propose a variable metric strategy that can be reinterpreted as a right-preconditioning method [1]. Consequently, we also investigate a left-preconditioned version of the same proximal gradient method, together with possible approximation techniques [2]. We prove the convergence of the preconditioned iterations under a suitable choice of the sequence of preconditioners. Numerical results show that preconditioning accelerates convergence while reducing the overall CPU time.

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Composite Designs for Second-Order Models

Stelios Georgiou[1]

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Abstract

This presentation considers the construction and evaluation of composite experimental designs for second-order response surface models. The focus is on designs that combine orthogonality, space-filling structure, and multi-criteria efficiency, motivated by experiments requiring accurate estimation of main effects, quadratic effects, and two-factor interactions under limited run sizes. Classical response surface designs are revisited alongside modern alternatives for second-order modelling and space-filling approaches, including definitive screening designs, orthogonal and structured space-filling designs, and approaches that address model uncertainty. These methods are examined through the information matrix of the full second-order model, with attention to estimability, conditioning, multicollinearity, and parameter-estimation precision.

The main contribution is the development of composite designs that combine two-level orthogonal factorial structures with axial components derived from orthogonal space-filling constructions, including Latin hypercube-based designs. This approach preserves the interpretability of coded response surface designs while improving coverage of the design region and enhancing information-matrix performance. The resulting designs are assessed using determinant-, trace-, and eigenvalue-based optimality criteria, together with norm-based measures that capture aggregate estimation uncertainty and support robustness under model uncertainty. Structural and geometric characteristics of orthogonal space-filling designs are used to guide the selection of axial components and to support systematic comparison across candidate designs.

Numerical comparisons with standard response surface and space-filling alternatives show that the proposed composite constructions can improve estimation efficiency, conditioning, and robustness, particularly in moderate- and high-dimensional settings.

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Eigenvector-based acceleration strategies for gradient-type methods

Marcos Raydan[1], Jean-Paul Chehab[2], Gaspard Kemlin[2], Yousef Saad[3]

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Abstract

Several strategies are described and analyzed to speed-up gradient-type methods when applied to the minimization of strictly convex quadratics and strictly convex functions. The proposed techniques focus on relaxing the traditional optimal step length associated with gradient methods, including the steepest descent (SD) and the minimal residual (MR) methods. Such a relaxation avoids the well-known negative zigzag effect and allows the iterates to move in the entire space which in turn implies that every so often the search direction approaches some eigenvector of the underlying Hessian matrix. The proposed speedups then rely on taking advantage of the properties of the Lanczos method once a search direction that approaches an eigenvector has been identified in order to accelerate the convergence towards the global minimizer. After analyzing the proposed strategies, we illustrate them on the global minimization of strictly convex functions.

Randomized iterative methods for inverse problems

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[2] *Emory University, Department of Mathematics, Atlanta, GA, USA*
[3] *Department of Mathematics, Kent State University, Kent, OH, USA*

Abstract

Randomized methods can be applied to speed up the computation of the singular value decomposition of a large matrix of low rank. They also can be used to accelerate the convergence of Krylov subspace methods for the solution of certain linear systems of equations. This talk discusses several approaches to apply randomized methods to the solution of large-scale linear systems of equations that arise when solving linear discrete inverse problems. These kind of problems appear when one seeks to determine the cause of an observed effect.

GLT $*$-algebras, low-rank matrix-sequences, and the GLH class

Stefano Serra-Capizzano[1]

[1] *DISAT - U. Insubria - Como & IT - U. Uppsala*

Abstract

The idea of Generalized Locally Toeplitz (GLT) sequences has been introduced as a generalization both of classical Toeplitz sequences and of variable coefficient differential operators and, for every sequence of the class, it has been demonstrated that it is possible to give a rigorous description of the asymptotic spectrum in terms of a function (the symbol) that can be easily identified. This generalizes the notion of a symbol for differential operators (discrete and continuous) or for Toeplitz sequences, where for the latter it is identified through the Fourier coefficients and is related to the classical Fourier Analysis. For every positive integers r, d the r-block d-level GLT class has nice $*$-algebra features and indeed it has been proven that it is stable under linear combinations, products, and inversion when the sequence which is inverted shows a sparsely vanishing symbol (sparsely vanishing symbol = a symbol whose minimal singular value vanishes at most in a set of zero Lebesgue measure). Furthermore, the GLT $*$-algebras virtually include any approximation of partial differential equations (PDEs), fractional differential equations (FDEs), integro-differential equations (IDEs) by local methods (Finite Difference, Finite Element, Isogeometric Analysis etc) and, based on this, we demonstrate that our results on GLT sequences can be used in a PDE/FDE/IDE setting in various directions, including preconditioning, multigrid, spectral detection of branches, fast matrix-less computation of eigenvalues, stability issues, asymptotic low-rank structures, and challenges such as the GLT use in tensors, stochastic, machine learning algorithms.

We discuss these issues in connection with the notion of low-rank matrix-sequences and with the recent class of Generalized Locally Hankel (GLH) matrix-sequences.

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Gradient-Type Subspace Iteration Methods for Symmetric Eigen-Problems

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[1] *University of Minnesota, Twin cities*

Abstract

Computing invariant subspaces is at the core of many applications, from machine learning to signal processing, and control theory, to name just a few examples. Often one wishes to compute the subspace associated with eigenvalues located at one end of the spectrum, i.e., either the largest or the smallest eigenvalues. It is also quite common that the data at hand undergoes frequent changes and that one is required to keep updating or tracking the target invariant subspace. For such problems, the subspace iteration algorithm is ideally suited. The talk will explores variants of the subspace iteration algorithm for computing approximate invariant subspaces. The talk will start by reviewing the subspace iteration approach and then discuss a few variants that exploit gradient-type techniques combined with a Grassmann manifold viewpoint. A gradient descent/ascent method as well as a conjugate gradient technique will be described and analyzed. Numerical experiments will illustrate the behavior of the algorithm on a few examples.

This talk will discuss the problem from a computational linear algebra viewpoint. It will present standard tools for computing invariant subspaces, and describe how these are adapted for situations where rapid updating is needed. We will also show the many connections that exist between different viewpoints adopted by practitioners.

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Kaniel–Stein Acceleration Revisited: Extrapolation, Projection Methods, and Anderson-Type Iterations

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[1] *Université du Littoral Côte d'Opale, LMPA, Calais, France*

Abstract

Least-squares acceleration techniques occupy an important place in the development of extrapolation methods for iterative linear solvers. Among the earliest contributions in this direction is the method introduced by Kaniel and Stein for accelerating linear fixed-point iterations through affine combinations of consecutive iterates determined by a constrained least-squares problem. Despite its elegant structure and its close connection with residual minimization, the Kaniel–Stein method has remained comparatively unexplored within the modern framework of projection and extrapolation methods.

In this work, we revisit the Kaniel–Stein acceleration and develop a unified interpretation that connects extrapolation procedures, projection techniques, and Anderson-type iterations. Our analysis reveals that two distinct accelerated vectors naturally arise in the Kaniel–Stein framework: an extrapolated approximation constructed from the current iteration window and a shifted vector obtained after application of the underlying fixed-point operator. We show that these vectors possess fundamentally different approximation and projection properties, although they are generated from the same least-squares coefficient system.

A central contribution of the paper is the clarification of the relationship between the Kaniel–Stein method and reduced rank extrapolation (RRE). While the least-squares systems involved in both approaches are structurally identical, the accelerated vectors produced by the two procedures are not the same. Consequently, the Kaniel–Stein scheme cannot be identified with RRE, and classical equivalence results linking RRE with minimal-residual Krylov methods do not extend to the Kaniel–Stein framework.

We further show that the Kaniel–Stein procedure is structurally much closer to Anderson acceleration than previously recognized. In particular, the method first extrapolates previously generated iterates and subsequently applies the fixed-point mapping to produce the propagated vector used for restarting the iteration. This interpretation provides a natural bridge between classical least-squares acceleration procedures and modern projection-based iterative methods.

The analysis developed in this paper sheds new light on the structure of least-squares acceleration methods, clarifies several ambiguities that persist in the extrapolation literature, and establishes new connections between extrapolation techniques, projection methods, and contemporary iterative solvers for large-scale linear systems.

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Contributed talks

Sylvester tensor equation

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Abstract

The Sylvester tensor equation is a multidimensional generalization of the classical Sylvester matrix equation and arises naturally in the discretization of high-order partial differential equations as well as in stability and control theory. In this work, we investigate low-multilinear-rank updating methods for efficiently solving large-scale Sylvester tensor equations. To enable the use of standard Krylov subspace methods, the original problem is projected onto lower-dimensional subspaces, yielding a reduced Sylvester tensor equation. The projection is constructed by forming a low-multilinear-rank right-hand side via the Tucker decomposition. We prove that when the right-hand side possesses a low-multilinear-rank structure, the solution of the Sylvester tensor equation also admits a low-multilinear-rank representation. This structural property significantly reduces computational cost and memory requirements, making the proposed approach suitable for large-scale problems.

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Asymmetric Spatial ORCA: A Panic-Dependent Collision Avoidance Framework For Heterogeneous Pedestrian Dynamics

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Abstract

We present a novel extension to the Optimal Reciprocal Collision Avoidance (ORCA) framework for pedestrian dynamics that addresses the given critical limitations of existing models: (1) the fixed temporal planning horizons that are inconsistent with human spatial cognition, (2) the unrealistic assumption of symmetric (equal) responsibility in avoidance maneuvers, (3) the inability to manage physical contact in dense crowds, and (4) the neglect of emotional state effects on navigation behaviour. Our proposed framework introduces a spatial-based half-plane formulation of the ORCA, couples collision-avoidance behaviour with panic intensity through a continuous dynamical system, and establishes asymmetric responsibility sharing that arises from differential emotional states. We replace the fixed temporal horizon with heterogeneous, agent-dependent spatial horizons d_h^i representing the maximal distance along each agent's trajectory within which collision-free constraints are imposed. Emotional heterogeneity is incorporated, and the responsibility factors asymmetrically distribute avoidance effort while maintaining reciprocity. The framework unifies anticipatory avoidance with non-smooth contact dynamics through conditional constraints: $\mathrm{AS}-\mathrm{ORCA}$ half-planes for separated agents $(d_{ij} > 0)$ and impulse-based non-penetration constraints for physical contact $(d_{ij} \leq 0)$. We prove the constraint sets are convex, enabling efficient quadratic programming solutions. Numerical simulations demonstrate realistic crowd phenomena, including bottleneck formation, panic propagation, and heterogeneous evacuation dynamics, validating the framework's ability to capture spatial perception and emotional effects in dense crowds.

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Convergence Enhancement of Lanczos-type Solvers by Multiple Residual Transformations

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Abstract

The bi-conjugate gradient (Bi-CG) [2] and bi-conjugate residual (Bi-CR) [5] methods are the underlying iterative solvers for linear systems $A\boldsymbol{x} = \boldsymbol{b}$, where $A \in \mathbb{R}^{n\times n}$ is a large sparse nonsymmetric nonsingular matrix and $\boldsymbol{b} \in \mathbb{R}^n$. Residual smoothing [4, 6] is a useful technique for converting a sequence of residuals generated by an iterative method to another residual sequence that has a smoother convergence behavior; additionally, it represents a transformation between different iterative solvers. It has recently been shown that the Bi-CG residuals can be transformed into the Bi-CR residuals using a residual smoothing scheme [3]. On the other hand, the hybrid procedure [1], which can be viewed as an extension of the residual smoothing, is a more general transformation technique to generate a residual sequence with superior convergence behavior by combining different sequences of residuals. In this study, we consider applying the hybrid procedure to the Bi-CG and Bi-CR residuals connected by the residual smoothing, and discuss further possibilities of multiple transformations for the residuals. These approaches enable us to enhance the convergence of the underlying residuals with low computational costs. Numerical experiments demonstrate the effectiveness of the presented methods.

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Discontinuous Galerkin Methods for the one-dimensional stochastic Stefan problem

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Abstract

We introduce a space-time discontinuous Galerkin method for the outer one-dimensional stochastic Stefan problem with spread. The non-smooth noise in time is defined as the formal derivative of a Wiener process $W(t)$. The stochastic process is first approximated by a C^∞ approximate process $W_\varepsilon(t)$, while the continuous problem by a smoother ε-problem. We apply a space-time discontinuous in time Galerkin method on the smooth problem and approximate the rough noise maximal solution by using the already constructed numerical solution and W. The numerical error is estimated by selecting properly ε in terms of the discretization parameter h and by using efficiently the error in ε of the approximate process and of its higher order derivatives.

A Variational Approach to Inverse Optimal Design of Chiral Scattering Structures

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Abstract

We discuss a variational framework for inverse optimal design in time-harmonic scattering with chiral material response. The design variables are the geometry of a scattering structure and a set of effective constitutive parameters (e.g. chirality admittance). After establishing well-posedness of the direct problem and uniqueness of the inverse problem in appropriate Sobolev trace spaces, we compute topological, shape and parameter sensitivities of an optimization functional and use them in an iterative design-reconstruction algorithm. Applications supported by numerical results illustrate the methodology and demonstrate how geometry and chiral material parameters can be optimized separately or jointly for various optimal design objectives (e.g. field enhancement, cloaking-type objectives and chiral-sensitive sensing).

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From Correlation to Causation in Machine Learning: A Systematic Review

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Abstract

Causal machine learning has become a central component of modern data analysis, as it addresses the limitations of traditional correlation based approaches. By explicitly identifying cause–effect relationships, it provides a rigorous framework for understanding the true impact of an intervention, a treatment, or a change in variables. This paper presents a systematic review of Causal Machine Learning, a field that has gained increasing importance as it overcomes the limitations of traditional predictive models by uncovering true cause–effect relationships. Building on the distinction between conventional machine learning and its causal counterpart. It then examines the core steps of causal machine learning problems. Particular attention is given to meta-learners, causal trees, and causal forests, which provide scalable and interpretable tools for estimating heterogeneous treatment effects in complex datasets. Following a systematic search strategy, an advanced search was performed in Google Scholar using the exact phrase "Causal Machine Learning", limited to publications from 2018 to 2025. Eligible studies were original articles published in Scopus- or Web of Science–indexed journals. After removing duplicates, articles were assessed for direct relevance to the study topic. Ultimately, 21 studies were included in the review. This approach provides a solid foundation for addressing the main research questions of the review: Do causal machine learning methods outperform traditional machine learning in predictive accuracy, or do they serve a different purpose? Can causal machine learning replace traditional machine learning, or do the two approaches complement each other in practical workflows? How can causal machine learning enhance supervised learning workflows to provide not only accurate predictions but also actionable causal insights? Why is causal machine learning predominantly applied in healthcare, and what unique advantages does it provide in clinical decision-making compared to other domains?

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A weak solution for a class of quasilinear elliptic Systems with nonstandard growth In Musielak-Orlicz space

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Abstract

Here we study existence of a weak solutions for some nonlinear elliptic systems like

$$\begin{cases} -\operatorname{div}\sigma(x,u,Du) = f(x,u,Du) \text{ in } \Omega \\ u(x) = 0 \quad \text{on } \partial\Omega, \end{cases}$$

where $\Omega \subset \mathbb{R}^n$ is a bounded open domain. The Term f satisfy the growth and sign condition. We establish the existence solution by using the idea of Young measure.

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A new approach for spectral analysis of matrix sequences and application to blocking structures.

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Abstract

The characterization of the spectral properties of matrix sequences is essential for building fast and effective iterative solvers for linear systems that usually arise when discretizing continuous real-world problems. The phrase *characterization* is intentionally used here instead of the *identification* since in most of the cases the spectral properties are given in connection with the range of a function, the so-called *spectral symbol*, adapted to the sequence. It turns out that the identification of the spectral symbol of a matrix sequence, if it exists, is equivalent to designing an effective preconditioner for a linear system with coefficient matrix a member of the sequence.

In the common approach, the spectral symbol of a matrix sequence is identified using the *affinity* of the sequence with others whose spectral symbol is known. The affinity is then searched within the *low norm* plus *low rank* perturbations of the sequence. This idea is culminated in the notion of the *approximating classes of sequences (a.c.s)* which is the core of the *Generalized Locally Toeplitz (GLT)* matrix sequences theory [3, 4]. However, following problems appeared in the literature recently [5] another approach emerged. Under this view, the corresponding matrices of the two matrix sequences in comparison are of different size, the one the result of a compression on the other, thus the approach is called *extradimensional*. The idea belongs to Tyrtyshnikov in a unpublished work. Then it was used in [5, Corollary 4.4], but the first systematic treatment can be found in [1].

This talk is an introduction to blocking structures where the extradimensional approach is used for identifying the spectral symbol of the corresponding matrix sequences. By using this idea we are able to prove that the whole matrix sequence carries properties that we can easily prove only for specific members of the sequence. For keeping things simple the case of 2×2 blocking structures is discussed. The analysis gives a clear idea of the kind of preconditioners that would be effective for such structures [2].

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High-order DG method for curved boundaries with polygonal meshes

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Abstract

Discontinuous Galerkin (DG) methods are widely recognized for their effectiveness in solving partial differential equations on complex geometries. However, they typically require the computational mesh to align with the geometry, which poses challenges when aiming to maintain optimal convergence in curved domains and across curved interfaces - a well-known issue, particularly relevant in modeling biological tissues.

We propose a numerical approach based on nodal discontinuous Galerkin methods, combined with a strategy tailored to handle the naturally occurring curved geometries in our application. This approach incorporates the DG-ROD (Reconstruction for Off-site Data) method [1], which applies a polynomial reconstruction of boundary conditions on the computational domain. Crucially, this technique does not depend on curved meshes and preserves both the stability and optimal convergence properties of the DG method.

A numerical benchmark is provided to assess the capability of the method with Dirichlet and Neumann boundary conditions prescribed on curved boundaries, demonstrating that the optimal convergence order is effectively achieved.

The performance of the method is further illustrated on a model arising from a biomedical application, involving geometries with curved anatomical features, in particular structures of the eye [2].

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3D Coronary Vessel Reconstruction from simulated single plane X-Ray Angiography

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Abstract

X-ray angiography is a commonly used imaging modality for the visualization of coronary vasculature, where the vessel anatomy is observed in real time through two-dimensional (2D) image projections [1]. In this work, we simulated the X-ray angiography process, including clinical geometric configurations derived from the meta-data of clinical studies, using a pinhole camera model for image formation. To this end, a voxel traversal algorithm, parallelized for GPU execution, was developed [2]. Synthetic vascular data were used to generate the angiographic image sets.

Using this simulator, we explore the feasibility of solving the inverse problem, i.e. the reconstruction of the three-dimensional (3D) vessel structure from multiple 2D projections. To this end, we formulate the problem as an optimization one to apply the well known Gradient Descent method [3]. We also investigate the use of the Expectation Maximization method [4]. Both of these methods update the 3D vessel model iteratively, to reduce the difference between the observed image and the simulated projections. Finally, possible extensions in real clinical data are discussed, which could prove useful in certain clinical cases, especially in the absence of biplane imaging system.

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Quantum Machine Learning in Image Analysis: A Survey with Focus on Medical Imaging Applications

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Abstract

The transformative potential of Quantum Machine Learning (QML) has been increasingly recognized across diverse scientific domains, including cryptography and pattern recognition, primarily due to the inherent advantages of quantum superposition and entanglement. While classical machine learning (CML) has demonstrated significant efficacy in medical image analysis, inherent constraints regarding computational complexity and the scarcity of high-quality labeled datasets persist. To mitigate these challenges, quantum-enhanced architectures are being explored, facilitating notable advancements in parameter optimization, algorithmic efficiency, and error reduction. In this survey, a comprehensive review and taxonomy of QML concepts and methodologies is established. The systematic review of recent literature is conducted with a dedicated focus on the integration of quantum computing principles within the specialized field of machine learning in medical imaging. The current study is synthesized, highlighting how the bridge between quantum computing , machine learning and medical informatics offers novel perspectives for diagnostic accuracy and data processing. Finally, emerging trends and future research trajectories are identified, providing a strategic roadmap for the continued evolution of quantum-assisted medical image analysis.

***Keywords*—** Quantum machine learning, Medical imaging, Quantum computing, Algorithmic optimization, Image analysis

Performance Analysis of the Parallel Shared-Memory Sparse Matrix-Vector Multiplication on Unstructured Matrices

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Abstract

In this talk, we evaluate the performance of various sparse matrix–vector multiplication (SpMV) methods, a fundamental kernel in Krylov-type iterative solvers. We specifically focus on unstructured sparse matrices, characterized by irregular and unpredictable nonzero patterns. Designing efficient SpMV algorithms for such matrices is challenging for two main reasons: load imbalance in parallel execution due to the irregular distribution of nonzero elements, and the inherently memory-bound nature of SpMV arising from low arithmetic intensity.

A wide range of techniques have been proposed to address these challenges, with much of the literature focusing on specialized sparse matrix storage formats and their corresponding algorithms. We present an overview of current state-of-the-art storage formats together with parallel SpMV implementations. Building on these approaches, we also introduce novel hybrid methods that combine multiple optimization strategies of the current methods.

When selecting an SpMV method, two key performance metrics must be considered. Obviously, SpMV execution speed is critical, since it is usually the dominant cost in Krylov solvers. However, the overhead associated with converting matrices into optimized storage formats can also be substantial. To capture this trade-off, we conduct an extensive experimental evaluation of both runtime performance and the conversion costs for all methods on a wide variety of sparse matrices and hardware platforms. We conclude with a detailed analysis of the results and discuss their implications for practical algorithm selection.

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Multilevel Preconditioning Strategies for Convex Optimisation Methods in Image Deblurring

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Abstract

Proximal gradient methods are widely used in imaging, and their speed of convergence can be accelerated by incorporating variable metrics and/or extrapolation steps. Recent works [1, 2] have shown that preconditioning strategies can significantly enhance this acceleration, in particular, for image deblurring problems. In parallel, a multilevel framework has been introduced in [3] to speed up inertial and inexact forward-backward schemes for image restoration problems.
In this talk, we combine preconditioning and multilevel strategies to design a robust and consistent acceleration framework for both standard and inexact forward-backward schemes applied to regularized convex optimization problems. Numerical experiments in image deblurring confirm that our approach yields a substantial improvement in convergence speed compared to standard methods.

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Some Numerical Results on Two-Dimensional Nonlinear Dispersive Equations

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Abstract

Nonlinear dispersive equations occur in many physical phenomena, such as optics, plasma physics, and water waves. We consider some well-known two-dimensional examples: Kadomtsev-Petviashvili equation and 2D-Nonlinear Schrödinger equation. Numerical experiments are conducted to investigate the dynamical properties of solitary wave solutions of these equations.

Complexity-Aware Training Time Prediction in Cybersecurity

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Abstract

Machine learning systems are increasingly deployed in operational environments where computational efficiency plays a central role. Beyond predictive accuracy, training time has become a decisive factor in experiment planning, model updating, and infrastructure management. In cybersecurity applications, where detection models must be frequently retrained to adapt to evolving threats, reliable runtime estimation is particularly important.

Classical asymptotic complexity analysis provides theoretical growth behavior but does not fully capture empirical execution time in practical settings where dataset size, feature dimensionality, optimization iterations, and hardware characteristics jointly influence performance. This limitation motivates the need for structured modeling approaches that explicitly relate measurable computational parameters to observed runtime.

In this work, we adopt the Full Parameter Time Complexity (FPTC) methodology to construct a parametric formulation of training time. The runtime is expressed as a function $F(n, v, Q)$, where n denotes the number of observations, v the feature dimension, and Q the number of optimization iterations. Binary logistic regression is considered as a case study due to its analytical tractability and its well-defined iterative optimization procedure.

The study includes the formal derivation of the computational cost model, the calibration of a hardware-dependent coefficient, and a systematic comparison between predicted and measured training times using the Web Page Phishing Detection Dataset. This framework provides a principled foundation for complexity-aware runtime prediction and supports the development of performance-aware machine learning systems in cybersecurity contexts.

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On the Feedback Stabilisation of Bilinear Systems

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Abstract

Bilinear systems form a particularly interesting subclass of nonlinear dynamical systems, with many important real-world applications. In this talk, I will introduce the fundamental structure of these systems and highlight their practical relevance. I will then present several new results that we established in a recent work, along with the control strategy that allows us to explicitly construct a family of quadratic feedback controls. Numerical simulations illustrating these results will also be discussed. Finally, I will briefly explain how the presence of time delays influences the behavior and controllability of such systems.

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Heterogeneous HPC: Leveraging CPU, GPU, and Vector Units for GEMM

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Abstract

New computing systems combine different hardware structures to achieve High Performance Computing, also known as Heterogeneous Computing. It is based on combining GPUs, CPUs, and vector units to solve complex problems. These problems are divided into smaller subproblems, and each subproblem is then given to the appropriate engine. This architecture is meant to deliver high throughput and better hardware optimization than homogeneous systems. However, effectively running these systems can be very challenging as it includes the orchestration of diverse resources that require workload partitioning, synchronization, and data movement between vectorized units, CPU threads, and GPUs [1]. GPUs have already gained a lot of momentum, but are still evolving. They have progressed into general-purpose accelerators offering a large number of cores and high-bandwidth memory. This progression comes with the development of different programming models, namely CUDA and OpenCL. They offer direct control over the device and manage data transfer efficiently, which enables potential speedup opportunities for parallel tasks. These models also make it possible and eventually easy to use GPUs with other processing engines [2]. New CPU systems feature wide-SIMD vector extensions namely AVX and AVX2. They allow instructions to work on several data points simultaneously. JIT frameworks can use them to accelerate loops. Vectorization can transform general-purpose CPUs into powerful engines for compute-intensive operations. The challenge remains paying additional attention to data alignment and memory hierarchy [3]. Our work presents a Heterogeneous HPC approach that makes use of CPUs, GPUs, and vectorized units within the same system to perform GEMM as a compute-intensive parallelizable task. GEMM is the base of several complex and multifold research problems like to deep learning, signal processing, and linear algebra. Its high arithmetic intensity and regular data access make it ideal for heterogeneous HPC approaches. In addition to the work in the literature, we introduce vectorized CPU units to enhance the performance for GEMM using Python. Through Numba, we tile and dispatch work to GPUs, vectorized CPU kernels, and CPU threads at runtime. The results show the different contributions of each engine to the overall performance of the system and lays the ground for more efficient partitioning approaches which would lead to better efficiency.

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T-IDR(s): Tensor-Induced Dimension Reduction Methods via the t-Product for High-Order Multilinear Systems

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Abstract

Induced Dimension Reduction (IDR) methods are a class of efficient short-recurrence algorithms, based on the induced dimension reduction theorem and introduced by Sonneveld and Van Gijzen [2], for solving large-scale non-symmetric linear systems. The main idea of these methods is to generate residual vectors that are constrained to lie in a sequence of nested subspaces. In this paper, we extend the IDR theorem to the tensor setting and propose a tensor-based generalization of the IDR(s) methods, denoted T-IDR(s), via the t-product for high-order multilinear systems. Numerical experiments are provided to illustrate the performance of the proposed algorithms.

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Efficient Updating of the Thin QR Factorization

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Abstract

Updating the factors in a QR decomposition after a rank one change is important for problems in optimization or recursive least-squares. Mature algorithms and software exist when updating the full QR. However, for large problems it is much more economic to store and maintain a thin QR. Updating the thin QR typically requires an orthogonal projection and is therefore different from updating the full QR. In this talk we propose a two phased algorithm. In phase one, the update is projected onto the orthonormal complement of Q. In phase two we use a sequence of rotations to restore the upper triangular factor R. We extend the method to rank-k updates and demonstrate its effectiveness on large sparse systems.

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Solution of large-scale inverse problems via preconditioned and constrained $\ell^2 - \ell^q$ with application to geophysics

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Abstract

In many fields of science and engineering we are faced with the solution of large-scale discrete inverse problems. Their solution is sensitive to the presence of noise in the data and they are of the form

$$A\mathbf{x} + \boldsymbol{\eta} = \mathbf{b}^\delta,$$

where $A \in \mathbb{R}^{m\times n}$ is a large severely ill-conditioned matrix, i.e., such that its singular values decrease rapidly to zero with no significant gap between the smallest ones, $\mathbf{b}^\delta \in \mathbb{R}^m$ represents the measured data that are corrupted by some additive noise $\boldsymbol{\eta} \in \mathbb{R}^m$. To compute stable solutions, the original problem is substituted by a well-posed one, whose solution well approximate the desired one. In this talk we consider the constrained $\ell^2 - \ell^q$ minimization

$$\arg\min_{\mathbf{x}\geq 0} \frac{1}{2}\left\|A\mathbf{x} - \mathbf{b}^\delta\right\|_2^2 + \frac{\mu}{q}\left\|L\mathbf{x}\right\|_q^q, \quad \mu > 0,\ 0 < q \leq 2, \tag{1}$$

where, the inequality is meant element-wise, $\|\cdot\|_2$ denotes the Euclidean norm, $L \in \mathbb{R}^{s\times n}$ is the so-called regularization operator, and $\|\mathbf{z}\|_q^q = \sum_{i=1}^n |z_i|^q$. We refer to the latter quantity as ℓ^q-norm, even though, for $q < 1$, it does not satisfy the triangular inequality. In [2] an algorithm for the solution of (1) was presented. In this talk we present a preconditioning strategy for this method stemmed from the seminal idea in [1] and obtained by either considering the Golub-Kahan partial bidiagonalization of A or its randomized SVD; see [4] and references therein.

We test our proposed approach on both image deblurring problems and on an inverse problem in geophysics, namely, the inversion of EM data for the investigation of the subsoil with non-invasive techniques; see [3].

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Voronoi integration of the rendering equation

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Abstract

In photorealistic image rendering, Monte Carlo methods [2] are the foundation for integration of the rendering equation in modern approaches. However, despite their effectiveness, traditional Monte Carlo methods often face challenges in controlling variance, resulting in noisy visual artifacts in some difficult to render regions of the image.

In this work, we propose a new approach to the integration of the rendering equation, introducing a Voronoi tessellation [1] reweighting backed by a Poisson point process sampling strategy to address some of the limitations of standard Monte Carlo methods.

From a theoretical point of view, we show that the variance based on a Poisson-Voronoi tessellation is smaller than that induced by the Monte Carlo method when the intensity of the underlying process is arbitrarily large and the function to be integrated satisfies a Hölder condition.

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A Theoretical Study of a Multi-Scale Hybrid Model for Plant Growth Dynamics

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Abstract

This work presents a theoretical study of a multi-scale hybrid model describing plant growth dynamics. The proposed framework integrates continuous and discrete processes to capture interactions between plant development, environmental conditions, and soil nutrient availability. We analyze the mathematical structure of the model and discuss its theoretical properties, highlighting its relevance for understanding plant growth across multiple spatial and temporal scales.

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Introducing Biplot Functionality in Radial Control Charts

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Abstract

Principal Component Analysis (PCA) is being used extensively in a multitude of disciplines. This is also true for the field of Statistical Process / Quality Control (SPC / SQC). The major benefit of implementing PCA is that it reduces the dimensionality of the parameter space of a process or the attribute space of a product, thereby, greatly facilitating subsequent analysis, since it reveals a reduced set of maximal–variance latent variables, deprived of any correlation. Statistical analysis and assessment using latent variables is very effective. In SPC though, one major post–analysis issue is to be able to trace back the root causes – in terms of the original variables – of an observed anomaly or a shift from the prescribed target values of parameters or attributes. When two major principal components (PC) are chosen for analysis, there exists a graphical representation, namely the Biplot, introduced by Gabriel in 1971, which serves this purpose. Biplots are 2D scatterplots in the plane of the two major PCs that represent simultaneously both entities: observations as points and original variables as concentric vectors, thereby revealing the relations between them. In a recent article, the authors introduced a new graphical tool, based on the Radial Visualization (RV) Star Coordinates (SC), which uses more than two major PCs to project observations on the SC–plane. The new tool, termed Radial Control Chart (RCC), serves as a multi-variate control chart. The present study aims at extending the concept of biplots by introducing biplot functionality to RCCs.

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D-optimal designs embedded in Hadamard matrices

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Abstract

Hadamard matrices have a central role in combinatorial matrix theory and optimal experimental design because they attain the maximal determinant bound for ± 1-matrices of order divisible by four. Closely related are D-optimal designs, which are ± 1-matrices maximizing the determinant and arise in the construction of statistically efficient experimental designs.

In this work we revisit the classical embedding problem, investigating when a D-optimal design D_k can appear as a submatrix of a Hadamard matrix H_n with $n > k$. Using properties of complementary minors of Hadamard matrices together with well established determinant bounds, we derive analytical conditions governing the embeddability of D-optimal designs. In particular, we provide an alternative approach to show that when k and n are multiples of four, a design D_k cannot be embedded in H_n whenever $n < 2k$, while embeddings may occur when $n \geq 2k$. For general orders k, computational criteria based on the determinant spectrum of ± 1-matrices allow the existence or non-existence of embeddings to be determined for several small orders.

We also study the reverse embedding problem. Using the excess property of Hadamard matrices, we extend earlier results and show that H_8 is embedded in D_9 and H_{16} is embedded in D_{17}. Additional analysis suggests structural limitations for larger orders and leads to a conjecture concerning the non-embeddability of H_n in D_{n+1} for $n > 16$. The obtained results clarify structural constraints between Hadamard matrices and maximal determinant designs and provide new insights into the embedding problem.

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The analysis of spherical data. New advancements and open challenges

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Abstract

In signal processing the time-frequency analysis of nonlinear and non-stationary processes, as well as the determination of the unknown number of active sub-signals of a blind-source composite signal are, in general, challenging inverse problem tasks. If we consider data sampled on a sphere, things get even more complicated. This is the reason why just a few techniques have been developed so far to study this kind of data. However, many real-life data are of this nature, like in Geophysics and Physics.

The idea is to extend the Iterative Filtering (IF) algorithm to work on the sphere. IF is a non-stationary signal decomposition method proposed a decade ago [1] to address the problem of extracting time-varying oscillatory components from a non-stationary multicomponent signal. This method proved to be really valuable in many applications, see [2] and references therein, and it was accelerated in what is known as Fast Iterative Filtering (FIF) [3] by leveraging the Toeplitz matrix theory.

In this talk, we introduce the generalization of IF to handle spherical data and show how we can address the question about its convergence [4]. We conclude with some examples of application to geophysical data.

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Infinite families of graphs and stable completion of arbitrary low rank matrices

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Abstract

We study deterministic constructions of graphs for which the stable completion of low rank matrices and tensors is generically possible regardless of the values of the entries. We relate the completability to the presence of some patterns (particular unions of self-avoiding walks) in the subgraph of the lattice graph generated from the support of the bi-adjacency matrix. Such patterns can also be related to the notion of ladder determinantal variety in algebraic geometry. The constructions make it possible to design infinite families of graphs on which exact and stable completion is possible for every fixed rank matrix through the sum-of-squares hierarchy.

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Stable hybrid upwinding VAG scheme for the incompressible diphasic model with discontinuous capillary pressure

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Abstract

The two-phase Darcy flow in porous media is a well known model to describe the evolution of fluids in porous rocks; it is of great interest for engineers and industrials with applications to geothermal energy, oil recovery, gas sequestration, and geological storage. The heterogeneity of natural porous media implies discontinuous spatial variations in physical properties; in particular, we focus on the numerical challenges raised by discontinuous permeability and capillary pressure laws, leading potentially to highly contrasted velocities and highly nonlinear transmission conditions at the interfaces between different rock-types.

In this work [1], we propose an improved discretization, in terms of stability and accuracy, of the one proposed in [2]. We use a Vertex Approximation Gradient method that enables us to avoid mixtures of different rock-types in the same control volume, captures the saturation discontinuities for mesh conforming to the heterogeneities, and such that one can reduce the discrete problem size at the solver stage. The incompressible nature of fluids allows us to express our system as a coupled system composed of a degenerate parabolic equation of conservation for the non-wetting phase and an elliptic pressure equation. We build a hybrid upwinding (more robust than classical phase potential upwinding) taking advantage of the total velocity formulation. Then, we link the discrete total velocity and the discrete global pressure by taking the right saturation at each interface by solving a nonlinear equation. This offers a couple of important mathematical properties. First, it entails the positivity of the discrete saturations. Secondly, one retrieves energy estimates by selecting key approximations of the fluxes. These stability results allow us to prove the existence of solutions to the scheme.

Numerical experiments on complex test-cases show the robustness of the new approach in terms of the accuracy as well as the nonlinear convergence.

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An equilibrated flux a-posteriori-steered error estimate and adaptivity for a high-order conforming discretization of the monodomain problem in cardiac electrophysiology

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Abstract

In this work, we consider the monodomain problem to simulate the electrical activity within the heart tissue. From a mathematical standpoint, it is modeled by a nonlinear parabolic partial differential equation coupled with an ordinary differential equation, whose numerical resolution is often challenging and computationally expensive. We employ the backward Euler scheme for the time discretization and the conforming $\mathbb{P}_p$ finite element method for the spatial discretization. We derive a guaranteed a posteriori error estimate on the error between the exact solution at the continuous level and the approximate solution that is valid at each time step and each iteration of the linearization solver. Our estimate, based on equilibrated flux reconstructions, also distinguishes the spatial and temporal components of the error. The spatial component further consists of the discretization error and the linearization error. At each time step of the simulation, we propose an adaptive version of the Newton algorithm based on stopping the Newton iterations when the estimators of the corresponding error components does not affect significantly the overall estimate. In addition, this adaptive procedure leads to a reduction of the total number of iterations while ensuring the accuracy of the solution. Numerical experiments are presented to demonstrate the effectiveness of the proposed approach.

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Deep Learning Supported Computer Vision for Sea-State Estimation under Dynamic Maritime Conditions

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Abstract

Precise evaluation and forecasting of sea states is crucial for safeguarding navigational safety, reviewing maritime incidents and optimizing energy efficiency in vessels. This study investigates innovative applications of computer vision and deep learning techniques for real-time sea-state recognition, with the aim of enhancing the operational safety and energy efficiency of maritime vessels. While traditional methods rely on moored buoys, maritime radar systems and satellite-based observations, these approaches are often limited by high excessive costs, low spatial resolution, or shadowing effects at low grazing angles. Recent advances in computer vision have demonstrated ship-borne optical cameras and Lidar as viable, high-resolution alternatives. Current state-of-the-art algorithms however frequently struggle with the dynamic motion of the vessel, variable lighting from sun glint and foam, and scale ambiguity due to the lack of fixed references on the open sea. This study proposes an integrated image processing framework that utilizes geometric rectification and advanced image processing algorithms to mitigate platform ego-motion and the other adverse effects present. By the utilization of stereo-vision configurations or temporal analysis of sea-surface texture, this study explores innovations on spatio - temporal image processing techniques to enhance the precision of sea state parameter estimations. These include techniques for geometric correction and stabilization, 3-D FFT, optical flow tracking, Gray-Level Co-occurrence Matrices and the Radon Transform. Deep learning-based semantic segmentation for identifying informative regions in frames. The fusion of measurements and analysis of the heave and pitch motions of a vessel in a seaway, recorded by a smartphone located onboard the ship are also being considered. The findings suggest that such optical sensing systems can provide a robust, non-intrusive solution for autonomous sea-state monitoring in diverse operational conditions. promising robust, calibration-free wave parameter estimation and potential innovations in edge-deployable real-time processing for autonomous maritime operations.

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Multi-level boosting for multimodal kernel learning

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Abstract

Multimodal data analysis has become a challenging problem in many scenarios because it combines several difficulties associated to feature selection, data fusion and dimensional ity. Among machine learning methods, kernel based learning strategies have shown their effectiveness to deal with multi modal data. These approaches are based on the famous kernel trick that allows to capture the non-linear nature of features in complex data set. Typically, kernel-based multimodal fusion methods can be divided into three categories: multi kernel learning based [1], subspace learning based [2] and co-learning based [3].

The method we propose here falls into the first two categories. Precisely, we introduce a novel kernel learning method to extract multiple categories from multimodal information sources. The principle of our algorithm is to build a strong learner from the stratified aggregation of task-specific learners. This network is composed of three levels of learners: the first level combines the output of distinct base kernel learners, the second level aggregates the output recorded by modalities, and lastly, the third level builds the final learner. Learning of network weights is based on an original multi-level extension of the SAMME algorithm [5], a multi-class version of the famous Adaboost algorithm [3]. In this work, the kernel ridge regression model is used as a multiclass base learner. The main contribution of this work is to propose a unique framework to simultaneously solve several key issues in kernel methods such as multiple kernel selection, multimodal data fusion, and scalability. The performance of the proposed algorithm is evaluated on various multimodal data sets from different fields such as multispectral remote sensing and brain activity using EEG recordings.

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The numerical approximation of 2D models for internal waves with spectral methods

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Abstract

The numerical approximation of some asymptotic models for the propagation of internal waves in 2D and under different physical regimes, proposed in [1], is studied. The talk will be focused on the semi-discretization in space of the corresponding periodic initial-value problem for the differential system with Fourier Galerkin methods. Some error estimates will be derived (extending the results obtained in [2] for the one-dimensional case) and numerical experiments will illustrate the performance and applicability of the use of spectral methods for the numerical treatment of these models.

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Preconditioning on blocking structures

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Abstract

The approximation of systems of Ordinary or Partial Differential Equations (ODEs or PDEs), the reconstruction of signals or images with incomplete data, all lead to block structured matrices, where the single blocks have (block) multilevel Toeplitz structure or, when there is no space invariance, a more general form. In fact, when dealing with ODEs and PDEs with variable coefficients, the resulting matrix-sequences belong to one of the (block) multilevel Generalized Locally Toeplitz (GLT) spaces (*-algebras when the blocks are square), with blocks having size that depends on the approximation scheme and on the dimensionality d of the physical domain, while the number of levels is exactly d.

The authors of [1] use the *extradimensional* technique to take advantage of the blocking structure's spectral symbol. However, since the distribution function's zeros and their order provide information about the conditioning as well as the size and type of subspaces where the ill-conditioning occurs [4], we look into appropriate preconditioning techniques for Krylov methods based on the theoretical analysis [2].

During this talk we will focus on the method of constructing such preconditioners and their clustering properties, accompanied by a wide range of numerical experiments showing its effectiveness on practical cases. Moreover, as example, we present the spectral features of the matrix sequences arising from the Taylor-Hood $\mathbb{P}_2$-$\mathbb{P}_1$ approximation of variable viscosity for $2d$ Stokes problem under weak assumptions on the regularity of the diffusion [3].

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Normalized Tensor Train Decomposition

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Abstract

Tensors with unit Frobenius norm are fundamental objects in many fields, including scientific computing and quantum physics, which are able to represent normalized eigenvectors and pure quantum states. While the tensor train decomposition provides a powerful low-rank format for tackling high-dimensional problems, it does not intrinsically enforce the unit-norm constraint. To address this, we introduce the normalized tensor train (NTT) decomposition, which aims to approximate a tensor by unit-norm tensors in tensor train format. The low-rank structure of NTT decomposition not only saves storage and computational cost but also preserves the underlying unit-norm structure. We prove that the set of fixed-rank NTT tensors forms a smooth manifold, and the corresponding Riemannian geometry is derived, paving the way for geometric methods. We propose NTT-based methods for low-rank tensor recovery, high-dimensional eigenvalue problem, estimation of stabilizer rank, and calculation of the minimum output Rényi 2-entropy of quantum channels. Numerical experiments demonstrate the superior efficiency and scalability of the proposed NTT-based methods.

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Variational Density Estimation for Non-Gaussian Distributions with Local Irregularities

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Abstract

Estimating probability density functions from finite samples is a classical problem in statistics, typically addressed by kernel-based or parametric methods under smoothness assumptions. However, in many physical and applied settings, the underlying density exhibits genuine non-smooth features such as sharp interfaces, discontinuities, or locally singular structures arising from censoring, partial observability, or intrinsic physical constraints. In such regimes, standard estimators may introduce severe bias or fail to capture the correct geometry of the distribution. In this work, we investigate a variational framework for non-Gaussian density estimation based on convex regularization, with a particular emphasis on total variation (TV), Sobolev-type, and entropy-based penalties. We formulate the estimation problem as a constrained optimization task on the space of probability densities and solve it efficiently using first-order primal–dual algorithms of Chambolle–Pock type. Through a series of controlled two-dimensional numerical experiments, including synthetic examples inspired by tomographic reconstruction and particle-based data, we systematically compare variational estimators with standard and adaptive kernel density estimation (KDE) techniques. Our results demonstrate that TV regularization provides a robust and geometrically faithful reconstruction of densities with sharp transitions, outperforming both KDE and smooth Sobolev regularization in the presence of true discontinuities. Sobolev and entropy-based methods, while effective for globally smooth densities, tend to oversmooth or smear singular features. Quantitative error metrics and qualitative visualizations support these findings and highlight the trade-offs between smoothness, bias, and structural preservation.

The proposed framework bridges ideas from variational imaging, statistical density estimation, and inverse problems, and offers a flexible and reproducible approach for density reconstruction in non-smooth regimes. We conclude by discussing theoretical perspectives, including consistency and Γ-convergence considerations, as well as extensions to censored data and hybrid regularization models [1, 2].

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A c-Product Tensor Framework for YOLO Enhanced by Golub–Kahan TSVD Compression

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Abstract

Recent advances in tensor linear algebra have highlighted the potential of structure-preserving decompositions to improve the efficiency and stability of deep-learning pipelines. We propose a novel integration of the Golub–Kahan Truncated SVD (TSVD) with c-product–based tensor contractions to enhance the representational compactness and numerical robustness of YOLO-style object detectors. In this framework, convolutional kernels, feature maps, and detection heads are modeled as third- and fourth-order tensors, enabling the Golub–Kahan TSVD to perform stable low-rank approximations that mitigate error amplification typically observed in standard tensor SVDs. The c-product provides a multilinear algebraic backbone for expressing YOLO's convolutional and attention-like operations as structured tensor contractions, allowing TSVD-compressed operators to be seamlessly substituted without altering the computational graph. Experimental analysis suggests that this combination yields significant reductions in parameter count and FLOPs, while preserving gradient stability during training and maintaining competitive detection accuracy. By unifying Golub–Kahan TSVD with c-product tensor calculus, this work introduces a principled pathway for designing numerically stable, low-rank, hardware-efficient variants of real-time object detectors.

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Prediction of Training Time for Perception Models in Autonomous Vehicles

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Abstract

Autonomous vehicles rely on deep learning models to perceive their environment, understand surrounding events, and make safe decisions in real time. These models must be highly accurate and fast, particularly when deployed on embedded systems with limited computing resources. However, training deep learning models is typically time-consuming and resource-intensive, which poses significant challenges for engineers during the development process.

This study investigates the main factors that influence training time, including dataset size and type, model complexity, and hardware capabilities. To address the inefficiencies of trial-and-error experiments, we propose a predictive approach based on regression analysis. Our method uses measurable parameters related to the dataset, the model architecture, and the computing resources to estimate training time before initiating the training process.

Specifically, we collect information such as the number of training samples, image sizes, model depth and number of parameters, and GPU or CPU specifications. By applying a regression model to these parameters, we can predict the expected training time for different configurations. This approach enables engineers to plan experiments more efficiently, compare multiple models, and optimize resource usage, ultimately reducing wasted effort, accelerating development, and supporting the reliable deployment of autonomous vehicle systems.

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Direct–Inverse Chiral Electromagnetic Scattering with Mixed Boundary Conditions: Variational Formulation and MFS

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Abstract

We study time-harmonic electromagnetic scattering in chiral media by impenetrable obstacles with mixed boundary conditions under a two-dimensional anti-plane reduction. The resulting problems are written in a variational form and analyzed in appropriate Sobolev trace spaces. We prove well-posedness of weak solutions. For the numerical approximation, we employ the Method of Fundamental Solutions (MFS), supported by density results for the traces of chiral fundamental solutions in the admissible trace spaces. We further consider the corresponding inverse problem of reconstructing the obstacle from scattering data, establish uniqueness of the reconstruction, and propose an MFS-based algorithm. Representative numerical results for both direct and inverse problems are presented.

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On the Condition Number of Vandermonde Matrices with Mock-Chebyshev Nodes

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Abstract

Polynomial interpolation on a set of distinct nodes, when expressed in the monomial basis, leads to a linear system with a Vandermonde-type coefficient matrix. A well-known drawback of the Vandermonde matrix is its tendency to become severely ill-conditioned when formed from real nodes [1], even for relatively low polynomial degrees. The level of ill-conditioning depends strongly on both the distribution of the interpolation points and the chosen basis. Although highly non-uniform node sets such as Chebyshev (or Chebyshev–Lobatto) points are often advocated to enhance numerical stability, in many applications the available data are restricted to equally spaced sampling locations. Under this constraint, polynomial interpolation may suffer not only from the Runge phenomenon but also from pronounced numerical instability. To address these issues, an effective strategy is to select mock-Chebyshev nodes from a dense set of uniformly spaced points, thereby retaining the favorable interpolation properties of Chebyshev-type distributions [2, 3, 4, 5].

In this study, we investigate the condition number of the Vandermonde matrix and show that mock-Chebyshev nodes provide an improvement comparable to that obtained with Chebyshev–Lobatto nodes. We also examine the conditioning behavior of closely related Chebyshev-type node selections extracted from uniform grids.

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Deflation approach for matrix function calculations based on double exponential-type numerical integral formula

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Abstract

This presentation focuses on integration-type methods [1, 2] that employ the double-exponential (DE) integral formula [3], *DE-type methods*, for computing matrix functions. DE-type methods exhibit high convergence rate thanks to the highly efficient DE integral formula; however, it is known that existence of eigenvalues near a specific region on the complex plane adversely affects the convergence. This presentation proposes a deflation approach that improves the convergence of the DE-type methods by extracting and separating the eigenspaces corresponding to the eigenvalues within such a region. To extract these interior eigenspaces, the proposed approach uses a complex moment-based eigensolver. The components of the matrix function corresponding to the interior eigenspace are directly obtained from the eigenpairs, whereas those corresponding to the exterior eigenspace are computed through the DE-type method with deflation. Error analysis and numerical experiments demonstrate the effectiveness of the proposed approach.

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Linearizing a class of eigenvector-dependent nonlinear eigenvalue problems

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Abstract

Nonlinear eigenvalue problems with eigenvector nonlinearities (NEPv) are algebraic eigenvalue problems whose matrix depends on the eigenvector. Applications range from computational quantum mechanics to machine learning. Due to its nonlinear behavior, existing methods almost exclusively rely on fixed-point iterations, the global convergence properties of which are only understood in specific cases. Recently, a certain class of NEPv with linear rational eigenvector nonlinearities has been exactly linearized, i.e., the spectrum of a linear eigenvalue problem contains the eigenvalues of the NEPv [1]. This linear problem is solved using structure exploiting algorithms to improve both convergence and reliability. We expand on this idea and propose a linearization for a different class of NEPv with quadratic rational nonlinearities, inspired by the discretized Gross-Pitaevskii equation [2]. The eigenvalues of this NEPv form a subset of the spectrum of a linear multiparameter eigenvalue problem which is equivalent to a system of generalized eigenvalue problems expressed in terms of operator determinants. A structure exploiting Arnoldi algorithm is used to filter a large portion of spurious solutions and to accelerate convergence [3].

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Riemannian manifold-based model reduction for large nonlinear dynamical systems

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Abstract

Model order reduction is a key enabler for the efficient simulation, analysis, and control of high-dimensional dynamical systems. Classical linear reduction techniques, such as Proper Orthogonal Decomposition (POD) and balanced truncation, are often inadequate when systems exhibit strong nonlinearities or evolve under intrinsic geometric constraints. In this work, we present a unified framework for model reduction based on Riemannian geometry, which explicitly accounts for the underlying manifold structure of the state space. The proposed approach exploits intrinsic geometric tools, including geodesic distances, tangent spaces, and exponential and logarithm maps, to construct reduced-order models in a coordinate-free and structure-preserving manner. We provide a mathematical formulation of Riemannian Proper Orthogonal Decomposition (R-POD), Riemannian balanced truncation, and Riemannian Krylov subspace methods, and discuss their application to nonlinear dynamical systems evolving on Lie groups, the manifold of symmetric positive definite (SPD) matrices, and other constrained state spaces. Numerical and theoretical considerations demonstrate that geometry-aware reduction techniques offer significant advantages in terms of stability preservation, constraint satisfaction, and physical interpretability when compared with their Euclidean counterparts.

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A Warm-basis Method for Bridging Learning and Iteration: A Case Study in Fluorescence Molecular Tomography

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Abstract

Fluorescence Molecular Tomography (FMT) is a widely used non-invasive optical imaging technology in biomedical research. It usually faces significant accuracy challenges in depth reconstruction, and conventional iterative methods struggle with poor -resolution even with advanced regularization. Supervised learning approaches can improve recovery accuracy but rely on large, high-quality paired training dataset that is often impractical to acquire in practice. This naturally raises the question of how learning-based approaches can be effectively combined with iterative schemes to yield more accurate and stable algorithms. In this work, we present a novel warm-basis iterative projection method (WB-IPM) and establish its theoretical underpinnings. The method is able to achieve significantly more accurate reconstructions than the learning-based and iterative-based methods. In addition, it allows a weaker loss function depending solely on the directional component of the difference between ground truth and neural network output, thereby substantially reducing the training effort. These features are justified by our error analysis as well as simulated and real-data experiments.

Accurate Computations with Totally Nonnegative Matrices of Any Rank

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Abstract

We will present new algorithms for performing virtually all computations with totally nonnegative matrices to high relative accuracy regardless of whether the matrix is singular generalizing the results of [3] for nonsingular totally nonnegative matrices.

The algorithms achieve high relative accuracy by completetely avoiding substractions and thus preserving the high relative accuracy. The matrix computations include the inverse, the eigenvalues, the SVD [2], the Schur complement, a submatrix, as well as any minor.

The new algorithms also include for the first time the computation of the singular vectors to high relative accuracy. It also completes computations in the nonsingular case, such as submatrices (and the properties thereof) which can be singular even when the initial matrix isn't.

Joint work with J. Delgado, A. Marco, J.M. Peña, J.J. Martines, R. Viaña.

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Minisymposium:
SafeRSM: Safety-Aware AI-Guided Experimental Design for Food Engineering with Robust Surrogates and Conformal Prediction

Organizer: SPhears AI

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Abstract: AI-driven experimental design promises to accelerate discovery in science and engineering by intelligently selecting experiments. However, in high-stakes applications, proposed experiments must satisfy safety or feasibility constraints with high confidence.

We present SafeRSM, a safety-aware framework for sequential experimental design that combines robust optimization principles with conformal prediction to ensure reliable performance. SafeRSM uses machine-learning surrogate models to predict experimental outcomes and incorporates domain knowledge via physics/chemistry-informed neural networks. To enforce safety, we calibrate the surrogate's uncertainty using conformal prediction, yielding distribution-free prediction intervals that guarantee a specified confidence level. We then formulate experiment selection as a robust optimization problem: at each iteration, SafeRSM chooses the experiment that maximizes the surrogate's predicted outcome under worst-case prediction error while satisfying safety constraints with high probability.

We derive theoretical bounds showing that, given mild assumptions (exchangeable data), SafeRSM will select only experiments that satisfy safety constraints with provable probability. We demonstrate SafeRSM on both synthetic benchmarks and a protein design case study involving safe optimization of biochemical reaction conditions. In experiments, SafeRSM achieves competitive objective values while incurring zero safety violations, outperforming baseline methods in terms of reliability and data efficiency.

Our results highlight that integrating conformal uncertainty quantification with robust optimization yields a principled and effective strategy for reliable, high-stakes experimental design. Ultimately, SafeRSM provides a mathematically grounded pathway to safely accelerate scientific discovery and process optimization in food engineering and other critical domains.

Speakers:

- **Kyritsis Georgios, Paraskevas Spyridon**
  SafeRSM: Safety-Aware AI-Guided Experimental Design for Food Engineering

Finite volume scheme for the Richards equation with different rock types on polygonal meshes

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Abstract

Drinking water reserves are steadily diminishing worldwide due to climate change, salinization, and overexploitation. Modeling and numerical simulation make it possible to predict subsurface contamination and monitor groundwater levels. In this study, we focus on the Richards equation which governs unsaturated flow in porous media due to the action of capillarity and gravity. In realistic subsurface environments, this equation must be solved in media where sharp discontinuities in hydro-geological properties arise at the interfaces between different rock types. These discontinuities introduce modeling and approximation challenges such as ensuring flux conservation at interfaces or reduced regularity of the solution. While previous studies have addressed the case of orthogonal meshes [1], such meshes cannot capture complex geometries, and existing methods face limitations in robustness, higher-order accuracy and computational cost [2]. The Discrete Duality Finite Volume method (DDFV) offers an interesting alternative by handling general polygonal meshes (that do not necessarily verify the orthogonality condition required by finite volume meshes) [3] and ensuring local conservation of fluxes. Modeling the Richards equation in heterogeneous hydrosystems requires a discretization that accounts for the multi-scale nature of the problem and an appropriate interface treatment while keeping a reasonable number of unknowns for the computational cost. This study explores the DDFV formulation combined with interface treatments to handle these discontinuities through several test cases. It also aims to develop a robust solver that achieves a better accuracy. This of great importance in applications such as groundwater management.

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AI-Enhanced Nano-Robotic On-Wafer Probe Station: YOLOv11 OBB-Based Detection of RF Calibration Standards

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Abstract

On-wafer RF characterization of high-frequency devices is often limited by manual probe station operation, leading to variability in alignment, reduced reproducibility, and limited throughput [1, 2]. In this work, we present a fully automated nano-robotic probe station in which probe positioning is driven by a vision-based deep learning detection system [3].

Platform. The station relies on SmarAct® piezoelectric nano-positioners providing 11 degrees of freedom across probe arms and chuck, with closed-loop position sensors ensuring sub-nanometer resolution. The full probing sequence – image acquisition, positioner commands and VNA data acquisition – is executed autonomously under LabVIEW®, using a FormFactor® ISS 101-190-C substrate as the calibration reference.

Detection model. A YOLOv11 Oriented Bounding Box (OBB) model is used to detect and classify calibration standards and probe states directly from 1920×1080 microscope frames. The model is trained on approximately 19 000 manually annotated images, augmented to around 90 000 samples to improve robustness to geometric variations. Ten object classes are defined: four calibration standards (OPEN, THRU, LOAD, SHORT), each represented by a center and a side crop annotation, and two probe state classes (PROBE_UP, PROBE_DOWN). The OBB formulation provides orientation-aware localization, which is particularly relevant when calibration structures appear at arbitrary angles in the field of view. Detection outputs are used directly to command the nano-positioners, enabling autonomous execution of probing sequences.

Validation. Experimental results demonstrate reliable detection performance and successful closed-loop positioning during automated probing sequences. Ongoing work focuses on quantifying positioning accuracy and repeatability, and on evaluating the impact on RF measurement performance across a wider range of calibration standards and operating conditions.

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Fast Iterative Algorithms for the Quaternion Moore-Penrose Pseudoinverse

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Abstract

The Moore-Penrose pseudoinverse is a key tool for least-squares problems, inverse problems, and low-rank approximations. When data are naturally represented by quaternions, for example in multi-channel or geometric signals, computing a quaternion pseudoinverse can become a major bottleneck. QSVD-based methods are robust but expensive, and embedding quaternion matrices into real or complex form often increases the computational cost and obscures structure.

In this talk, we present recent work on quaternion-native, decomposition-free iterative methods for computing the Moore-Penrose pseudoinverse. The algorithms are developed and analyzed directly over $\mathbb{H}$, with no real/complex embeddings. Our main focus is a damped Newton-Schulz iteration that handles noncommutativity and rectangular matrices, together with a simple spectral scaling that guarantees convergence. We also discuss faster local variants using higher-order (hyperpower) updates, as well as practical factorizations that reduce per-iteration cost. Beyond Newton-Schulz, we briefly introduce two complementary approaches: a randomized sketch-and-project method (including a hybrid global-then-local strategy), and a matrix-form conjugate-gradient method based on the normal equations.

We conclude with numerical results on synthetic benchmarks and three case studies, CUR image/video completion, Lorenz filtering, and FFT-based deblurring. The experiments show that the Newton-Schulz family can achieve excellent accuracy with competitive computational cost. The implementations are available in QuatIca (PyPI: https://pypi.org/project/quatica/;
source: https://github.com/vleplat/QuatIca), a new open-source Python library for quaternion numerical linear algebra.

A Fast Direct Solver for Nonuniform Discrete Fourier Transform of Type 3

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Abstract

Nonuniform discrete Fourier transform (NUDFT) and its inverse are widely used in various fields of scientific computing. In this talk, we introduce a novel fast direct inversion method for type 3 NUDFT. The proposed method approximates the type 3 NUDFT matrix as a product of a type 2 NUDFT matrix and an HSS matrix, where the type 2 NUDFT matrix is further decomposed as the product of an HSS matrix and uniform DFT matrix. Based on the decomposition of the type 3 NUDFT matrix, both matrix forward application and backward inversion could be accomplished in quasi-linear complexity. Our fast backward inversion can serve as a fast direct solver or as an efficient preconditioner. Additionally, we provide an error bound for the approximation under specific sample distributions. Numerical results are presented to verify the relevant theoretical properties and demonstrate the efficiency of the proposed methods.

Low cost estimations of matrix inverses

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Abstract

Let A be a symmetric positive definite matrix. We address the problem of efficiently approximating the diagonal entries of its inverse A^{-1} without explicitly computing the inverse. To this end, we develop a heuristic approach that exploits structural properties of the matrix to produce accurate and computationally efficient estimates.

The proposed method is based on proximity-based quadratic form estimators and avoids the need for full matrix inversion by relying only on matrix-vector products and inner products. As a result, the computational complexity is reduced from cubic to quadratic, making the approach suitable for large-scale problems. We provide a theoretical analysis of the method, including error bounds and a backward stability analysis, demonstrating that the approximation remains reliable even in moderately ill-conditioned settings.

Extensive numerical experiments on various classes of symmetric positive definite matrices, including structured matrices, covariance matrices, and randomly generated systems, confirm the accuracy, robustness, and significant computational gains of the proposed approach compared to classical inversion techniques. Furthermore, we highlight the practical relevance of the method in statistical inference, particularly in the computation of F-statistics in linear regression, where only the diagonal elements of the inverse matrix are required.

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Spectral analysis and approximation of Quaternion Toeplitz matrix sequences with numerical applications

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Abstract

Many discretizations of inverse problems or integro-differential equations yield linear systems whose matrices have structured forms (common examples are Toeplitz matrices, their variable coefficient or blocks generalizations, or perturbations of them). Further, in several physical or signal-processing applications, particularly multi-channel problems, quaternion-valued matrices naturally model the corresponding discretized linear inverse problems. This is appealing for modeling and computation, but it introduces two well-known difficulties: quaternions are noncommutative, and, due to this property, left and right spectra don't coincide. Even for Hermitian matrices, the spectral properties of structured quaternionic matrices generally differ from those of their complex counterparts. A first analysis of unilevel Hermitian scalar Toeplitz matrices bounded in the spectral norm is done in [2], which includes an analysis of the preconditioned conjugate gradient method with Strang preconditioners.

In this talk, we present general frameworks that overcome these problems for the asymptotic spectral analysis of quaternion block multilevel Toeplitz sequences, and can be used as tools for the design and analysis of preconditioners. Indeed, we construct complex matrix-valued symbols that provide the Weyl-type singular value and eigenvalue distributions for quaternion block Toeplitz sequences, along with a quaternion notion of approximating classes of sequences. The two methods provide criteria and tools for constructing fast preconditioners that significantly reduce Krylov iterations count for quaternion linear systems. As an example, we present the structure and preconditioning criteria of preconditioners arising from quaternion trigonometric matrix algebras. We also discuss future directions, including extensions to quaternion GLT algebras and other open problems in approximation and spectral analysis of quaternion Toeplitz structures.

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Rational Approximations in Nonoverlapping Domain Decomposition Preconditioning

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Abstract

Domain decomposition methods are powerful tools in large-scale scientific computing. Nonoverlapping preconditioning, in particular, has a long record of success. The key novelty of this work is replacing local fractional-order approximations of the Schur complement with a global approach.

We consider the elliptic boundary value problem $\mathcal{L}\mathbf{u} = \mathbf{f}$ in a three-dimensional domain $\Omega \subset \mathbb{R}^3$, discretized by the finite element method (FEM) on an unstructured tetrahedral mesh $\mathcal{T}_h$. The resulting linear system $\mathbb{A}\mathbf{u} = \mathbf{f}$ is large-scale, sparse, symmetric, and positive definite, with an unstructured stiffness matrix $\mathbb{A}$. To efficiently solve this system, we investigate a nonoverlapping domain decomposition (DD) preconditioner based on a graph partitioning of the computational domain, $\Omega = \cup_{i=1}^{p} \Omega_i$, obtained using general-purpose partitioning algorithm.

The preconditioner is derived from a block factorization of $\mathbb{A}$, where the blocks correspond to degrees of freedom internal to the subdomains Ω_i and to those located on the interface γ. The subdomain problems are independent and can be solved in parallel, while the interface problem involves the associated Schur complement. The subdomain problems are independent and can be solved in parallel. Its inverse is approximated using a best uniform rational approximation (BURA) of order k to $\Lambda^{-1/2}$, where Λ denotes the discrete Laplace-Beltrami operator on the interface.

We prove that the proposed preconditioner delivers optimal convergence:the condition number remains uniformly bounded, independently of the mesh size and the number of subdomains. These results significantly extend our earlier work on structured two-dimensional meshes [3] to the three-dimensional, unstructured setting. Further theoretical background on BURA methods and their application to preconditioning can be found in [2] and [1], respectively.

Numerical experiments on sequences of nested meshes, with both fixed and varying graph-based partitions generated by PARMETIS, confirm the theoretical optimality. We also study the influence of the BURA order and the accuracy of the subdomain solvers on the overall efficiency and robustness of the preconditioned iterative method.

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Robust inner-outer Krylov solvers with deflated restarting for linearized analyses of turbulent compressible flows

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Abstract

Many applications in Computational Fluid Dynamics (CFD) require the solution of real, large, sparse, non-symmetric, and ill-conditioned linear systems. Main areas concern gradient-based optimization, linear stability analysis, data assimilation, or fixed-point iterations. Robust and efficient parallel strategies are of main concern to cope with the resulting matrices whose size can grow up to millions and number of non-zero elements to billions. Not only must they be able to deliver solutions within a prescribed error tolerance if required but also to perform it in an affordable time on hundreds of computing cores.

In this talk, we propose robust hybrid direct-iterative approaches based on several numerical ingredients: flexible inner-outer Krylov methods with Krylov subspace recycling [1], Restricted Additive Schwarz preconditioner [2] applied on MPI partitions extended by one level of overlapping, fast approximate direct solvers per extended partitions [3, 4], and mixed precision algorithms to exploit benefits of single precision arithmetic for the resulting global preconditioning operator [5]. Such approaches are then evaluated on large complex problems issuing from the analysis of 2D and 3D turbulent transonic flows with RANS modelling and high-order approximation within the discontinuous Galerkin ONERA CFD solver *Aghora* [6]. More specifically, we focus on accurate solutions of linear systems arising from stiff adjoint-based aerodynamic shape optimization problems to assess the potential of the proposed approaches.

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The Long-Run Behavior of Stochastic Gradient Descent: A Large Deviations Analysis

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Abstract

Even though it's been around for more than 70 years, stochastic gradient descent (SGD) remains the go-to method for solving large-scale non-convex optimization problems and training deep learning models and networks. However, we know surprisingly little about the algorithm's long-run behavior—for example, which local minimizers are more likely to be observed in the long run (and by how much)?

In this talk, we examine the long-run distribution of SGD in general, non-convex problems using an approach based on the theory of large deviations and randomly perturbed dynamical systems, we show that the long-run distribution of SGD resembles the Boltzmann-Gibbs distribution of equilibrium thermodynamics with temperature equal to the method's step-size, and energy levels determined by the problem's objective and the statistics of the noise. In particular, we show that, in the long run, (a) the problem's critical region is visited exponentially more often than any non-critical region; (b) the iterates of SGD are exponentially concentrated around the problem's minimum energy state (which does not always coincide with the global minimum of the objective); (c) all other connected components of critical points are visited with frequency that is exponentially proportional to their energy level; and, finally (d) any component of local maximizers or saddle points is "dominated" by a component of local minimizers which is visited exponentially more often.

In addition, we also examine the time it takes for SGD to reach the global minimum of a general, non-convex loss function. To that end, we provide a tight characterization of the global convergence time of SGD via matching upper and lower bounds which are dominated by the most "costly" set of obstacles that the algorithm may need to overcome to reach a global minimizer from a given initialization, coupling in this way the global geometry of the underlying loss landscape with the statistics of the noise entering the process. Finally, motivated by applications to the training of deep neural networks, we also provide a series of refinements and extensions of our analysis for loss functions with shallow local minima.

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Energy-Preserving Finite Volume Discretizations for a Thermo-Hydro-Mechanical Model

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Abstract

The storage of hydrogen, produced via water electrolysis, in cementitious cavities offers a solution to the overproduction of electricity from wind farms. However, hydrogen infiltration into the materials could lead to chemical degradation, structural damage, loss of mechanical strength, and possibly an increased leak risk. It is necessary to predict and prevent these issues to ensure safe and efficient storage.

This work aims to propose a Thermo-Hydro-Mechanical model that describes a non-isothermal, compressible gas flow in a porous medium characterized by small deformations and porosity variations. Linear isotropic thermo-poroelastic constitutive laws are considered for the solid skeleton, assuming small temperature variations around a reference temperature, and thermal equilibrium is assumed between the fluid and the skeleton. This model consists of a system of nonlinear PDEs representing the conservation of fluid mass, the conservation of entropy under reversible mechanical deformations, and the momentum conservation equation.

First, we derive energy estimates for the compressible flow to obtain a control over the solution under certain assumptions. Next, we focus on the numerical analysis by discretizing our model using an implicit Euler scheme for the time discretization and a two-point flux approximation (TPFA) scheme for the space discretization. A particular attention is given to the definition of the discrete density at cell interfaces, which is crucial for ensuring that the energy estimates are well-preserved at the discrete level. Finally, we present some numerical experiments to show the strength of the proposed approach.

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Long-Time Behavior of Solutions for the Higher-Order Benjamin-Ono Equation

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Abstract

In this talk, we focus on the nonlocal higher-order Benjamin-Ono equation proposed by Craig, Guyenne, and Kalisch in [1]. We prove the existence and non-existence of solitary wave solutions to the nonlocal higher-order Benjamin-Ono equation. We generate solitary wave solutions by using a Petviashvili's iteration method. An efficient and accurate Fourier spectral method is proposed to investigate the long-time dynamics of solitary wave solutions.

This study is supported by Scientific and Technological Research Council of Türkiye (TUBITAK) under the Grant Number MFAG-124F363.

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Algorithmic methods for optimising experiments

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Abstract

Finding the best experimental design is computationally difficult, particularly in high-dimensional spaces or multi-objective problems. Real-world applications frequently involve competing design criteria that must be reconciled. Other experimental designs may include functional factors. Examples can be found in the fields of chemistry, engineering, the environment, the pharmaceutical industry, and more. Algorithmic tools that strike a balance between computing speed and efficiency will be presented.

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High-resolution positivity-preserving vertex-centered finite volume scheme for degenerate anisotropic convection-diffusion equations

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Abstract

In this study, we introduce an advanced control volume finite element (CVFE) scheme specifically designed for nonlinear convection-diffusion problems characterized by anisotropic and potentially degenerate diffusion operators. The formulation utilizes vertex unknowns and skillfully handles the complex and heterogeneous diffusion tensors. To address the challenge of maintaining solution positivity, the scheme incorporates a nonlinear correction that mitigates the anti-diffusive flux components without expanding the stencil. This adjustment ensures that the discrete solution remains within physical bounds and supports energy stability. For the convective term, a second-order spatial reconstruction is performed using a median dual-edge-based gradient, and a Barth-Jespersen-type flux limiter is applied to control spurious oscillations near discontinuities. The method demonstrates robustness and accuracy across various test configurations, with numerical results confirming its ability to preserve key qualitative properties while enhancing the standard CVFE approach.

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Learning Incomplete Factorization Preconditioners for GMRES

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Abstract

Incomplete LU factorizations of sparse matrices are widely used as preconditioners in Krylov subspace methods to speed up solving linear systems. Unfortunately, computing the preconditioner itself can be time-consuming and sensitive to hyper-parameters. Instead, we replace the hand-engineered algorithm with a graph neural network that is trained to approximate the matrix factorization directly. To apply the output of the neural network as a preconditioner, we propose an output activation function that guarantees that the predicted factorization is invertible. Further, applying a graph neural network architecture allows us to ensure that the output itself is sparse which is desirable from a computational standpoint. We theoretically analyze and empirically evaluate different loss functions to train the learned preconditioners and show their effectiveness in decreasing the number of GMRES iterations and improving the spectral properties on synthetic data.

Personalized Generative Adversarial Networks using Generator-Side Quantum Clustering for recommender systems

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Abstract

Generative adversarial networks (GANs) have been extensively studied in recommender systems for data augmentation , but existing models are often unable to capture the multimodal and overlapping structure of user preferences, which leads to limited diversity and mode collapse. To address this issue, clustering-aware GANs have been proposed, including mixture-based generators , clustering regularization in the latent space, and ClusterGAN-type architectures , which introduce explicit modal structure into classical latent spaces. Related approaches also mitigate mode collapse through regularization strategies. On the other hand, quantum generative adversarial networks have been proposed, focusing mainly on quantum generators, quantum discriminators, or distance-based objectives. However, using quantum clustering as an organizer of the latent space within a classical GAN generator has not been explored. In this work, we propose a classical–quantum hybrid GAN framework that integrates a quantum clustering subroutine into the generator to structure latent representations using quantum fidelity-based similarity. This architecture introduces prototypes to guide the generator, encouraging it to focus on different data modes and reducing mode collapse, while maintaining training stability. The proposed approach is evaluated on recommender systems using the MovieLens dataset , generating synthetic user preference profiles derived from explicit ratings. Experimental results demonstrate improved diversity, enhanced coverage of user preference modes, and improved recommendation performance compared to conventional GAN and clustering-based GAN benchmarks, highlighting the practical potential of quantum clustering for recommender system data generation .

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Logarithmic Convexity and impulse Approximate Controllability for Degenerate Parabolic Equations with Robin Boundary Conditions

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Abstract

Impulsive systems are a class of dynamical systems that experience sudden changes at specific moments in time. In this work, we investigate the approximate controllability of a class of one-dimensional degenerate parabolic equations with Robin boundary conditions. The degeneracy occurs at one endpoint of the spatial domain, and we apply an impulsive control in a small region at a fixed moment. Our main result establishes an observability inequality for the adjoint system, from which we deduce approximate controllability at final time . The proof relies on a logarithmic convexity argument, developed through a Carleman commutator approach.

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A Provably-Correct and Robust Convex Model for Smooth Separable NMF

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Abstract

Nonnegative matrix factorization (NMF) is a linear dimensionality reduction technique for nonnegative data, with applications such as hyperspectral unmixing and topic modeling. NMF is a difficult problem in general (NP-hard), and its solutions are typically not unique. To address these two issues, additional constraints or assumptions are often used. In particular, separability assumes that the basis vectors in the NMF are equal to some columns of the input matrix. In that case, the problem is referred to as separable NMF (SNMF) and can be solved in polynomial-time with robustness guarantees, while identifying a unique solution. However, in real-world scenarios, due to noise or variability, multiple data points may lie near the basis vectors, which SNMF does not leverage. In this work, we rely on the smooth separability assumption, which assumes that each basis vector is close to multiple data points. We explore the properties of the corresponding problem, referred to as smooth SNMF (SSNMF), and examine how it relates to SNMF and orthogonal NMF. We then propose a convex model for SSNMF and show that it provably recovers the sought-after factors, even in the presence of noise. We finally adapt an existing fast gradient method to solve this convex model for SSNMF, and show that it compares favorably with state-of-the-art methods on both synthetic and hyperspectral datasets.

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Randomized Sketching for Tucker Tensors: From Compressed Summation to GMRES

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Abstract

Tensor equations of the form $\mathcal{L}(X) = B$, with $\mathcal{L}$ a sum of Kronecker products, arise across scientific computing, from high-dimensional PDEs to large-scale inverse problems. When the tensor order is moderate but mode sizes are very large, the Tucker format is an attractive choice, yet using it inside iterative solvers is notoriously hard, as operator applications, orthogonalization, and linear combinations all trigger rank growth and force expensive truncations of large intermediate tensors.

In this talk, I will present a line of work that addresses these bottlenecks through randomized sketching applied directly to Tucker factors. The first part introduces sketching-based methods for Tucker tensor summation [1] that exploit the structure of Khatri–Rao and Kronecker products to perform compressed arithmetic without ever forming dense intermediates. Building on this foundation, the second part develops a randomized Tucker-sketched GMRES solver [2] in two variants: a robust method based on the randomized HOSVD with adaptive accuracy control, and a faster one built on the multilinear Nyström approximation, which at the price of a prescribed maximal rank accelerates orthogonalization, avoids storing the Krylov basis, and assembles the solution at negligible cost. Numerical experiments on image deblurring, a parameter-dependent elliptic problem, a transport equation, and a convection–diffusion problem illustrate the efficiency and robustness of the framework.

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Enriching Krylov Subspaces for General Form Linear Least-Squares Problems

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Abstract

In this talk, we present a projection-based method for computing solutions to large scale linear least-squares problems $\min_{\mathbf{x}} \|A\mathbf{x} - \mathbf{b}\|$. To ensure physically meaningful solutions, a priori information is incorporated into the formulation through a regularization matrix L, leading to the constrained problem

$$\begin{cases} \min\limits_{\mathbf{x}} \|L\mathbf{x}\|^2 \\ \mathbf{x} \in \left\{ \arg\min\limits_{\mathbf{x}} \|A\mathbf{x} - \mathbf{b}\|^2 \right\}. \end{cases}$$

Standard Krylov subspaces generated by projection methods depend on the right-hand side $\mathbf{b}$ and on the matrix A (and on A^T, in some occasion), but they do not reflect the influence of the regularization matrix L. For many relevant choices of L, the null space $\mathcal{N}(L)$ is nontrivial, and it is therefore desirable for the solution subspace to include this null space. We investigate some strategies for enriching the Krylov subspace generated by the Arnoldi partial decomposition of A with starting vector $\mathbf{b}$, by incorporating a basis of $\mathcal{N}(L)$ in the Krylov subspace. Numerical experiments are presented to illustrate the effectiveness and performance of the proposed approaches.

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Cloud implementation for parallel solution of discretized and linearized complementary problems

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Abstract

The presented talk deals with the parallel solution of stationary complementary problems. Such problems occur particularly on one hand for the discretized and linearized Hamilton-Jacobi-Bellman equations (H.J.B.) modeling numerous applications in stochastic control, management, economics, mechanics, and optics [1] and on the other hand for the discretized obstacle problem that arises, for example, in the study of the electroplastic torsion of a cylindrical bar with a simply connected cross-section and also in economics and mechanics (see for example [2]). These two previous problems are formulated by using the three-dimensional convection - diffusion operator.

In particular the obstacle problem can be formulated by various ways like the solution of variational inequation or like a multivalued formulation [3] and also by a complementary formulation. In the present presentation, we consider only the latter formulation, which in fact, models the projection on the convex set modeling the constraints to which the solution is subject, and we refer to [3] for a performance study on cloud architecture in the case of a multivalued formulation.

For the two types of problems considered, i.e. the discretized and linearized H.J.B. and obstacle problems, appropriate discretization schemes are considered for the numerical solution on decentralized memory machines by using parallel synchronous and asynchronous Schwarz alternating algorithms. In the considered applications the discretization matrices are either strongly, either irreducible diagonal dominant. Consequently for the H.J.B. problem the matrix of the algebraic linear system resulting from the Newton like linearization is also irreducible diagonal dominant. Concerning the obstacle problem, this property of irreducibility is not preserved since the linearization matrix is reducible; then in this latter case the discretization matrix modeling the obstacle problem must be strongly diagonal dominant which is verified in financial problems classically modeled by evolution problems. Then these assumptions ensure the convergence of the parallel synchronous or asynchronous Schwarz alternating methods for the solution of the linearized problems. Finally the results of parallel simulations performed on clusters and cloud architectures will be presented.

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A preconditioned majorization-minimization method for ℓ^p-ℓ^q regularization

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Abstract

Many inverse problems can be formulated as the minimization of a functional that balances a data fidelity term with a sparsity-promoting regularization term, leading to ℓ^p–ℓ^q minimization problems. For large-scale applications such as image deblurring and computerized tomography, Majorization–Minimization (MM) methods combined with Generalized Krylov Subspace (GKS) techniques provide an effective computational framework. However, their performance may be limited by slow convergence and growing subspace dimensions.

In this talk, we present a preconditioning strategy for the MM-GKS method designed to accelerate convergence while preserving the quality of the reconstructed solutions. The construction of the preconditioner is shown to be compatible with different quadratic majorants within the MM framework. This flexibility allows, in particular, the use of different criteria for automatic selection of the regularization parameter, such as generalized cross-validation (GCV) and discrepancy principle (DP).

Numerical experiments in image deblurring and computerized tomography illustrate that the proposed preconditioning strategies significantly reduce computational cost without degrading reconstruction accuracy.

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Numerical integration of the fractional nonlinear Schrödinger equation with a high order method

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Abstract

In this work we will integrate numerically the fractional nonlinear Schrödinger equation with the aim of studying the dynamics of solitary wave solutions. The numerical scheme used to perform this study is based on applying the mehod of lines to the periodic initial value problem. A Fourier spectral method will be considered for the discretization in space and a fourth-order Runge-Kutta of composition type as time integrator.

Similarity-Based Cross-Project Software Defect Prediction Using Vector Databases

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Abstract

Cross-project defect prediction (CPDP) at software class level remains a critical challenge in improving software quality while maintaining lower testing costs. Traditional machine learning approaches rely on supervised models trained on historical software metrics, yet they often struggle to generalize across different software projects, since not all projects share the same statistical characteristics. In this paper, we investigate an alternative approach inspired by retrieval-augmented generation (RAG) systems, using vector databases to perform similarity-based CPDP for software classes.

We propose a framework in which each software class is represented as an embedding obtained using UniXcoder by Microsoft. Each project is stored as a separate collection in a vector database (Qdrant), containing the embedding vectors of its software classes. Given a target class, the vector database is queried to retrieve similar classes from relevant source project collections. The retrieved embeddings combined with software static metrics are then used to estimate the defect-proneness of the target software class and to rank classes for testing prioritization.

Experiments are conducted on the 5 Java projects from the PROMISE dataset, which provides labeled defect data for multiple software projects. The proposed retrieval-based framework is compared against naive predictors such as random and majority-Class predictors requiring no-learning, metrics only K-nearest neighbor (kNN), and CPDP models utilizing Logistic Regression (LR), XGBoost classifier, and Random Forest (RF). Our results demonstrate that the proposed framework consistently outperforms classical supervised models when used in software CPDP, particularly in maintaining good Precision@ and Recall@ at multiple stages.

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On block Krylov and matrix polynomials

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Abstract

The deep connection between Krylov methods, scalar orthogonal polynomials, and moment matrices is well established, particularly for Hermitian and unitary matrices. In this talk, we extend this framework to block Krylov methods and orthogonal matrix polynomials.

By representing the elements of a block Krylov subspace via matrix polynomials, we consider the matrix-valued inner product introduced in [1], which, under a non-degeneracy assumption, defines a linear isometry. This establishes a one-to-one correspondence between orthonormal matrix polynomials and orthonormal bases of the block Krylov subspace.

For normal matrices, the block Gauss discretization [1, 2] of such an inner product admits an integral representation familiar from the theory of orthogonal matrix polynomials. As an application, we extend a Szegő-type short recurrence, originally developed for matrix polynomials on the unit circle [3], to the block Arnoldi algorithm applied to unitary matrices.

Finally, we analyze the structure of the block moment matrix and explore its connection to orthogonal matrix polynomials and recurrence coefficients via a Cholesky-like factorization.

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Restarted Lanczos methods for the Linear Response eigenvalue problem

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Abstract

The Linear Response Eigenvalue Problem (LREP) is defined as

$$Hz = \lambda z, \qquad \text{with} \quad H = \begin{bmatrix} A & B \\ -B & -A \end{bmatrix}, \tag{1}$$

where A and B are $n \times n$ real symmetric matrices such that $\left[\begin{smallmatrix} I & 0 \\ 0 & -I \end{smallmatrix}\right] H$ is positive definite. This problem is very relevant in computational quantum chemistry and physics, for instance to study the absorption spectra of molecules or solids. It can be seen as a particular case of the more general Bethe-Salpeter eigenproblem (BSE), where A and B are complex.

In recent years, significant progress has been made in the numerical solution of the LREP, see the survey [1]. We are interested in Lanczos-type methods. In particular, we consider the methods proposed by Teng and Li [2] and Zhong and Xu [3], which rely on Lanczos tridiagonalization and bidiagonalization, respectively. Our goal is to provide robust and efficient solvers in the SLEPc library [4], and one of the key ingredients for this is to design effective restarting strategies.

It turns out that the two mentioned methods resemble the first two methods for the BSE that we have analyzed in [5]. We adapt the restarting methods and explore the equivalence between the LREP and BSE cases.

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Piecewise quadratic optimization of risk linked to innovative products

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Abstract

We consider the marketing of innovative products and the associated risk. The decision variables are four vector quantities. These are the quantities of innovative and non-innovative products sold, and the respective prices of these products. These are chosen at the beginning of the period. We hereby introduce two random vectors, with components representing the quantities of innovative or non-innovative products left on the market. In that case, the risk is piecewise quadratic with respect to prices and quantities. This is due to the construction of the products chosen for sale, which depends on all previous quantities. It also involves the traditional ReLU σ function. We then proceed to examine the structure of the Jacobian matrix of the risk, which is highly dependent on correlations between the products. The objective is optimised by introducing signatures of the arrangements of hyperplanes that underlie the risk. The combinatorics of this problem are addressed through a learning process, as opposed to an exhaustive search of optimal signatures. The walk in the combinatorial set of signatures may be considered as Markovian. However, we have opted for a deterministic approach to allow minor alterations of signatures measured through ℓ^1 distances.

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Bound-preserving finite scheme in a porous media flow problem

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Abstract

We present a finite numerical scheme for porous media flow that rigorously preserves physical bounds on saturation and pressure. The method is designed to prevent nonphysical overshoots and undershoots that commonly arise in standard discretizations. By combining appropriate flux approximations with a bound-preserving mechanism, the scheme ensures stability and robustness for strongly nonlinear flow regimes. We establish discrete maximum principles for both saturation and pressure without constraint mesh and time conditions. Numerical experiments demonstrate the effectiveness of the approach on typical porous media flow problems, including heterogeneous and degenerate cases. The results confirm that the proposed scheme maintains accuracy while enforcing essential physical constraints. This makes it particularly suitable for reliable simulations of multiphase flow in porous media.

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On structure-preserving reduction to Hessenberg-like form of a Hamiltonian matrix

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Abstract

The reduction of a Hamiltonian matrix to a condensed Hessenberg-like form, is needed for designing structure preserving methods for computing eigenpairs of such matrix.
To preserve the original Hamiltonian's structure, the reduction is usually handled via symplectic similarity transformations. JHESS and its variant JHMSH algorithms are the main algorithms used for such reduction. The later is involved in the SR-algorithm (which is a QR-like algorithm), structure-preserving, for computing eigenpairs of a Hamiltonian matrix.

Fatal breakdowns or near-breakdowns may be encountered in these algorithms, causing brutal stops of the computations or producing serious numerical instability.

In this talk, we discuss some different aspects of these algorithms.

A Shrink-and-Expand Technique for Symmetric Block Eigensolvers

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Abstract

In symmetric block eigenvalue algorithms, such as the subspace iteration algorithm and the locally optimal block preconditioned conjugate gradient (LOBPCG) algorithm, a large block size is often employed to achieve robustness and rapid convergence. However, using a large block size also increases the computational cost. Traditionally, the block size is typically reduced after convergence of some eigenpairs, known as deflation. We propose a non-deflation-based, more aggressive technique, where the block size is adjusted dynamically during the algorithm. This technique can be applied to a wide range of block eigensolvers, reducing computational cost without compromising convergence speed. Both theoretical analysis and numerical experiments support the efficiency of the proposed technique. In practice, an overall acceleration of 20% to 30% is observed.

This is a joint work with Yuqi Liu and Yuxin Ma [1].

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A fast two-grid ADI method for two-dimensional nonlinear time-fractional reaction-diffusion equations on fitted meshes

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Abstract

Efficient numerical treatment of two-dimensional nonlinear time-fractional reaction–diffusion equations remains a challenging task due to nonlocality and weak initial singularities. In this work, we propose a novel fast two-grid alternating direction implicit (ADI) method for solving such problems governed by the Caputo derivative of order $\mu \in (0, 1)$. The weak initial singularity is effectively captured using a fitted temporal mesh, while the fractional derivative is discretized via a high-order sum-of-exponentials approximation, leading to significant reductions in storage and computational cost. An ADI framework is constructed to decompose the two-dimensional problem into a sequence of one-dimensional subproblems, thereby improving computational efficiency. To further enhance performance, a spatial two-grid strategy is employed, wherein the nonlinear system is solved on a coarse grid and a corresponding linearized system is solved on a fine grid. A rigorous theoretical analysis is carried out using a discrete energy method, local truncation error estimates, and a fractional Grönwall inequality, establishing unconditional stability and optimal convergence rates. Numerical experiments validate the theoretical results and demonstrate the accuracy and efficiency of the proposed method.

Termination of parallel asynchronous linear iterations on clusters and cloud architectures

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Abstract

Large scale numerical simulations occurring for solving coupled problems modeling multiphysics applications require powerful means of computation. Only massively parallel efficient computer architectures are now able to offer this power. In this context, grid computing, peer to peer and cloud computing appear to be challenging paradigms in order to match this need in high speed computing. Concerning parallel numerical methods, note that parallel asynchronous iterative algorithms deserve particular attention since the synchronizations of the processors of heterogeneous and massively parallel architectures significantly degrade the performance of these methods when convergence is slow [1]. Among the challenging issues related to the efficient use of parallel asynchronous algorithms on new parallel distributed architectures, such as convergence study, and performance analysis, the derivation of stopping criteria is particularly difficult for defining reliable termination for such iterative methods. Several approaches for the convergence detection of parallel asynchronous iterations using computer science approaches have been proposed in the literature [1]. Nevertheless, in such computer science approaches, the accuracy of the parallel computations is not easy to evaluate when the convergence of the parallel iterations is reached. Thus error bounds allowing to evaluate the accuracy of iterative computations must be estimated.

Thus the present talk is only devoted to numerical approach for defining efficient stopping criteria for parallel asynchronous algorithms. For solving large linear algebraic systems the study is based on the use of mathematical tools used for studying the convergence of parallel asynchronous iterations and consider mainly the perturbation by round-off errors or by lossy compression of parallel asynchronous fixed point problems. Consequently, in the finite dimensional case, various ideas tackled in the context of numerical perturbation are developed to obtain upper bounds of the error. In particular, several various stopping criteria with respect to the absolute error and also to the relative error and to a mixed vectorial norm error are presented allowing estimations of errors bounds based on the estimate of the diameter of the embedded sets centered on the exact solution of the linear system [2] and using sliding macro iteration. Such criteria are particularly well suited to specific contexts such as the use of distributed memory machines, grid computing, peer to peer computing and cloud computing. Various parallel experiments for the resolution of discretized boundary value problem performed on clusters or on cloud computing architectures will be presented and analyzed.

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Symbol-Based Analysis of a Multigrid Method for a PDE-Constrained Optimal Control Problem

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Abstract

This work investigates optimal control problems constrained by the heat equation, which are typically solved using an all-at-once system formulation. Multigrid methods are a promising approach for such problems, offering optimal convergence where computational cost grows linearly with the number of unknowns.

When the problem is discretised on a structured grid, the system matrix exhibits a block-Toeplitz-like structure. In this setting, symbol-based techniques provide an elegant analytical framework for describing the behaviour of multigrid methods. Indeed, the matrix-valued symbol characterises the asymptotic spectral behaviour of the system matrix and, in different applications, has provided multigrid convergence analyses irrespective of the number of levels employed [1, 2].

While the symbol accurately describes the spectral properties in this application, a naïve multigrid construction based solely on this analysis suffers from slow convergence. The stalling occurs on a low-dimensional subspace associated with the time boundary of the all-at-once system. This contribution analyses the behaviour of the multigrid method on this problematic subspace and exploits the structure of the system matrix to introduce a suitable modification to improve convergence.

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Quantum Machine Learning in image analysis: A survey with focus on medical and defense applications

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Abstract

The transformative potential of Quantum Machine Learning (QML) has been increasingly recognized across diverse scientific domains, including cryptography[1] and pattern recognition [2], primarily due to the inherent advantages of quantum superposition and entanglement. While classical machine learning (CML) has demonstrated significant efficacy in medical image analysis [3] and defense applications [4], inherent constraints regarding computational complexity [5] and the scarcity of high-quality labeled datasets [6] persist. To mitigate these challenges, quantum-enhanced architectures are being explored, facilitating notable advancements in parameter optimization [7], algorithmic efficiency [8], and error reduction [9]. In this survey, a comprehensive review and taxonomy of current QML concepts and methodologies is established. The systematic review of recent literature is conducted with a dedicated focus on the integration of quantum computing principles within the specialized field of machine learning in medical imaging and defense applications. The current study is synthesized, highlighting how the bridge between quantum computing and machine learning offers novel perspectives for inference accuracy and robustness for critical medical and defense applications. Finally, emerging trends and future research trajectories are identified, providing a strategic roadmap for the continued evolution of image analysis using quantum-assisted machine learning.

A Study of Supersaturated Design-Based Computational Methods for Variable Selection in High-Dimensional Observational Data

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Abstract

In experimental studies, Supersaturated Designs (SSDs)-based statistical methods are widely used to screen relevant factors when the number of factors exceeds the number of experimental runs. Simulation studies have demonstrated that several SSD-based approaches perform well in such experimental settings. This has motivated the exploration of their potential application to high-dimensional observational data for variable selection.

Variable selection is a commonly used technique for identifying important predictors in statistical models based on observational data; however, it has also been widely criticised due to concerns such as model instability and selection bias. In response, we first review recent recommendations and methodological developments for variable selection in observational studies.

We then evaluate the performance of SSD-based statistical methods in the context of high-dimensional observational data using both simulated and real-world datasets. Their performance is further compared with existing variable selection approaches. The results provide insight into the suitability and robustness of SSD-based methods beyond experimental designs and highlight their potential as an alternative tool for high-dimensional data analysis.

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On error estimates for computing the exponential of matrices arising from finite element discretization

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Abstract

Several methods for computing the action of the matrix exponential $\mathrm{e}^{A}b$ are expressed in the form of substituting the matrix A into a rational approximation of the scalar exponential function, such as Padé approximation [1], numerical quadrature [2], or polynomial interpolation [3]. The error of such methods can be evaluated using the numerical range of A. Hence, if the numerical range (or its bounding box) can be computed numerically, the error can also be evaluated numerically.

In this study, we consider the case where A has the structure $A = M^{-1}K$, where M is a well conditioned symmetric positive definite matrix. In this situation, efficient computation of the bounding box of the numerical range is difficult, and the error estimate can result in an overestimation. In this talk, we propose considering the numerical range of a similarity-transformed matrix of A to estimate the error. The numerical range of the transformed matrix is not only numerically computable but also is bounded theoretically depending on the properties of K.

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Determining the space dependent coefficients in space-time fractional diffusion equations via Krylov preconditioning

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Abstract

We consider a time-space fractional diffusion equation with a variable coefficient and investigate the inverse problem of reconstructing the source term, after regularizing the problem with the quasi-boundary value method to mitigate the ill-posedness. The equation involves a Caputo fractional derivative in the space variable and a tempered fractional derivative in the time variable, both of order in $(0, 1)$. A finite difference approximation leads to a two-by-two block linear system of large dimensions.

We focus on a spectral and invertibility analysis of the associated matrix sequences, employing tools from Generalized Locally Toeplitz (GLT) theory, and construct the preconditioner guided by the GLT analysis. Numerical experiments regarding the convergence speed of iterative methods are reported and commented.

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Gauss-type quadrature rules with quasi-prescribed nodes

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Abstract

Consider the numerical approximation of integrals over a finite interval $[a, b]$ by Gauss-type quadrature rules with prescribed nodes $x_k \in \mathbb{R} \setminus (a, b)$, $k = 1, 2, ..., m$. In particular, if these nodes coincide with the zeros of the integrand, one can effectively obtain an n-point quadrature formula that achieves a degree of exactness $2n - 1 + m$.

Motivated by this observation, we propose a decomposition of the given integral into two parts. The first part can be evaluated analytically and therefore does not contribute to the quadrature error. The second part has x_k, $k = 1, 2, ..., m$, as zeros of a suitably modified integrand. This approach enables the construction of Gauss-type quadrature rules with enhanced accuracy for the remaining integral. In the proposed framework, the nodes x_k, $k = 1, 2, ..., m$, are referred to as quasi-prescribed, since they do not appear explicitly in the final quadrature formula.

Particular attention is given to cases corresponding to Gauss–Radau and Gauss–Lobatto formulas. Several numerical examples are presented to illustrate the theoretical results.

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Fast Estimates of Quadratic Forms with Matrix Powers

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Abstract

We will discuss a class of efficiently computable estimates of the quadratic form $x^T A^k x$ for a symmetric positive definite matrix A and a general $k \in \mathbb{R}$. We extend the validity of the approach developed in papers [1] and [2], and present certain explicit bounds on the error.

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Solving an inverse eigenvalue problem for Multiple Orthogonal Polynomials

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Abstract

We discuss new algorithms for computing the recurrence coefficients corresponding to multiple orthogonal polynomials on the step-line. We start by reformulating the problem as an inverse eigenvalue problem (IEP), which can be solved using numerical linear algebra techniques.

Then, two approaches to solve this IEP are considered: the first is based on the link with block Krylov subspaces and results in a biorthogonal Lanczos process with multiple starting vectors; the second consists of applying a sequence of Gaussian eliminations on a diagonal matrix to construct the banded Hessenberg matrix containing the recurrence coefficients.

Finally, we analyze the accuracy and stability of the algorithms with numerical experiments on the ill-conditioned IEP related to Kravchuk and Hahn polynomials, as well as on other better conditioned examples.

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Numerical Linear Algebra Approach to Efficient Score Computation for Diffusion Models

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Abstract

Stable diffusion models have emerged as a powerful paradigm for generative modeling, achieving state-of-the-art results in image synthesis. However, this approach comes at a significant computational cost: training requires thousands of epochs on large datasets, and inference demands hundreds of denoising steps. This paper presents a novel framework to accelerate score-based diffusion models. It first converts the standard diffusion model into a Fokker-Planck formulation. Thus, computing the score functions can be done via solving large sparse linear systems for each image. However, for training involving many images, it can still lead to high computational costs. To address this, we introduce a cross-matrix Krylov projection method that exploits mathematical similarities between matrices, using a shared subspace built from "seed" matrices to rapidly solve for subsequent "target" matrices. Our experiments show that this technique achieves a 15.8% to 43.7% time reduction over standard sparse solvers. Additionally, we compare our method against DDPM baselines in denoising tasks, showing a speedup of up to 115 times. As a result, under a fixed computational budget, our model is able to produce high-quality images while DDPM fails to generate recognizable content, illustrating our approach is a practical method for efficient image generation in resource-limited settings. Qualitative and quantitative results are presented to demonstrate the performance of our method.

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A Quantum Block Power Method for Singular Value Decomposition via QSVT

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Abstract

We present a quantum algorithm for estimating the singular values and the associated left and right singular vectors of a rank-deficient operator $A \in \mathbb{R}^{N\times M}$. Our method assumes block-encoding access to A and combines the block-encoding framework with quantum singular value transformation (QSVT) to implement polynomial spectral filters that selectively amplify the dominant singular subspace. Inspired by the classical block power method for SVD, the algorithm iteratively projects onto the span of the k largest singular vectors and outputs approximations of the leading singular values together with corresponding singular vector states. The query complexity is $O(d)$ calls to the block-encoding, where d is the degree of the QSVT polynomial required to achieve a target precision and depends on parameters such as the desired error tolerance and spectral separation. Compared with the $O(k^2N)$ scaling of the classical block power method in analogous access settings, our approach offers a substantial reduction in query cost, making it promising for large-scale low-rank approximation tasks and related applications such as principal component analysis and least-squares problems.

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Regularisation in deep neural networks

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Abstract

Regularisation is widely used in deep neural networks and physics informed neural networks because, it is claimed, it solves the problem of overfitting. There is, however, no evidence for this claim, and furthermore, theoretical and computational evidence that overfitting and regularisation are unrelated is in [1, 3, 5]. Regularisation is not benign because its application to the least squares (LS) problem $\min_x \|Ax - b\|_2^2$ when a condition on the decay of the singular values of A is not satisfied leads to a large error in the solution of the regularised LS problem [2, 4]. There are several forms of regularisation, including weight decay (also known as Tikhonov regularisation and ridge regression), dropout and Jacobian regularisation, that are used in deep neural networks, and all these forms require a regularisation parameter λ that controls the severity with which the regularising constraint is imposed on the objective function. It is implicitly assumed that regularisation is necessarily required, but this requirement is never verified, and λ is considered a hyperparameter whose value is determined from training data.

A detailed and rigorous consideration of the application of regularisation to deep learning will be presented, and examples from the MNIST dataset will be included. The presentation will include several condition numbers of a deep neural network, the effect of noise on the training data, and the use of regularisation to mitigate the adverse effects of adversarial attacks.

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Randomized Generalized Error Minimizing Method for Linear Ill-Posed Problems

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Abstract

For solving noisy linear ill-posed problems arising from the practical applications, the residual based iterative methods may suffer semi-convergence phenomenon, where the iterates initially get closer to the desired solution but then degrade as the iteration continues. Building upon the randomized Gram-Schmidt algorithm, a random sketching technique known to reduce inner product computational costs over classical Gram-Schmidt and numerical stability comparable to modified Gram-Schmidt, we develop a novel randomized generalized error minimizing (GMERR) Krylov subspace method. This process extends the application of randomized Gram-Schmidt in methods such as randomized GMRES and LSQR. We further introduce a block variant, resulting in a block randomized Arnoldi process and a block GMERR method for large-scale ill-posed problems. A theoretical analysis of the regularization properties and numerical stability of the proposed methods is provided, leveraging random projection theory. Numerical experiments demonstrate the efficacy of the proposed algorithms.

Direct–Inverse Chiral Electromagnetic Scattering with Mixed Boundary Conditions: Variational Formulation and MFS

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Abstract

We study time-harmonic electromagnetic scattering in chiral media by impenetrable obstacles with mixed boundary conditions under a two-dimensional anti-plane reduction. The resulting problems are written in a variational form and analyzed in appropriate Sobolev trace spaces. We prove well-posedness of weak solutions. For the numerical approximation, we employ the Method of Fundamental Solutions (MFS), supported by density results for the traces of chiral fundamental solutions in the admissible trace spaces. We further consider the corresponding inverse problem of reconstructing the obstacle from scattering data, establish uniqueness of the reconstruction, and propose an MFS-based algorithm. Representative numerical results for both direct and inverse problems are presented.

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