Abstracts

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1 Plenary Talks

Mathematical approximation, risk, and confidence for statistical learning

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Certain flexible models such as artificial neural networks permit accurate approximation high-dimensional function under appropriate conditions. Penalized empirical loss criteria and especially penalized log-likelihood criteria permit realization of such accurate approximations from finite samples. In particular, an information-theoretic property yields a clean one-sided penalized empirical process bound that permits adaptation of various aspects of the network, including the ℓ_1 path norm of the parameters and optionally the size and architecture of the network. Both statistical risk bounds and statistical confidence bounds arise as consequences of the empirical process inequality. The statistical risk is shown to be controlled by an index of the resolvability of the target by functions of moderate complexity relative to the sample size. The confidence bounds illuminate the phenomenon of "benign over-fitting". In particular, accuracy of generalization is established for over-fit models, if the ℓ_1 norm of the fitted parameters is small compared the square root of the sample size divided by the log of the parameter dimension.

Computational fluid–structure interaction: methods, breakthroughs and applications

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In this talk I will present recent breakthroughs in advanced fluid-structure interaction (FSI) modeling that enable the application of what is largely considered by some "academic" methods to accurate and effective simulation of mechanical and structural systems. The presentation will focus on describing the modeling approaches involved and showing several convincing examples/studies from wind energy to air-blast FSI.

An arbitrarily high order finite element method for arbitrarily shaped domains with automatic mesh generation

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Partial different equations with discontinuous coefficients having complex interface geometry are of great interests in practical applications. The design of body-fitted high-order finite element methods requires the construction of shape regular body-fitted meshes for complex geometry and also nonlinear element transforms from the reference element to the elements with curved boundary. In practical applications, it may be challenging to satisfy the conditions imposed on the nonlinear element transforms in the literature which depend on the geometry of the interface.

In this talk we study high-order unfitted finite element methods on Cartesian meshes with hanging nodes for elliptic interface problems, which release the work of body-fitted mesh generation and provide a natural way to design high-order methods without resorting to nonlinear element transforms. We introduce new concepts of large element and interface deviation to solve the small cut cell problem of unfitted finite element methods. We construct a reliable algorithm to merge small interface elements with their surrounding elements to automatically generate the finite element mesh whose elements are large with respect to both domains. We show novel *hp*-domain inverse estimates which allow us to prove the stability of the finite element method under practical interface resolving mesh conditions and prove *hp* a priori and a posteriori error estimates. We propose new basis functions for the interface elements to control the growth of the condition number of the stiffness matrix in terms of the finite element approximation order, the number of elements of the mesh, and the interface deviation. Numerical examples are presented to illustrate the competitive performance of the method. This talk is based on joint works with Ke Li, Yong Liu and Xueshuang Xiang.

Digital twins through reduced order models and machine learning

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The vision of building digital twins for complex infrastructure and systems is old. However, realizing it remains very challenging due to the need to combine advanced computational modeling, reduced order models, data infusion for calibration, updating and uncertainty management, and sensor integration to obtain models with true predictive value for decision support. Nevertheless, the perspectives of using digital twins for predictive maintenance, operational optimization, and risk analysis are very substantial and the potential for impact significant, from safety, planning, and financial points of view.

In this talk we shall first discuss the importance of reduced models in the development of digital twin technologies and continue by discussing different aspects of the challenges associated with developing digital twins through a few examples, combining advanced model and data driven technologies, e.g., classifiers, Gaussian regression and neural networks, to enable failure analysis, optimal sensor placement and, time permitting, multi-fidelity methods and risk analysis for rare events.

These are all elements of the workflow that needs to be realized to address the challenge of building predictive digital twins and we shall demonstrated the value of such technologies through a number of different examples of increasing complexity.

The finite element method and isogeometric analysis: mathematical and engineering perspectives

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I will begin by probing into the past to discover the origins of the Finite Element Method (FEM), and then trace the evolution of those early de-

velopments to the present day in which the FEM is ubiquitous in science, engineering, mathematics, and medicine, and the most important discretization technology in Computational Mechanics. However, despite its enormous success, there are still problems with contemporary technology, for example, building meshes from Computer Aided Design (CAD) representations is labor intensive, and a significant bottleneck in the design-through-analysis process. Other deficiencies are the introduction of geometry errors in computational models that arise due to feature removal, geometry clean-up and CAD "healing," necessary to facilitate mesh generation, the inability of contemporary technology to "close the loop" with design optimization, and the failure of higher-order finite elements to achieve their full promise in industrial applications. These issues are addressed by *Isogeometric Analysis* (IGA), the vision of which was first presented in a paper published October 1, 2005 [1]. Since those seminal ideas, the subject has progressed enormously and a number of advantages of IGA-FEM over traditional FEM have become manifest. I will very briefly present the motivation leading to IGA, its status, mathematical properties, recent progress, areas of current activity, and what it offers for analysis model development and the design-through-analysis process. Finally, I will speculate on the future of Computational Mechanics, the technologies that will prevail, computer developments, and the role of Machine Learning and AI.

Reference

[1] T.J.R. Hughes, J.A. Cottrell and Y. Bazilevs, "Isogeometric Analysis: CAD, Finite Elements, NURBS, Exact Geometry and Mesh Refinement," Computer Methods in Applied Mechanics and Engineering, 194, (2005) 4135-4195.

Modeling, estimation, and applications of generalized heteroscedastic Gaussian processes

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For one-dimensional continuous time series, the stochastic volatility model and its inference methods have long been a subject of active research. Their

extensions to multi-dimensional cases, however, have met a lot challenges ranging from modeling to computation. We here introduce a generalized mixture model and variational Bayes inference procedures for handling multi-dimensional volatility processes. The introduced model is then used as a latent structure for constructing heteroscedastic Gaussian processes, which is an attempt to address a key drawback of the standard Gaussian process that its structure is completely by one kernel function. We further demonstrate how to use variational approximations to carry out an explicit marginalization of the hidden functions, resulting in efficient parameter estimation and process forecasting. We demonstrate its advantages by both simulations and applications to real-data examples of regression, classification and state-space models.

Extreme superposition: models for large-amplitude rogue waves

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Rogue waves or freak waves are spatially-localized disturbances of a background field that are also temporally localized. In the setting of the focusing nonlinear Schrödinger equation, which is a universal model for the complex amplitude of a wave packet in a general one-dimensional weakly-nonlinear and strongly-dispersive setting that includes water waves and nonlinear optics as special cases, a special exact solution exhibiting rogue-wave character was found by D. H. Peregrine in 1983. Since then, with the help of complete integrability, Peregrine's solution has been generalized to a family of solutions of arbitrary "order" where more parameters appear in the solution as the order increases. These parameters can be adjusted to maximize the amplitude of the rogue wave for a given order. This talk will describe several recent results concerning such maximal-amplitude rogue wave solutions in the limit that the order increases without bound. For instance, it turns out that there is a limiting structure in a suitable near-field scaling of the peak of the rogue wave; this structure is a novel exact solution of the focusing nonlinear Schrödinger equation — the "rogue wave of infinite order" — that is also connected with the hierarchy of the third Painlevé equation. This is joint work with Deniz Bilman and Liming Ling.

Modeling COVID-19 incidence and reproduction number by the renewal equation

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The COVID-19 pandemic has undergone frequent and rapid changes in its local and global infection rates, driven by governmental measures, or the emergence of new viral variants. The COVID-19 daily count of incident cases i_t and its associated reproduction number R_t have become the main metrics used by policy makers and journalists to monitor the spread of the pandemic. The daily reproduction number R_t is defined as the average number of new infections caused by a single individual that was infected at time t. It is therefore a key indicator of the spread of an epidemic and a crucial tool for policy makers. R_t can be deduced from the incidence i_t through the inversion of the *renewal equation* linking both quantities. Yet, a timely computation of R_t from i_t is a challenging inverse problem, because of a combination of case detection delays, administrative delays and measurement noise. In this talk, I'll explain how to faithfully reconstruct i_t and R_t using the renewal equation. I'll show that thanks to a rigorous inversion of the renewal equation, R_t can be estimated up to 9 days in advance with respect to a prevalent anterior method, EpiEstim, thus enabling a much faster reaction to the pandemic spread. The daily results for all countries of this method, *EpiInvert*, are published online daily since July 2021.

The symbiosis of applied mathematics and statistics

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Recent years have seen many examples of fields that have benefitted from the complementary perspectives of both applied mathematicians and statisticians, including compressed sensing/ℓ_1 regularisation, the theoretical analysis of deep learning and the analysis of tensor data. I will present some further examples drawn from my own research on nonparametric inference under shape constraints and matrix perturbation theory, and will offer some thoughts on what the communities can learn from each other.

Mathematics and biology: search, a case study

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Eugene Wigner was a theoretical physicist who won the Nobel prize in 1963. In 1960 he published a now famous paper "The Unreasonable Effectiveness of Mathematics in the Natural Sciences". It seems an appropriate time to consider the effectiveness of mathematics and computer science in the biological sciences. Genetic sequence database search where mathematics plays a central role is used to illustrate some of the issues that arise.

2 Invited Talks

Variational multiscale moment methods for the Boltzmann equation

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Integrating the Boltzmann equation against the collision invariants leads to the conservation laws of mass, momentum and energy. These equations require closure relations to balance the number of unknowns with the number of equations. Such closure may be attained by the Chapman-Enskog method which assumes that the distribution conforms to a perturbation series in powers of the Knudsen number scaled by a Maxwellian [1]. By using a scaled Boltzmann equation to solve for successive orders of the perturbation series, we obtain familiar fluid dynamic equations: Euler, Navier-Stokes-Fourier, Burnett, and so on. However, the equations on the Burnett level, and beyond, are not well-posed [2].

Instead of a perturbation series, we use the variational multiscale (VMS) method [3] to split our unknown into a coarse scale term from the space of collision invariants and a fine scale term from the orthogonal complement to the collision invariants. We show that the Chapman-Enskog method can be viewed as particular way of approximating the fine scale term under the VMS formulation. By approximating the fine scale term differently, we are able to derive an alternative to the Burnett equations (i.e. a correction to the Navier-Stokes-Fourier) for which we can show entropy stability. We conclude our discussion with a derivation of analytical solutions to benchmark problems to elucidate the approximation properties of the proposed model.

[1] L. Saint-Raymond, "A mathematical PDE perspective on the Chapman–Enskog expansion". *Bulletin of the American Mathematical Society*, (2014).
[2] A. V. Bobylev, "Instabilities in the Chapman-Enskog expansion and hyperbolic burnett equations", *Journal of Statistical Physics*, (2006).
[3] T. J. R. Hughes and G. Sangalli. "Variational multiscale analysis: the fine-scale green's function, projection, optimization, localization, and stabilized

methods". *SIAM Journal on Numerical Analysis*, (2007).

Provably convergent plug & play linearized ADMM, applied to deblurring spatially varying kernels

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Bayesian methods to solve inverse problems in imaging usually combine an explicit likelihood function with a prior distribution on natural images. Many recent works have proposed and studied the use of learned priors that are only known implicitly via a neural network denoiser that approximates the proximal operator of the negative log-prior. In combination with proximal descent schemes like ADMM, such Plug & Play (PnP) approches achieved state-of-the-art visual performance for many image restoration tasks. Nevertheless, two shortcomings prevent PnP-ADMM algorithms from large adoption in some real-world problems: *(i)* convergence guarantees only hold under tight conditions on the denoiser training or regularization parameters that may lead to suboptimal results, and *(ii)* the proximal operator of the data-fitting term may be intractable for some applications such as nonuniform deblurring.

This presentation introduces the PnP-LADMM, where a linearization allows to bypass the intractable proximal operator. In addition, based on recent progress in non-convex optimization, we show the convergence of the PnP-LADMM under less constrained conditions than previous results on PnP-ADMM. Our experiments show that the proposed algorithm reaches state-of-the-art performance in a fraction of the time required by other provably convergent PnP algorithms. Furthermore, when unrolling a few iterations of our PnP-LADMM algorithm into a single network that is trained end-to-end we can further improve both visual quality and computational cost, and still generalize to a large family of blur kernels, noise levels and super-resolution factors.

Provable sample-efficient sparse phase retrieval initialized by truncated power method

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We investigate the sparse phase retrieval problem, which involves recovering an s-sparse signal of length n using m magnitude-only measurements. Recently, two-stage non-convex approaches have gained considerable interest due to their provable linear convergence towards the underlying solution when properly initialized, despite their non-convex nature. However, the sample complexity of these algorithms is often constrained by the initialization stage. Commonly, spectral initialization is employed in the initialization stage, which necessitates $m = \Omega(s^2 \log n)$ measurements to generate a suitable initial guess. This results in a total sample complexity that is order-wisely higher than necessary. To decrease the required number of measurements, we introduce a truncated power method as a substitute for spectral initialization in non-convex sparse phase retrieval algorithms. We prove that $m = \Omega(\bar{s}s \log n)$ measurements, with $\bar{s}$ representing the stable sparsity of the underlying signal, are adequate for generating a desired initial guess. In cases where the underlying signal consists of only a few significant components, our proposed algorithm achieves an optimal sample complexity of $m = \Omega(s \log n)$. Numerical experiments further validate the enhanced sample efficiency of our method compared to existing state-of-the-art algorithms.

Dynamic fracture for geological applications

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We present an energy-preserving mechanic formulation for dynamic quasi-brittle fracture in an Eulerian-Lagrangian formulation, where a second-order phase-field equation controls the damage evolution. The numerical formulation adapts in space and time to bound the errors, solving the mesh-bias

issues these models typically suffer. The time-step adaptivity estimates the temporal truncation error of the partial differential equation that governs the solid equilibrium. The second-order generalized-α time-marching scheme evolves the dynamic system. We estimate the temporal error by extrapolating a first-order approximation of the present time-step solution using previous ones with backward difference formulas; the estimate compares the extrapolation with the time-marching solution. We use an adaptive scheme built on a residual minimization formulation in space. We estimate the spatial error by enriching the discretization with elemental bubbles; then, we localize an error indicator norm to guide the mesh refinement as the fracture propagates. The combined space and time adaptivity allows us to use low-order linear elements in problems involving complex stress paths. We efficiently and robustly use low-order spatial discretizations while avoiding mesh bias in structured and unstructured meshes. We demonstrate the method's efficiency with numerical experiments that feature dynamic crack branching, where the capacity of the adaptive space–time scheme is apparent. The adaptive method delivers accurate and reproducible crack paths.

Image segmentation problems: models, algorithms and challenges

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Imaging technology has been developing in an extremely rapid pace in the last three decades to the extent that the established models for processing were struggling all along to deal with new and emerging imaging modalities and varying degrees of imaging quality. Image segmentation is commonly studied task that remains challenging. The recently popular method of deep learning offers a potentially promising approach for fast segmentation but it has its own set of challenges to tackle real life problems. The demand of a large number of training data that contain manually labelled segmentation is found unrealistic in many real-life scenarios.

In this talk, I first review variational models with a view to assess their successes and failures, focusing on image segmentation and co-registration. Then I discuss a new semi-supervised learning approach for deep learning to

solve image segmentation tasks where few manual labels are available. Instead of self-learning, we propose the use of variational segmentation models, assisted by image registration, for computing pseudo-labels. Results by few labels are completive to cases where many labels are given. Finally I show some recent results on merging algorithms based on learning and mathematical ideas for microscopic images in grading cores of colorectal cancer tissue microarrays, where the two approaches must work together – learning alone cannot decompose irregular image features within region of interests (RoIs) and mathematical models alone cannot distinguish different RoIs. The talk contains joint works with many CMIT and LCMH colleagues including Dr L Borrows, Prof F Torella, Dr Daoping Zhang, Mr H R Zhang, Mr D Sculthorpe, Dr S Mills, Dr J Patel, Dr A Islim, Prof M Jenkinson and Dr A Mukherjee.

Nonsmooth nonconvex-nonconcave min-max problems and generative adversarial networks

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This talk considers a class of nonsmooth nonconvex-nonconcave min-max problems in machine learning and games. We first provide sufficient conditions for the existence of global minimax points and local minimax points. Next, we establish the first-order and second-order optimality conditions for local minimax points by using directional derivatives. These conditions reduce to smooth min-max problems with Fréchet derivatives. We apply our theoretical results to generative adversarial networks (GANs) and propose a quasi-Newton subspace trust region method for min-max problems. Examples of OCT image segmentation are used to illustrate the efficiency of the new theory and method.

Total stability of localized learning

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Many regularized kernel-based methods do not only depend on the underlying probability measure P, but also on some regularization parameter λ and on a kernel k. We investigate the *joint* influence of small pertubations of (P, λ, k), as such pertubations are common in practice. Existing results from the literature are generalized and improved. In order to also make such learning methods applicable to big data, where such methods suffer from their super-linear computational requirements, we show how our results can be transferred to the context of localized learning. Here, the effect of slight variations in the applied regionalization, which might for example stem from changes how the whole data set is split up into regions, is considered as well. The talk is based on the paper by Köhler, H. and Christmann, A. (2022). Journal of Machine Learning Research, 23, 1–41.

Approximation of eigenproblems of incompressible materials using a stabilised finite element formulation. Application to modal analysis

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In this work we describe a finite element formulation to approximate eigenproblems of incompressible materials. In particular, the problem considered is the Stokes one, modelling either an incompressible fluid or an incompressible elastic solid, and having as unknowns the displacement field (or velocity, in the case of fluids) and the pressure. The standard Galerkin method is unstable unless interpolations satisfying the inf-sup conditions are used. To avoid this restriction, we use a stabilised finite element method. It is explained why residual based formulations are not appropriate in this case, and a formulation involving only the pressure gradient is employed. We provide the results of the numerical analysis, which shows that both eigenvalues and eigenvectors are optimally approximated by the formulation proposed. This

formulation is then applied to the modal analysis of the vibrations of incompressible elastic solids, which is derived in detail for the stabilised formulation proposed. Finally, an error estimate for a truncated modal expansion is provided, also considering the effect of the stabilisation. Numerical results show that the proposed formulation behaves as the theoretical results predict.

RankSEG: a consistent ranking-based framework for segmentation

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Segmentation has emerged as a fundamental field of computer vision and natural language processing, which assigns a label to every pixel/feature to extract regions of interest from an image/text. To evaluate the performance of segmentation, the Dice and IoU metrics are used to measure the degree of overlap between the ground truth and the predicted segmentation. In this paper, we establish a theoretical foundation of segmentation with respect to the Dice/IoU metrics, including the Bayes rule and Dice/IoU-calibration, analogous to classification-calibration or Fisher consistency in classification. We prove that the existing thresholding-based framework with most operating losses are not consistent with respect to the Dice/IoU metrics, and thus may lead to a suboptimal solution. To address this pitfall, we propose a novel consistent ranking-based framework, namely RankDice/RankIoU, inspired by plug-in rules of the Bayes segmentation rule. Three numerical algorithms with GPU parallel execution are developed to implement the proposed framework in large-scale and high-dimensional segmentation. We study statistical properties of the proposed framework. We show it is Dice-/IoU-calibrated, and its excess risk bounds, and the rate of convergence are also provided. The numerical effectiveness of RankDice/mRankDice is demonstrated in various simulated examples and Fine-annotated CityScapes and Pascal VOC datasets with state-of-the-art deep learning architectures.

Some recent advances of quadratures for isogeometric analysis

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In this talk, I will focus on the use of quadratures rules for the integrals in the isogeometric analysis discretization. I will start by reviewing some of the classic Gaussian-type quadratures, followed by recent rules including weighted quadratures, reduced Gauss rules, and Gauss-Greville rules. I will then introduce a new set of quadratures and compare their performance in the setting of isogeometric analysis with various splines. Finally, I will close my talk with an open question on completing a table of quadrature rules for C^k-continuous and p-th ($p > k, k = -1, 0, 1, \cdots$) order spline spaces. This talk is based on joint work with Pouria Behnoudfar (CSIRO) and Victor Calo (Curtin University).

Bayesian image restoration: from deep prior to uncertainty estimation

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Recovering high-quality images/videos from those degraded versions are often needed before further image/video processing and analysis. While most of current deep CNNs solve the image restoration (IR) problems by directly mapping a low-quality image to its high-quality versions, the rich domain knowledge of IR has largely been ignored. To address this issue, we formulated the IR problem as a MAP estimation problem, and proposed to unfold the optimization into a deep neural network. The explicit estimation of the uncertainty associated with the estimates also allow us to construct a new class of uncertainty-driven loss (UDL) functions for deep unfolded networks. Extensive experiments on typical IR and video denoising tasks verified the effectiveness of the proposed methods.

Multicontinuum homogenization and applications

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In this talk, I will discuss an approach for multicontinuum homogenization. The main idea of this approach is to identify multiple continua at each macroscopic point. I will discuss a short history and the derivation. Further, I will discuss its relation to previously developed multiscale methods and to solvers.

Learning nonlinear functionals using deep ReLU networks

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Functional neural networks have been proposed and studied in order to approximate nonlinear continuous functionals defined on $L^p([-1,1]^s)$ for integers $s \geq 1$ and $1 \leq p < \infty$. However, their theoretical properties are largely unknown beyond universality of approximation or the existing analysis does not apply to the rectified linear unit (ReLU) activation function. In this talk we investigate the approximation power of functional deep ReLU networks and establish their rates of approximation under mild regularity conditions.

Bayesian cancer subtyping based on paired methylation data

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The comparison between tumour tissue and its neighbouring normal tissue can provide cleaner information for identifying cancer-related genetic and epigenetic markers. Here we analyse DNA methylation profiles from such paired samples. A Bayesian algorithm is provided to stratify patients into epigenetically relevant subtypes and capture the methylation signatures of different subtypes.

From data to modeling: exploration at the whole brain scale

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We will first present some of our recent results on tackling brain disorders with the aim to establish nonlinear association, prediction, subtype, and spatio-temporal pattern analyzing for data ranging from genetic, MRI imaging and phenotypes. With the aid of AI algorithms (usually developed by ourselves), the analysis above is usually carried out at the whole brain scale (data-driven approach) to avoid possible bias. A digital twin brain (DTB) platform including the whole brain for human (86 B neurons), monkey and zebrafish (100,000 neurons) is established to simulate the activity both in the resting-state and in action. The activity of the DTB at voxel level shows a correlation coefficient of 0.9 with its biological counterpart in the resting state. We also test the DTB in actions including visual and auditory tasks. Finally, we are working on developing the DTB platform for brain-machine interfaces (DBS for example) and applications in other brain disorders.

Optimal analysis of non-uniform Galerkin-mixed FE approximations to the Ginzburg–Landau equations in superconductivity

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This talk is concerned with new error analysis of a lowest-order backward Euler Galerkin-mixed finite element method for the time-dependent Ginzburg–Landau equations. The method is based on a commonly-used non-uniform approximations, in which linear Lagrange element, the lowest order Nédélec edge element and Raviart–Thomas face element are used for the order parameter ψ, the magnetic field **curlA** and the magnetic potential $\mathbf{A}$, respectively. This mixed method has been widely used in practical simulations due to its low cost and ease of implementation. In the Ginzburg–Landau model, the order parameter ψ is the most important variable, which indicates the

state of the superconductor. An important feature of the method is the inconsistency of the approximation orders. A crucial question is how the first-order approximation of $(\mathbf{curlA}, \mathbf{A})$ influences the accuracy of ψ_h. The main purpose of this paper is to establish the second-order accuracy for the order parameter in spatial direction, although the accuracy for $(\mathbf{curlA}, \mathbf{A})$ is in the first order only. Previous analysis only gave the first order convergence for all three variables due to certain artificial pollution involved in analysis. Our analysis is based on a nonstandard quasi-projection for ψ and the corresponding more precise estimates, including in H^{-1}-norm. With the quasi-projection, we prove that the lower-order approximation to $(\mathbf{curlA}, \mathbf{A})$ does not pollute the accuracy of ψ_h. Our numerical experiments confirm the optimal convergence of ψ_h. The approach can be extended to many other multi-physics models.

Structured mesh generation for IGA

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Structured surface quadrilateral mesh generation and volume hexahedral mesh generation are crucial for Isogeometric Analysis. But the structured meshing problem is intrinsically challenging. This talk focuses on the recent development to tackle these challenges based on modern topological and geometric theories.

It is well known that a closed torus does not admit a quad-mesh with only two singularities, whose valences are 3 and 5 respectively. But the theoretic proof is highly non-trivial. Although it seems to be a combinatorial problem, it has deep roots in the characteristic class theory of holomorphic line bundles, especially the Abel-Jacobi theorem. This discovery leads to the governing equations of the configurations of quad-mesh singularities. By solving these equations using Hodge theory and surface Ricci flow, the high quality, automatic quad-mesh generation algorithms can be developed.

The singularity configuration of volumetric hex-meshes becomes more complicated, due to the fact that the fundamental group of the manifold of crosses is non-Abelian, hence the classical topological obstruction theory for fiber bundles can not be applied. Instead, the recent breakthrough of

the proof of Thurston's virtual Haken conjecture offers novel insights to the problem, by using the cube-complex theory it is promising to conquer the problem with theoretic guarantees.

Estimation of leading multi-block canonical correlation directions via ℓ_1-norm constrained proximal gradient descent

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Multi-block CCA constructs linear relationships that explain coherent variations across multiple data blocks. We view it as a generalized eigenvalue problem and estimate the leading mCCA direction using ℓ_1-constrained proximal gradient descent. Rather than fixing one constraint value, we propose a decaying sequence of constraints over successive iterations and show that the resulting estimate is rate-optimal under suitable assumptions. While previous work has demonstrated such optimality with a fixed ℓ_0 constraint, the same level of theoretical understanding is still lacking for the ℓ_1 constrained formulation. It is unclear whether there exists a ℓ_1-constrained formulation that can achieve the optimal rate, despite being widely used in practice. In addition, we describe a simple deflation procedure for sequentially estimating multiple directions. We compare our proposal to several existing methods whose implementations are available on R CRAN, and the proposed method outperforms its competitors in both simulations and a TCGA cancer data set.

Wavelets on bounded intervals and wavelet methods for Helmholtz equations

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Many problems such as image processing and numerical PDEs are given in bounded domains. Hence, wavelets on bounded domains are important in many applications. For image processing, the boundary wavelets must have

high vanishing moments to reduce the boundary artifacts, while for numerical computing, the boundary wavelets must satisfy certain boundary conditions. In this talk, we shall propose a general direct approach for adapting any biorthogonal (multi)wavelets on the real line to wavelets on the interval $[0, 1]$ having vanishing moments or satisfying boundary conditions. The Helmholtz equation is challenging to solve numerically due to the pollution effect, which often results in a huge ill-conditioned linear system. For large wavenumbers, iterative solvers are probably the only feasible way of solving such huge ill-conditioned linear systems. Wavelet methods are particularly suitable for this purpose, because wavelets are known to have sparsity and uniformly bounded condition numbers. In this talk, we first prove that our constructed wavelets on bounded intervals are Riesz bases in the Sobolev space $H^1([0, 1]^2)$. Then we apply them to numerically solve an electromagnetic scattering problem involving 2D Helmholtz equations having nonlocal boundary conditions. For given tolerance, our numerical experiments show that the wavelet Galerkin method has much fewer iteration steps than the standard finite element method. This talk is based on the following papers:

1. B. Han and M. Michelle, Wavelets on intervals derived from arbitrary compactly supported biorthogonal multiwavelets, *Applied and Computational Harmonic Analysis*, **53** (2021), 270-331.

2. B. Han and M. Michelle, Wavelet Galerkin method for an electromagnetic scattering problem, preprint (2023).

PIFE-PIC: parallel immersed-finite-element particle-in-cell for 3-D kinetic simulations of plasma-material interactions

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In this presentation, we present a recently developed particle simulation too PIFE-PIC, which is a novel three-dimensional (3-D) Parallel Immersed-Finite-Element (IFE) Particle-in-Cell (PIC) simulation model for particle simulations of plasma-material interactions. This framework is based on the recently developed non-homogeneous electrostatic IFE-PIC method, which

is designed to handle complex plasma-material interface conditions associated with irregular geometries using a Cartesian-mesh-based PIC. Three-dimensional domain decomposition is utilized for both the electrostatic field solver with IFE and the particle operations in PIC to distribute the computation among multiple processors. A simulation of the orbital-motion-limited (OML) sheath of a dielectric sphere immersed in a stationary plasma is carried out to validate PIFE-PIC and profile the parallel performance of the code package. Parallel efficiency up to approximately 110 superlinear speedup was achieved for strong scaling test. Furthermore, a large-scale simulation of plasma charging at a lunar crater containing 2 million PIC cells (10 million FE/IFE cells) and about 1 billion particles, running for 20,000 PIC steps in about 154 wall-clock hours, is presented to demonstrate the high-performance computing capability of PIFE-PIC.

Image vectorization by affine shortening flow

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Image vectorization aims at converting pixel images to vector graphics, which allows geometric transformations without degrading the resolution. In this talk, we introduce a novel vectorization method based on affine shortening flow. We will see that this geometric PDE offers various benefits including efficient depixelization and natural splittings for piecewise polynomial curve fitting. Then we will briefly discuss its extension to color images. Finally, we shall demonstrate experiments and comparison sudies to show the proposed method's effectiveness in preserving details while removing pixelization effects.

Statistical approaches to genome wide association analysis of complex diseases

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Genome wide association analysis (GWAS) has provided numerous insights into the genetic etiology of complex diseases. In this talk, I will talk about

genetic correlation analysis and risk prediction using GWAS summary statistics. First, I will introduce LOGODetect, a powerful and efficient statistical method to identify small genome segments harboring local genetic correlation signals. LOGODetect automatically identifies genetic regions showing consistent associations with multiple phenotypes through a scan statistic approach. It uses summary association statistics from genome-wide association studies (GWAS) as input and is robust to sample overlap between studies. Next, I will discuss the challenges in genetic risk prediction, and introduce NeuPred, a novel Bayesian polygenic risk score.

DeepRHP: a hybrid variational autoencoder for designing random heteropolymers as protein mimics

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Synthetic random heteropolymers (RHPs), consisting of a predefined set of monomers, offer an approach toward the design of protein-like materials. These RHPs, if designed appropriately, can mimic protein behavior and function. As such, there is a need for computational tools to efficiently guide RHP design. We bridge this gap by developing DeepRHP, a modified variational autoencoder (VAE) model under a semi-supervised framework. By equipping a classical VAE with an additional feature-based VAE, DeepRHP forces the latent space to capture structures of critical chemical features as well as individual RHP sequence patterns. In this sense, our method is versatile by allowing any relevant features to be incorporated in a hybrid manner. We demonstrate the effectiveness of DeepRHP by suggesting potential monomer compositions that stabilize membrane proteins (e.g. Aquaporin Z) in non-native environments and cross-validating our prediction with published results. The concordance between our model and true RHP function suggests strong potential in utilizing hybrid autoencoder architectures to guide RHP design for proteins and other biological compounds.

Covariance estimators for the ROOT-SGD algorithm in online learning

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Online learning naturally arises in many statistical and machine learning problems. The most widely used methods in online learning are stochastic first-order algorithms. Among this family of algorithms, there is a recently developed algorithm, Recursive One-Over-T SGD (ROOT-SGD). ROOT-SGD is advantageous in that it converges at a non-asymptotically fast rate, and its estimator further converges to a normal distribution. However, this normal distribution has unknown asymptotic covariance; thus cannot be directly applied to measure the uncertainty. To fill this gap, we develop two estimators for the asymptotic covariance of ROOT-SGD. Our covariance estimators are useful for statistical inference in ROOT-SGD. Our first estimator adopts the idea of plug-in. For each unknown component in the formula of the asymptotic covariance, we substitute it with its empirical counterpart. The plug-in estimator converges at the rate $O(1/\sqrt{t})$, where t is the sample size. Despite its quick convergence, the plug-in estimator has the limitation that it relies on the Hessian of the loss function, which might be unavailable in some cases. Our second estimator is a Hessian-free estimator that overcomes the aforementioned limitation. The Hessian-free estimator uses the random-scaling technique, and we show that it is an asymptotically consistent estimator of the true covariance. Our paper is available at https://arxiv.org/abs/2212.01259.

Variational approach to image vectorization

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We propose a novel algorithm for converting quantized raster color images to resolution-independent scalable vector graphics (SVG). Starting from the

discontinuity set of the input image, we pay attention to T-junctions, the topology of the discontinuity set, and intensity differences in adjacent regions to properly denoise and vectorize the image. We propose methods using affine scale-space and Mumford-Shah-type functional to vectorize images in geometrically meaningful way. These methods compare favorably to the state-of-art (SOTA) vectorization methods.

Minimax bounds for estimating multivariate Gaussian location mixtures

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We prove minimax bounds for estimating Gaussian location mixtures on $\mathbb{R}^d$ under the squared L^2 and the squared Hellinger loss functions. Under the squared L^2 loss, we prove that the minimax optimal rate is upper and lower bounded by a constant multiple of $n^{-1}(\log n)^{d/2}$. Under the squared Hellinger loss, we consider two subclasses based on the behavior of the tails of the mixing measure. When the mixing measure has a sub-Gaussian tail, the minimax rate under the squared Hellinger loss is bounded from below by $(\log n)^d/n$, which implies that the optimal minimax rate is between $(\log n)^d/n$ and the upper bound $(\log n)^{d+1}/n$ obtained by Saha and Guntuboyina(2017). On the other hand, when the mixing measure is only assumed to have a bounded p^{th} moment for a fixed $p > 0$, the minimax rate under the squared Hellinger loss is bounded from below by $n^{-p/(p+d)}(\log n)^{-3d/2}$. This rate is minimax optimal up to logarithmic factors.

Concordant changes among multiple large-scale data sets

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With the rapid developments of biomedical technologies, large-scale data have been increasingly collected. In practice, concordant/discordant changes

among a series of data sets can be of biological and clinical interest. It is also important to evaluate the overall reproducibility for a biomedical study with large-scale data. Statistically, the changes of a large number of variables are analyzed. Therefore, we have developed a mixture model based framework for the analysis of concordance/discordance as well as the evaluation of reproducibility among multiple large-scale biomedical data sets. The mixture model is based on the z-scores transformed from test p-values, and it is generally applicable to many different types of large-scale data. It is simple with three normal distribution components for each data set to represent negative changes, no changes and positive changes. When the number of data sets increases, the model parameter space increases exponentially due to the component combinations from different data sets. We have also developed two model reduction strategies so that efficient statistical inference can be achieved. To illustrate the advantages of our approach, we consider some recent genome-wide expression data sets as well as brain magnetic resonance imaging data sets as the applications.

Weak and strong stabilization of cut elements

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Cut finite element and isogeometric methods are based on embedding a computational domain into a background mesh that is not required to match the boundary leading to so-called cut or trimmed elements at the boundary. Adding stabilization terms we can control the variation of the discrete functions close to the boundary, which allows us to prove stability, condition number estimates, and optimal order a priori error estimates. Alternatively, we may use a discrete extension operator and solve the problem in a subspace of the finite element space where the unstable degrees of freedom are eliminated in such a way that optimal order approximation bounds are retained. These two approaches, the first weak and the second strong, have the same goal: to stabilize the method but appear very different at first glance.

We show that the definition of stabilization terms, added to the weak statement, may be generalized in two ways: (1) The stabilized quantity may be some functional of the discrete function, for instance, finite element de-

grees freedom. This allows us to stabilize the unstable modes more precisely than standard approaches. (2) The choice of elements that are connected. Typically, face neighbors, or connected patches are used, but we may stabilize by connecting elements intersecting the boundary to an element within a distance proportional to the mesh parameter. We show that the generalized stabilization form fits into the standard abstract requirements, and as a consequence, we obtain stable and optimal order convergent methods for second-order elliptic problems.

We also show that for a modified robust design of the ghost penalty, one may let the stabilization parameter tend to infinity without introducing locking. The limit corresponds to strong enforcement of certain algebraic constraints, which are identical to constraints implemented in specific extension operator frameworks. This illustrates the very close connection between stabilization and extension approaches.

Stability and generalization of stochastic gradient descent

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Stochastic gradient descent (SGD) has become the workhorse behind many machine learning problems. Optimization and estimation errors are two factors responsible for the statistical behavior of SGD. In this talk, I will report generalization analysis of SGD by considering simultaneously the optimization and estimation errors. I will introduce new algorithmic stability concepts to relax the existing restrictive assumptions and to improve the existing learning rates. Our results show new connections between generalization and optimization, which illustrate how a best learning performance can be achieved by early stopping.

Quasi-Monte Carlo finite element approximation of the Navier–Stokes equations with initial data modeled by log-normal random fields

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In this paper, we analyze the numerical approximation of the Navier–Stokes problem over a bounded polygonal domain in $\mathbb{R}^2$, where the initial condition is modeled by a log-normal random field. This problem usually arises in the area of uncertainty quantification. We aim to compute the expectation value of linear functionals of the solution to the Navier–Stokes equations and perform a rigorous error analysis for the problem. In particular, our method includes the finite element, fully-discrete discretizations, truncated Karhunen–Loéve expansion for the realizations of the initial condition, and lattice-based quasi-Monte Carlo (QMC) method to estimate the expected values over the parameter space. Our QMC analysis is based on randomly-shifted lattice rules for the integration over the domain in high-dimensional space, which guarantees the error decays with $\mathcal{O}(N^{-1+\delta})$, where N is the number of sampling points, $\delta > 0$ is an arbitrary small number, and the constant in the decay estimate is independent of the dimension of integration.

Determining a random Schrödinger equation with unknown source and potential

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This talk studies the direct and inverse scattering problem associated with a time-harmonic random Schrödinger equation with a Gaussian white noise source term. We establish the well-posedness of the direct scattering problem and obtain three uniqueness results in determining the variance of the source term, the potential and the mean of the source term, sequentially, by the corresponding far-field measurements. The first one shows that a single realization of the passive scattering measurement can uniquely recover the variance of the source term, without knowing the other two unknowns. The second shows that if active scattering measurement is further used, then a

single realization can uniquely recover the potential function without knowing the source term. The last one shows that if full measurements are used, then both the potential and the random source can be uniquely recovered.

From apes to human the cis-regulatory modules underwent a phase transition with ALU as one key driving force

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We consider the fundamental question: what genetic changes made us uniquely human? One perspective to answer the question is comparative genomics. Phylogenetic studies based on DNA sequences infer that the chimpanzee is our closest living relative. However, when we examine the genomic regions of human and chimpanzee that can be aligned, the divergence rate at the nucleotide level is as little as 1.23%. In this study, we constructed a cis-regulatory element frequency (CREF) matrix for each species. We proposed to decompose the regulatory information by dual-eigen module and polarized gene and cis-motif eigenvectors. Then we align and compare the CREF dual-eigen modules across human, chimpanzee, great ape and orangutan. The top three CREF modules are highly conserved. They comprise the key processes of life. Surprisingly between the fourth and fifth level, the CREF modules underwent a phase transition. Mathematically, it corresponds to a degenerate 2-D eigen-space due to identical singular values. The phase transition led to a human-specific fourth CREF module that regulate long-term memory, cochlea development that is crucial for language and music, social behaviors, and sympathetic nerve systems. The dual-eigen analysis indicates that one key genetic driving force for the phase transition of regulatory modules from apes to human are mutations relating to Alu. Evidences were collected by checking the cis-regulatory motifs present on Alu elements along the polarized motif eigenvectors. In addition, human-specific repetitive sequences constitute 4.6% of the human genome. We reported 47 human-specific Alu insertions into the proximal gene regulatory regions, most of which are indeed participate in long-term memory, cochlea development, and cognition.

Generalization ability of wide neural networks on $\mathbb{R}$

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We perform a study on the generalization ability of the wide two-layer ReLU neural network on $\mathbb{R}$. We first establish some spectral properties of the neural tangent kernel (NTK): *a*) K_d, the NTK defined on $\mathbb{R}^d$, is positive definite; *b*) $\lambda_i(K_1)$, the i-th largest eigenvalue of K_1, is proportional to i^{-2}. We then show that: *i*) when the width $m \to \infty$, the neural network kernel (NNK) uniformly converges to the NTK; *ii*) the minimax rate of regression over the RKHS associated to K_1 is $n^{-2/3}$; *iii*) if one adopts the early stopping strategy in training a wide neural network, the resulting neural network achieves the minimax rate; *iv*) if one trains the neural network till it overfits the data, the resulting neural network can not generalize well. Finally, we provide an explanation to reconcile our theory and the widely observed "benign overfitting phenomenon".

A revisit of a viscoelasticity theory

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The viscoelasticity theory proposed in [1,2] has gained popularity over the years, largely because it is amenable to finite element implementation and convenient in accounting for material anisotropy. Recently, a finite-time blow-up solution has been identified [3], signifying an alerting issue concerning its theoretical root. The lack of a thermodynamic foundation has been viewed as a major drawback of this model.

In this talk, I will address the issue by providing a complete thermomechanical theory for the aforementioned finite viscoelasticity model [4]. The derivation elucidates the origin of the evolution equations of that model, with a few non-negligible differences. It is also shown that the conjugate variable and non-equilibrium stress should be differentiated, an issue that has been ignored in prior works. I will discuss the relaxation property of

the non-equilibrium stress in the thermodynamic equilibrium limit and its implication on the form of free energy, which clarifies the failure of a classical model based on the identical polymer chain assumption.

Based on the consistent framework, a set of energy-momentum consistent schemes is constructed for finite viscoelasticity using a *strain-driven* constitutive integration scheme and a generalized *directionality property* for the stress-like variables. I adopt a suite of smooth generalization of the Taylor-Hood element based on Non-Uniform Rational B-Splines for spatial discretization. The element is further enhanced by the grad-div stabilization to improve the discrete mass conservation. I will also discuss recent advancements in designing non-singular algorithmic stresses for energy-momentum consistent schemes [5]. Numerical examples will be provided to justify the effectiveness of the proposed methodology.

[1] J.C. Simo. On a fully three-dimensional finite-strain viscoelastic damage model: formulation and computational aspects. *Computer Methods in Applied Mechanics and Engineering*, 60:153-173, 1987.
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[3] S. Govindjee, T. Potter, and J. Wilkening. Dynamic stability of spinning viscoelastic cylinders at finite deformation. *International journal of solids and structures*, 51:3589-3603, 2014.
[4] J. Liu, M. Latorre, and A.L. Marsden. A continuum and computational framework for viscoelastodynamics: I. Finite deformation linear models. *Computer Methods in Applied Mechanics and Engineering*, 385:114059, 2021.
[5] J. Liu, On the design of non-singular, energy-momentum consistent integrators for nonlinear dynamics using energy splitting and perturbation techniques. *Journal of Computational Physics*, accepted.

Medical imaging analysis in clinical scene

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In clinical scenarios, we often encounter some difficulties when we are engaged in medical image analysis research, such as small samples, lack of modality, multimodality modeling, and model interpretability. In this talk, we will

discuss how artificial intelligence methods can solve the above difficulties for problems such as tumor detection and diagnosis. We will discuss the application of small sample learning, generative adversarial network, radiomics, pathomics, multi-task learning in medical image analysis through specific problems.

Numerical analysis of a fully discrete finite element method for incompressible vector potential MHD system

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We investigate a fully discrete finite element scheme for the three dimensional incompressible magnetohydrodynamic (MHD) problem based on magnetic vector potential formulation. Using a mixed finite element approach, we discretize the model by the fully discrete semi-implicit Euler scheme with the velocity and the pressure approximated by stable MINI finite elements and the magnetic vector potential by edge elements. The formulation enjoys the novel feature that it can always produce an exactly divergence free magnetic induction discretized solution. However, its computational difficulty and efficiency are comparable to the traditional MHD model. We will also discuss some strong convergence results and error estimates for the numerical solutions of the model, as well as the existence and well-posedness of the weak solution of the model. Finally, some numerical examples are carried out to demonstrate both accuracy and efficiency of the fully discrete scheme.

Color image inpainting via robust pure quaternion matrix completion

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In this talk, we study color image inpainting as a pure quaternion matrix completion problem. Our main aim is to propose a new minimization problem with an objective combining nuclear norm and a quadratic loss weighted among three channels. We obtain the error bound in both clean and cor-

rupted regimes. Experimental results are presented to confirm and demonstrate our theoretical findings.

Graph Laplacians and operator networks - ML tools for computational mechanics

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In this talk I will describe two popular concepts in Machine Learning that can play an important role in solving challenging problems in Computational Mechanics. This includes Operator Networks which can be used to construct inexpensive, differentiable surrogates for complex differential and integral operators. It also includes Graph Laplacians which can be used for constructing multi-fidelity models. I will present illustrative examples, and where possible, discuss theoretical estimates for the performance of these algorithms.

TandemAligner: a new parameter-free framework for fast sequence alignment

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The recent advances in complete genomics revealed the previously inaccessible genomic regions (such as centromeres) and enabled analysis of their associations with diseases. However, analysis of variations in centromeres, immunoglobulin loci, and other biomedically important extra-long tandem repeats (ETRs) faces an algorithmic challenge since there are currently no tools for accurate sequence comparison of ETRs. Counterintuitively, the classical alignment approaches, such as the Smith-Waterman algorithm, that work well for most sequences, fail to construct biologically adequate alignments of ETRs. This limitation was overlooked in previous studies since the ETR sequences across multiple genomes only became available in the last year. We present TandemAligner — the first parameter-free sequence alignment algorithm with sequence-dependent alignment scoring that automati-

cally changes for any pair of compared sequences. The inherent limitation of the standard alignment is that the less significant matches of frequent k-mers have the same contribution to the score as the more significant matches of rare k-mers. To address this limitation, TandemAligner prioritizes matches of rare substrings that are more likely to be relevant to the evolutionary relationship between two sequences. We apply TandemAligner to various human centromeres and primate immunoglobulin loci, arrive at the first accurate estimate of the mutation rates in human centromeres, and quantify the extremely high rate of large duplications and deletions in centromeres. This extremely high rate (that the standard alignment algorithms fail to uncover) suggests that centromeres represent the most rapidly evolving regions of the human genome with respect to their structural organization.

This is a joint work with Andrey Bzikadze.

A robust fifth order finite difference Hermite WENO scheme for compressible Euler equations

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In this presentation, we would like to present a robust fifth order finite difference Hermite weighted essentially non-oscillatory (HWENO) scheme for compressible Euler equations following the HWENO with limiter (HWENO-L) scheme (*J. Comput. Phys., 472:111676, 2023*). The HWENO-L scheme reduced storage and increased efficiency by using restricted derivatives only for time discretizations, however, it cannot control spurious oscillations well when facing strong shocks since the derivatives are directly used in spatial discretizations without any restrictions. To address such an issue, our proposed HWENO scheme performs flux reconstructions in the finite difference framework without using the derivative value of a target cell, which can result in a simpler and more robust scheme. The resulting scheme is simpler while still achieving fifth order accuracy, so is more efficient. Besides, numerically we find it is very robust for some extreme problems even without positivity-preserving limiters. The proposed scheme also inherits advantages of previous HWENO schemes, including arbitrary positive linear weights in the flux reconstructions, compact reconstructed stencils, and high resolution. Numerical tests are performed to demonstrate the fifth order accuracy,

efficiency, robustness, and high resolution of proposed HWENO scheme.

Motifs in multiple sequence alignments

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We present a novel approach to the information processing of multiple sequence alignments (MSA). The framework is based on deriving relational signatures, obtained from small subsamples of sequences of the MSA. It is well suited for the early detection of emerging variants. Typically sequence similarities are used in order to infer lineages, partitioning into blocks of sequences exhibiting specific characteristic mutations. We suggest here the inference of an inherent organization of the MSA based on a notion of relational phenotype (motif). Such a motif is realized by small numbers of sequences. The relations manifest via co-evolving sites and are consequently not directly tied to mutations. However, in the presence of selection pressure, this co-evolution is non random. Motifs can be expressed in terms of a particular type of simplicial complex, whose simplices are endowed with specific weights, affecting the homology of the complex.

An EMA-conserving, pressure-robust and *Re*-semi-robust reconstruction method for simulation of incompressible Navier–Stokes equations

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Proper EMA-balance (E: kinetic energy; M: momentum; A: angular momentum), pressure-robustness and *Re*-semi-robustness (*Re*: the Reynolds number) are important properties of Navier-Stokes simulations with exactly divergence-free elements. However, the construction of these elements is not trivial in most cases. In this talk, based on the pressure-robust reconstruction methods in [cf. A. Linke and C. Merdon, Comput. Methods Appl. Mech. Engrg. 2016], we propose a novel reconstruction method for a class of non-divergence-free simplicial elements which admits almost all the above

properties. The only exception is the energy balance, where kinetic energy should be replaced by a properly discrete form. Some numerical comparisons with exactly divergence-free methods, pressure-robust reconstructions and the EMAC scheme are provided to confirm our theoretical results.

This is a jointed work with Dr. Xu Li.

Surface reconstruction based modified Gauss formula

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Surface reconstruction aims at reconstructing continuous surface from discrete point cloud. This is a fundamental problem in computer vision, 3D modeling and many other applications. In this talk, we introduce several surface reconstruction methods based famous Gauss formula in potential theory. Gauss formula provide an explicit integral formula for indicator function. Then surface reconstruction can be transformed to be an integral over the surface which can be computed efficiently by proper quadrature rule and fast multipole method (FMM). For point cloud without oriented normals, Gauss formula also gives effective reconstruction in an implicit manner. Extensive experiments show that our methods are very effective and efficient, even outperform learning based methods.

Computational approaches for metagenomic contig binning using Hi-C data

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Recovering high-quality metagenome-assembled genomes (MAGs) from complex microbial ecosystems remains challenging. Recently, high-throughput chromosome conformation capture (Hi-C) has been applied to simultaneously study multiple genomes in natural microbial communities. We developed several statistical and computational approaches including HiCZin, HiCBin and ViralCC to resolve high-quality bacterial and viral MAGs utilizing Hi-C con-

tact maps. Applications of these algorithms to several metagenomic data sets enable discovery of novel microbial genomes and virus-host interactions.

Bound-preserving and phase-wise conservative schemes for multi-phase flow in porous media

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Multi-phase flow in porous media has wide applications in energy and environment. Petroleum reservoir engineers spent great efforts in the development and production of oil and gas reservoirs by conducting and interpolating the simulation of multiphase flow in porous geological formation. Meanwhile, environmental scientists use subsurface flow and transport models to investigate and compare for example various schemes to inject and store CO2 in subsurface geological formations. One basic requirement for accurate modeling and simulation of multiphase flow is to have the predicted physical quantities sit within a physically meaningful range. For example, the predicated saturation should sit between 0 and 1. Unfortunately, popular simulation methods used in the industries do not preserve physical bounds. A commonly used fix to this problem is to simply apply a cut-off operator, say, to the computed saturation at each time step whenever it becomes larger than one. However, this cut-off practice does not only destroy the local mass conservation, but it also damages the global mass conservation, which seriously ruins the numerical accuracy and physical interpretability of the simulation results. In this talk we present our work on semi-implicit algorithms for multiphase flow in porous media with possibly multiple capillary pressure functions, one in each subdomain. Our proposed algorithms are locally mass conservative for all phases. They are able to accurately reproduce the spatial discontinuity of saturation due to different capillary pressure functions, and they correctly ensure that the total velocity is continuous in the normal direction. Moreover, the new schemes are unbiased with regard to the phases and the saturations of all phases are bounds-preserving (under certain conditions). The proposed semi-implicit algorithms are derived from our novel splitting of variables based on the underlying physics. Numerical examples are presented to demonstrate the efficiency and robustness of the new algorithms. This presentation is based on our joint work with Huangxin

Chen (Xiamen University), Jisheng Kou (Shaoxing University), Xiaolin Fan (Guizhou Normal University), and Tao Zhang (KAUST).

Optimal transport for single-cell data analysis

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Advances in single-cell technologies enable comprehensive studies of heterogeneous cell populations that make up tissues, the dynamics of developmental processes, and the underlying regulatory mechanisms that control cellular functions. The computational integration of single-cell datasets is drawing heavy attention toward making advancements in machine learning and data science. Optimal transport (OT) is a powerful tool in the analysis of complex data, as it learns an optimal cost-effective mapping between data distributions. In this talk, I will report our recent work on developing OT-based data analysis methods for single-cell multi-omics integration and dynamic inference of time series single-cell data.

Approximation of curved domains with polygonal meshes

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In the finite element discretization of second order elliptic equations on 2D domains with curved boundary, it is well-known that the discrepancy between the curved physical domain and the polygonal approximation domain leads to a loss of accuracy for high order discretizations. Popular treatments, for example the isoparametric elements and the isogeometric analysis, do not apply directly to discretizations on polygonal meshes, such as the weak Galerkin methods and the virtual element methods, etc. In this work, we explore possible ways for these discretizations to achieve optimal convergence, by using properties of the polygonal mesh and boundary correction techniques.

Applied harmonic analysis and particle dynamics for designing neural message passing on graphs

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Graph representation learning has broad applications applications from recommendation systems to drug and protein designs. In this talk, I will talk about using harmonic analysis and particle systems to design useful neural message passing with theoretically guaranteed separability and efficient computation. These message passings are proved to have strictly positive lower bounded Dirichlet energy and thus to circumvent the oversmoothing problem appearing in many spatial GNNs, when the node features are indistinguishable as the network deepens.

Geometric quasilinearization (GQL) for bound-preserving schemes

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Solutions to many partial differential equations satisfy certain bounds or constraints. For example, the density and pressure are positive for equations of fluid dynamics, and in the relativistic case the fluid velocity is upper bounded by the speed of light, etc. As widely realized, it is crucial to develop bound-preserving numerical methods that preserve such intrinsic constraints. Exploring provably bound-preserving schemes has attracted much attention and is actively studied in recent years. This is however still a challenging task for many systems especially those involving nonlinear constraints.

Based on some key insights from geometry, we systematically propose a novel and general framework, referred to as geometric quasilinearization (GQL), which paves a way for studying bound-preserving problems with nonlinear constraints. The essential idea of GQL is to equivalently transfer all nonlinear constraints into linear ones, through properly introducing some free auxiliary variables. We establish the fundamental principle and general theory of GQL via the geometric properties of convex regions, and propose three simple effective methods for constructing GQL. We apply the

GQL approach to a variety of partial differential equations, and demonstrate its effectiveness and remarkable advantages for studying bound-preserving schemes, by diverse challenging examples and applications which cannot be easily handled by direct or traditional approaches.

Discontinuous Galerkin methods for magnetic advection-diffusion problems

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We devise and analyze a class of the primal discontinuous Galerkin methods for magnetic advection-diffusion problems based on the weighted-residual approach. In addition to the upwind stabilization, we find a new mechanism under the vector case that provides more flexibility in constructing the schemes. For the more general Friedrichs system, we show the stability and optimal error estimate, which boil down to two core ingredients – the weight function and the special projection – that contain information of advection. Numerical experiments are provided to verify the theoretical results.

Optimal clustering by Lloyd algorithm for low-rank mixture model

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We investigate the computational and statistical limits in clustering matrix-valued observations. We propose a low-rank mixture model (LrMM), adapted from the classical Gaussian mixture model (GMM) to treat matrix-valued observations, which assumes low-rankness for population center matrices. A computationally efficient clustering method is designed by integrating Lloyd algorithm and low-rank approximation. Once well-initialized, the algorithm converges fast and achieves an exponential-type clustering error rate that is minimax optimal. Meanwhile, we show that a tensor-based spectral method delivers a good initial clustering. Comparable to GMM, the minimax optimal clustering error rate is decided by the separation strength, i.e, the minimal

distance between population center matrices. By exploiting low-rankness, the proposed algorithm is blessed with a weaker requirement on separation strength. Unlike GMM, however, the statistical and computational difficulty of LrMM is characterized by the signal strength, i.e, the smallest non-zero singular values of population center matrices. Evidences are provided showing that no polynomial-time algorithm is consistent if the signal strength is not strong enough, even though the separation strength is strong. The performance of our low-rank Lloyd algorithm is further demonstrated under sub-Gaussian noise. Intriguing differences between estimation and clustering under LrMM are discussed. The merits of low-rank Lloyd algorithm are confirmed by comprehensive simulation experiments. Finally, our method outperforms others in the literature on real-world datasets

Joint inference of clonal structure using single-cell genome and transcriptome sequencing data

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Latest developments in high-throughput single-cell genome (scDNA) and transcriptome (scRNA) sequencing technologies enabled cell-resolved investigation of tissue clones. However, it remains challenging to cluster and couple single cells for heterogeneous scRNA and scDNA data generated from the same cell population. In this work, we present a computational framework – CCNMF, which uses a novel Coupled-Clone Non-negative Matrix Factorization technique to jointly infer clonal structure for scDNA and scRNA data generated from the same specimen. CCNMF couples single cells by linking copy number and gene expression profiles through their general concordance. We validated CCNMF using both simulated and real cell mixture bench-

marks and fully demonstrated its robustness and accuracy. As real world applications of CCNMF, we analyzed scRNA and scDNA data from an ovarian cancer cell mixture, a gastric cancer cell line, and a primary gastric cancer. We resolved the underlying clonal structures and identified dosage-sensitive genes between coexisting clones. In summary, CCNMF is a coherent computational framework that simultaneously resolves genome and transcriptome clonal structures, facilitating understanding of how cellular gene expression changes along with clonal genome alternations. Availability: The R package of CCNMF is available at https://github.com/labxscut/CCNMF.

High order numerical scheme for the nonlinear quantum Zakharov system

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In this paper, we design an energy conserving local discontinuous Galerkin (LDG) method to solve the quantum Zakharov system (QZS). We first give theoretical proof for the conservation of mass and energy and then focus our discussion on the priori estimates for the semi-discrete approximation of the QZS. With the proof for the L^2 boundedness of the numerical solutions and the discrete Poincaré inequalities, we obtain the optimal error estimates. Next, we develop a decoupled and implicit linear fully-discrete scheme using the semi-implicit spectral deferred correction (SISDC) method for temporal discretization. Another strength of our approach is the arbitrary high accuracy which depends only on the degree of the approximating piecewise polynomials. Finally, several numerical examples are reported to validate it and the conservation properties. Especially, the second-order convergence rate of the QZS to its limiting model in the semi-classical limit is achieved as expected.

Energy dissipation preserving Runge-Kutta methods for phase-field models

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As gradient flows, energy dissipation is an intrinsic property of phase-field models. High performance energy stability preserving numerical schemes are highly desired. Recent decades, many such well known numerical schemes are developed, such as convex splitting, stabilization technique, IEQ approach, SAV approach, and etc. Basically, most high-order energy stability preserving schemes are multistep methods and the so-called energy stability is established via modified energy. In this talk, I will introduce several single step linear Runge-Kutta (RK) methods, including explicit RK (EX-RK) methods, implicit explicit RK (IMEX-RK) methods and exponential time differencing Runge-Kutta (ETD-RK) methods. All these RK methods are shown to preserve the original energy decaying property. For EX-RK and IMEX-RK methods, only using the butcher table we provide a systematical framework to determine whether a scheme can preserve the energy stability or not. We prove the original energy stability based on the Lipschitz continuity assumption of nonlinear terms and a transformation of the nonlinear stability into quadratic form stability via a novel technique.

Towards an understanding of soft sparsity in regression learning

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Sparsity has played a key role in statistical and machine learning theories. Since hard sparsity in terms of the ℓ_0 constraint on effects of the predictors involved is often unlikely to be proper, soft sparsity is more realistic and useful in many applications. In this talk, we will examine how soft sparsity quantifications are linked to the ability to learn a target function. A contrast will be made between model selection and model averaging: How does the sparsity nature of the coefficients in series expansions determine if and when model averaging can significantly improve over model selection. We will also

provide an insight on compressibility of a deep neural network via a theoretical bounding of the compression error in terms of soft sparsity measures of the weight parameters in the pre-trained network. A backward pruning method is proposed and shown to be effective in compressing a deep network while maintaining its predictive accuracy.

Controlling the false discovery rate in structural sparsity: split knockoffs

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Controlling the False Discovery Rate (FDR) in a variable selection procedure is critical for reproducible discoveries, which receives an extensive study in sparse linear models. However, it remains largely open in the scenarios where the sparsity constraint is not directly imposed on the parameters, but on a linear transformation of the parameters to be estimated. Examples include total variations, wavelet transforms, fused LASSO, and trend filtering, etc. In this paper, we propose a data adaptive FDR control in this transformational or structural sparsity setting, the Split Knockoff method. The proposed scheme exploits both variable and data splitting. The linear transformation constraint is relaxed to its Euclidean proximity in a lifted parameter space, yielding an orthogonal design for improved power and orthogonal Split Knockoff copies. To overcome the challenge that exchangeability fails due to the heterogeneous noise brought by the transformation, new inverse supermartingale structures are developed for provable FDR control. Simulation experiments show that the proposed methodology achieves desired FDR and power. An application to Alzheimer's Disease study is provided that atrophy brain regions and their abnormal connections can be discovered based on a structural Magnetic Resonance Imaging dataset (ADNI). This is a joint work with CAO, Yang and SUN, Xinwei.

Cross-linked peptide identification using a protein-feedback method

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Improving the sensitivity of protein-protein interaction detection and protein structure probing is a principal challenge in cross-linking mass spectrometry (XL-MS) data analysis. In this talk, we propose an exhaustive cross-linking search method with protein feedback (ECL-PF) for cleavable XL-MS data analysis. ECL-PF adopts an optimized α/β mass detection scheme and establishes protein-peptide association during the identification of cross-linked peptides. Existing major scoring functions can all benefit from the ECL-PF workflow to a great extent. In comparisons using synthetic datasets and hybrid simulated datasets, ECL-PF achieved three-fold higher sensitivity over standard techniques. In experiments using real datasets, it also identified 65.6% more cross-link spectrum matches and 48.7% more unique cross-links.

This is a joint work with C. Zhen, S. Dai, S. Lai, Y. Lin, S. Lian, X. Fan, and N. Li.

Balanced augmented Lagrangian method with applications to compressive sensing and imaging

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We consider the canonical convex minimization model with both linear equality and inequality constraints, and reshape the classic augmented Lagrangian method (ALM) by better balancing its subproblems. The resulting subproblems of the balanced ALM handle the objective function and the coefficient matrix separately. The balanced ALM improves the classic ALM, as well as primal-dual type methods that are widely used in imaging, by its larger applicable range and easier subproblems. We also show its efficiency for some applications in compressive sensing and image restoration.

Rank-one prior: real-time scene recovery

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Scene recovery is a fundamental imaging task with several practical applications, including video surveillance and autonomous vehicles, etc. In this talk, we provide a new real-time scene recovery framework to restore degraded images under different weather/imaging conditions, such as underwater, sand dust and haze. A degraded image can actually be seen as a superimposition of a clear image with the same color imaging environment (underwater, sand or haze, etc.). Mathematically, we can introduce a rank-one matrix to characterize this phenomenon, i.e., rank-one prior (ROP). Using the prior, a direct method with the complexity O(N) is derived for real-time recovery. For general cases, we develop ROP + to further improve the recovery performance. Comprehensive experiments of the scene recovery illustrate that our method outperforms competitively several state-of-the-art imaging methods in terms of efficiency and robustness.

Recent progress on multiscale computational methods

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Complex nonlinear interplays of multiple scales give rise to many interesting physical phenomena and pose significant difficulties for the computer simulation of multiscale PDE models in areas such as reservoir simulation, high-frequency scattering, radiative transfer, and crack propagation. In this talk, we report our recent work on multiscale computational methods, which are either more "conventional" multiscale methods for PDEs with heterogeneous coefficients or variational models for crystalline defects, or machine learning-based model reduction methods.

Intelligent spatial transcriptomics: paving the way for deciphering tissue architecture

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Technological advances in spatial transcriptomics are critical for a better understanding of the structure and function of tissues in biological research. Recently, the combination of intelligent/statistical algorithms and spatial transcriptomics are emerging to pave the way for deciphering tissue architecture. In this talk, I will introduce our efforts to advance intelligent spatial transcriptomics. We first develop a graph attention auto-encoder framework STAGATE to accurately identify spatial domains by learning low-dimensional latent embeddings via integrating spatial information and gene expression profiles. We validate STAGATE on diverse spatial transcriptomics datasets generated by different platforms with different spatial resolutions. STAGATE could substantially improve the identification accuracy of spatial domains, and denoise the data while preserving spatial expression patterns. Importantly, STAGATE could be extended to multiple consecutive sections to reduce batch effects between sections and extract three-dimensional (3D) expression domains from the reconstructed 3D tissue effectively. Based on this, we also 1) develop STAMarker for identifying spatial domain-specific variable genes, 2) design STAligner for integrating spatial transcriptomics of multiple slices from diverse biological scenarios, and 3) illustrate the effectiveness of the graph attention auto-encoder for spatial clustering of spatial metabolomics.

Learning the underlying unified coordinate system in single-cell data

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Building an atlas of all human cell types with their gene expression properties at single-cell resolution can provide a fundamental reference to future human biology and medicine. Cells exhibit multifaceted heterogeneity at multiple

scales. Finding the major attributes that can be used to index or sort the cells with regard to different aspects of the heterogeneity is important for building and utilizing cell atlases. For this purpose, we developed a multidimensional coordinate system UniCoord for different physical and biological attributes of cells by adopting a supervised variational autoencoder (VAE) neural network model. We trained UniCoord on the first cell-centric assembled human single-cell atlas hECA to make it represent the diversity of healthy human cells. Experiments showed that UniCoord is able to capture key cellular features of spatial, temporal and functional gradients from massive data. These features are sufficient for accurate data reconstruction and label identification and can be interpolated to predict intermediate cell states between two discrete cell groups for studying cell state transition and cell type differentiation. UniCoord provides a prototype for a learnable universal coordinate framework for organizing sophisticated cell atlases to enable better analyzing the highly orchestrated functions and multifaceted heterogeneities of diverse cells of an organ, a system or the whole human body.

Numerical methods for nonlinear Schrödinger equations with random potentials

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In this talk, we consider the numerical solution of a nonlinear Schrödinger equation with spatial random potential. The randomly shifted quasi-Monte Carlo lattice rule combined with the time-splitting pseudospectral discretization is applied and analyzed. The nonlinearity in the equation induces difficulties in estimating the regularity of the solution in random space. By the technique of weighted Sobolev space, we identify the possible weights and show the existence of QMC that converges optimally at the almost-linear rate without dependence on dimensions. The full error estimate of the scheme is established. Finally, we present numerical results to verify the accuracy and investigate the Anderson localization phenomenon.

Statistical inference of cell-type-specific gene co-expression from single cell and bulk RNA-seq data

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The inference of gene co-expressions from microarray and RNA-sequencing (RNA-seq) data has led to rich insights on biological processes and disease mechanisms. However, the bulk samples analyzed in most studies are a mixture of different cell types. As a result, the inferred co-expressions are confounded by varying cell type compositions across samples and only offer an aggregated view of gene regulations that may be distinct across different cell types. In this talk, we introduce two new statistical methods for inferring cell-type-specific co-expressions. Firstly, we discuss CS-CORE, a method that explicitly accounts for the high sequencing depth variations and measurement errors present in single cell data for estimating and testing cell-type-specific co-expression. When applied to analyze multiple scRNA-seq datasets, CS-CORE identified cell-type-specific co-expressions and differential co-expressions that were more reproducible and/or more enriched for relevant biological pathways than those inferred from the existing methods. Secondly, we introduce CSNet, a flexible framework to estimate cell-type-specific gene co-expressions from the rich collection of bulk RNA-seq data in the past 15 years. The general framework in CS-CORE and CSNet can be adopted to integrate single cell and bulk RNA-seq data for more efficient use of the accumulating data in different diseases.

A mass conservative scheme for the coupled Brinkman-Darcy flow and transport

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In this talk, I will present a strongly mass conservative scheme for the coupled Brinkman-Darcy flow and transport. Staggered DG method and mixed finite element method are judiciously balanced to ensure the mass conservation. Moreover, the interface conditions are naturally incorporated into the formulation without resorting to Lagrange multiplier. In particular, the

scheme is robust with respect to the values of the viscosity, which makes it highly flexible for a variety of applications. Using the velocity generated from the coupled Brinkman-Darcy flow, the upwinding staggered DG method is devised for the transport equation. A rigorous convergence error analysis is performed for the proposed scheme, showing the optimal convergence error estimates. Several numerical experiments will be presented to demonstrate the performance of the proposed scheme.

3 Contributed Talks

Velocity and energy of periodic travelling internal waves

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For a periodic travelling irrotational wave propagating at the interface between two homogeneous, incompressible and inviscid fluids, we generalise the Stokes definitions for the velocity of the wave propagation in a two-layer fluid framework. We prove, under certain monotonic conditions imposed on the horizontal velocity of the motion at the interface, that the mean horizontal velocity of propagation of the wave is greater than the generalised mean horizontal velocity of the mass of the fluid. We show that, for internal waves of small amplitude, the excess kinetic and potental energy densities of the fluid per horizontal unit area have the same magnitude, but different signs. For the nonlinear setting, we prove that the excess potential energy density is positive, whereas the kinetic is negative.

Multi-classification using one-versus-one deep learning strategy with joint probability estimates

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The One-versus-One (OvO) strategy is a stream of multi-classification models which focus on training binary classifiers between each pair of classes. While the OvO strategy takes the advantage of balanced training data, the classification accuracy is usually hindered by the voting mechanism to combine all the binary classifiers. In this paper, a novel OvO multi-classification model incorporating joint probability measure is proposed under the deep learning framework. In the proposed model, a two-stage algorithm is developed to estimate the class probability from the pairwise binary classifiers. Given the binary classifiers, the pairwise probability estimate is calibrated by a distance measure on the separating feature hyperplane. From that, the class probability of the subject is estimated by solving a joint probability based distance minimization problem. Numerical experiments in different applica-

tions show that the proposed model achieves generally higher classification accuracy than other state-of-the-art models.

Hyperspectral image analysis with spatial-spectral reconstruction and diffusion geometry-based clustering

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Hyperspectral images, containing a hundred or more spectral bands of reflectance, have become a crucial data source in various disciplines such as natural and social sciences, agriculture, and environmental monitoring. With the advancements in remote sensing technology, these images are often generated in large quantities and at a relatively coarse spatial resolution. This situation necessitates the development of unsupervised machine learning algorithms for automatic analysis, enabling researchers to efficiently process and interpret this vast amount of data.

In response to this need, we introduce the Spatial-Spectral Image Reconstruction and Clustering with Diffusion Geometry (DSIRC) algorithm, specifically designed for partitioning pixels in highly mixed hyperspectral images. DSIRC mitigates measurement noise and enhances image quality through a shape-adaptive reconstruction procedure, ensuring accurate representation of the underlying spatial and spectral information. In particular, the DSIRC algorithm identifies spectrally correlated pixels within a data-adaptive spatial neighborhood for each pixel, taking into account the inherent spatial relationships. It then reconstructs the pixel's spectral signature using its neighbors' signatures, preserving the essential characteristics of the scene. Subsequently, the algorithm locates high-density, high-purity pixels distant in diffusion distance, a data-dependent metric that captures the inherent structure of the hyperspectral data. These pixels are treated as cluster exemplars and assigned a unique label. For the remaining non-modal pixels, the DSIRC algorithm labels them based on their diffusion distance-nearest neighbor of higher density and purity that has been previously labeled. This approach ensures a consistent and accurate clustering of the entire dataset.

The strong numerical results obtained from the application of DSIRC indicate that incorporating spatial information through image reconstruc-

tion significantly improves the performance of pixel-wise clustering. Consequently, DSIRC offers an efficient tool for analyzing large-scale hyperspectral imagery, paving the way for more accurate and comprehensive understanding of land use and land cover.

Deep learning-based 3D localization on rotating point spread function with applications on telescope imaging

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We consider the high-resolution imaging problem of 3-dimensional (3D) point source image recovery from 2-dimensional data using a method based on point spread function (PSF) engineering. The method involves a new technique based on the use of a rotating PSF with a single lobe to obtain depth from defocus. The amount of rotation of the PSF encodes the depth position of the point source. Applications include high-resolution single-molecule localization microscopy as well as the localization of space debris using a space-based telescope. Instead of applying a model-based optimization, we introduce a convolutional neural network (CNN)-based approach to automatically localize space debris in full 3D space. A hard sample training strategy is proposed to further improve the performance of CNN. Contrary to the traditional model-based method, our technique is efficient and outperforms the current state-of-the-art method by more than 11% precision with a comparable improvement in the rate of recall.

Generalization analysis of pairwise learning for ranking with deep neural networks

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Pairwise learning is widely employed in ranking, similarity and metric learning, AUC maximization, and many other learning tasks involving sample pairs. Pairwise learning with deep neural networks was considered for ranking, but there lacks enough theoretical understanding about this topic. In this talk, we apply symmetric deep neural networks to pairwise learning for

ranking with a hinge loss ϕ_h and carry out generalization analysis for this algorithm. A key step in our analysis is to characterize a function which minimizes the risk. This motivates us to firstly find the minimizer of ϕ_h-risk and then design our two-part deep neural networks with shared weights, which induces the anti-symmetric property of the networks. We present convergence rates of the approximation error in terms of function smoothness and a noise condition and give an excess generalization error bound by means of properties of the hypothesis space generated by deep neural networks. Our analysis is based on tools from U-statistics and approximation theory.

Mathematical modelling of blood flow through multiple stenoses in a narrow artery

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In this work, blood is considered as a non-Newtonian Kuang-Luo (K-L) fluid model, with no-slip conditions at the arterial wall. In fact, the main properties of K-L fluid model are that the plasma viscosity and yield stress play a very important role. These param- eters make this fluid remarkably similar to blood, however, when we change these parameters the flow characteristics change significantly. We have derived a numerical expression for the blood flow characteristics such as resistance to blood flow, blood flow rate, axial velocity, and skin friction. These numerical expressions have been solved by MATLAB 2021 software and discussed graphically. Furthermore, these results have been compared with Newtonian fluid and observation made that resistance to blood flow and skin friction is decreased when blood is changed from non-Newtonian to Newtonian fluid.

Spherical signal processing via framelets and convolutional neural networks

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Wavelet/Framelet analysis has been one of the central topics in applied and computational harmonic analysis and has achieved remarkable success in

many real-world applications. However, in practice, signals defined on a spherical surface rather than in Euclidean spaces arise in various situations and thus extending the theory and algorithms to spherical data is in great demand. In this work, we develop a general theoretical framework for constructing Haar-type tight framelets on any compact set with a hierarchical partition. In particular, we construct a novel area-regular hierarchical partition on the 2-sphere and establish its corresponding spherical Haar tight framelets with directionality. We conclude by evaluating and illustrating the effectiveness of our area-regular spherical Haar tight framelets in several denoising experiments. Furthermore, we propose a convolutional neural network (CNN) model for spherical signal denoising which employs the fast framelet decomposition and reconstruction algorithms. The experiment results show that our proposed CNN model is generative, robust, and outperforms threshold methods.

A 3-stage spectral-spatial method for hyperspectral image classification

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Hyperspectral images often have hundreds of spectral bands of different wavelengths captured by aircraft or satellites that record land coverage. Identifying detailed classes of pixels becomes feasible due to the enhancement in spectral and spatial resolution of hyperspectral images. In this work, we propose a novel framework that utilizes both spatial and spectral information for classifying pixels in hyperspectral images. The method consists of three stages. In the first stage, the pre-processing stage, the Nested Sliding Window algorithm is used to reconstruct the original data by enhancing the consistency of neighboring pixels and then Principal Component Analysis is used to reduce the dimension of data. In the second stage, Support Vector Machines are trained to estimate the pixel-wise probability map of each class using the spectral information from the images. Finally, a smoothed total variation model is applied to ensure spatial connectivity in the classification map by smoothing the class probability tensor. We demonstrate the superiority of our method against three state-of-the-art algorithms on six benchmark hyperspectral datasets with 10 to 50 training labels for each

class. The results show that our method gives the overall best performance in accuracy even with a very small set of labeled pixels. Especially, the gain in accuracy with respect to other state-of-the-art algorithms increases when the number of labeled pixels decreases, and, therefore, our method is more advantageous to be applied to problems with a small training set. Hence, it is of great practical significance since expert annotations are often expensive and difficult to collect.

A generic algorithm framework for distributed optimization over the time-varying network with communication delays

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In this talk, we will discuss the distributed optimization problem (DOP) over the time-varying communication network with communication delays. The existing distributed optimization algorithms (DOAs) cannot be directly applied to DOPs over the time-varying network with communication delays. In our work, by adding new virtual agents and redefining communication links, some delay properties are realized and existing DOAs can then be reused to solve the DOPs. Thus, a generic algorithm framework is established which can apply to many important DOAs, such as the mirror descent algorithm and dual averaging algorithm, to solve DOPs over the time-varying network with communication delays. The convergence results of the DOAs are established and verified under the generic algorithm framework.

Localized necking and bulging of finitely deformed residually stressed solid cylinder

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In this paper we investigate the influence of residual stress on the stability of a solid circular cylinder subject to axial extension. The nonlinear theory of

elasticity is used to derive the equations governing the linearized incremental deformations superimposed on a known finitely deformed configuration. Specialized to the neo-Hookean model with residual stress, the bifurcation analysis results in the exact bifurcation condition for zero and periodic modes, based on the Stroh formalism. An expansion technique is adopted to treat singularities in the governing equations. We investigate three loading scenarios, specifically, an increase in axial stretch with constant residual stress, an increase in residual stress with fixed axial length or fixed axial force. In each case the zero mode, corresponding to a localized bifurcation, occurs first. The explicit bifurcation condition for zero mode is derived, which accounts for the geometric dimensions, the residual stress and the axial elongation on the stability of the solid cylinder. The critical values of the residual stress and the axial force for localized necking or bulging to occur are identified. In particular, we show that a reduction in residual stress delays the onset of localized necking. At constant values of pre-stretch, with $1.5 < \lambda < 2.10692$, localized necking occurs at a critical residual stress, localized bulging occurs when $\lambda > 2.10692$. We use Maxwell's equal-area rule to characterize the two-phase deformation consisting of necked and bulged regions. It is shown that the Maxwell values of stretch identify the radii of the two regions, which are connected by a transition zone that translates along the cylinder. At the completion of two-phase deformation the stretch is again uniform.

Approximation of smooth functionals using deep ReLU networks

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In recent years, deep neural networks have been employed to approximate nonlinear continuous functionals F defined on $L^p([-1,1]^s)$ for $1 \leq p \leq \infty$. However, the existing theoretical analysis in the literature either is unsatisfactory due to the poor approximation ability, or does not apply to the rectified linear unit (ReLU) activation function. This paper aims to investigate the approximation power of functional deep ReLU networks in two settings: F is continuous with a modulus of continuity, and F has higher order Fréchet derivatives. A novel functional network structure is proposed

to extract features of higher order smoothness harbored by the target functional F. Quantitative rates of approximation in terms of the depth, width and total number of weights of neural networks are derived for both settings. We give logarithmic rates when measuring the approximation error on the unit ball of a Hölder space. In addition, we establish nearly polynomial rates (i.e., rates of the form $\exp\left(-a(\log M)^b\right)$ with $a > 0, 0 < b < 1$) when measuring the approximation error on a space of analytic functions. Lastly, our work may also shed some light on improving rates of approximation when using deep ReLU networks to learn nonlinear operators.
Keywords: Approximation theory, deep learning theory, ReLU, smooth functionals, Fréchet derivative, polynomial rates.

Computing diffraction anomalies as nonlinear eigenvalue problems

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When planar electromagnetic waves illuminate on a diffraction grating or other periodic structures, reflected and transmitted waves in different radiation channels are excited and propagate away. Diffraction anomalies such as zero reflection, zero transmission and perfect absorption may arise for incident waves with specific frequencies and/or wavevectors, and these phenomena can be used to manipulate electromagnetic waves and light. The frequencies and wavevectors of anomalies are discretely distributed in the spectrum, and some anomalies may appear only on structures with specific physical parameters. Existing methods for computing anomalies are usually computationally expensive and not very effective, as they require repeatedly solving a boundary value problem in a small parameter region. In this study, different anomalies are computed using an efficient numerical method based on nonlinear eigenvalue formulations, and a contour-integral method is used to solve the nonlinear eigenvalue problems. With this method, all solutions in the selected solution domain can be obtained by a fixed number of calculations, and the results are highly accurate. To demonstrate the new method, numerical examples on structures with periodic arrays of cylinders are provided.

A portfolio optimization problem with consumption constraints

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We consider a portfolio optimization problem of Merton's type in which there is a positive lower bound on the consumption to reflect the minimum living standard constraint in the real world. The problem is formulated as a stochastic control problem with some control constraint. The constraint, although simple, makes the problem much more complicated. The state space consists of two regions: constrained region and unconstrained region, which are part of the solution. We derive the Hamilton-Jacobi-Bellman equations and obtain the explicit solutions and the optimal strategies on both regions. This is a join work with Weidong Tian.

Imaging with localized solutions

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Several applications comprises both image processing and the solution of a differential equation. An example is the inverse problem of seismic migration, where the reconstruction of an underground structure should be carried out with known fields at the source and receivers on the Earth's surface. From a mathematical point of view, the initial-boundary value problem for the wave equation in a half-plane should be solved, where the boundary data are obtained as a result of measurements, can be multiscale and contain a noise.

We present a representation of the solution of the wave equation with built-in processing of boundary data. It is based on continuous wavelet analysis. At the boundary, this representation turns into a decomposition in space-time wavelets. Each wavelet is the boundary data for some highly localized solution of the wave equation. If the propagation velocity is constant, this solution is the exact solution of the wave equation, given by an explicit formula. If the propagation velocity depends on the coordinates, then the

elementary solution is the asymptotic solution, called the Gaussian packet or quasi-photon. It is localized near a point traveling along the rays with a wave speed.

The talk is based on papers joint with Evgeny Gorodnitskiy and on the paper with Ru-Shan Wu and Yu Geng.

Autonomous vehicle active safety control system based on roadside LiDAR and V2X communication

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Safety issues remain the biggest concern for the widespread adoption of autonomous driving. Due to the limited detection range of traditional onboard sensors and the consequent blind spots, accidents could happen if the autonomous vehicle (AVeh) could not detect traffic in the blind spots. This issue is exacerbated in urban environments where there is mixed pedestrian and vehicular traffic.

To address this issue, an AVeh active safety control system for eliminating blind spots is proposed. This system is based on a roadside LiDAR system with V2X communication. 3D LiDAR sensors are placed on the roadside providing a bird's-eye view of the surrounding road areas to perceive, identify and keep track of the road users including traffic in the blind spots. A complete road traffic condition will continuously be communicated to an AVeh via a V2X communication system. The vehicle can then perform necessary analysis for taking required actions to avoid accidents and save lives.

A prototype of the proposed system was built and tested in an AVeh. The test results demonstrated that the system could perceive the complete traffic condition of the surrounding road areas eliminating blind spots, resulting in a greatly improved safety performance.

Generalization guarantees of gradient descent for multi-layer neural networks

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Recently there is considerable progress on understanding the generalization of neural networks (NNs) trained by gradient descent (GD) using the algorithmic stability approach. However, most of them focused on one-hidden-layer NNs and did not systematically address the effect of different network scaling parameters. In this paper, we significantly extend the previous work by establishing the stability and generalization of GD for multi-layer NNs with generic network scaling factors. In particular, we establish the excess population risk bound $\mathcal{O}(1/\sqrt{n})$ for GD in both two-layer and three-layer NNs when the network width satisfies certain qualitative conditions related to the scaling parameter, the size of training data n, and its network complexity (i.e., the norm of the minimizer of the population risk). Our results indicate sufficient or necessary conditions for under-parameterized and over-parameterized NNs trained by GD to achieve the risk rate $\mathcal{O}(1/\sqrt{n})$. Furthermore, we show the larger the scaling parameter or the simpler the network complexity is, the less over-parameterization is needed for GD to achieve the desired error rates. Under a low-noise condition, we obtain a fast risk rate $\mathcal{O}(1/n)$ for GD in both two-layer and three-layer NNs.

Spherical framelets from spherical designs

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We investigate in detail the structures of the variational characterization $A_{N,t}$ of the spherical t-design, its gradient $\nabla A_{N,t}$, and its Hessian $\mathcal{H}(A_{N,t})$ in terms of fast spherical harmonic transforms. Moreover, we propose solving the minimization problem of $A_{N,t}$ using the trust-region method to provide spherical t-designs with large values of t. Based on the obtained spherical t-designs, we develop (semi-discrete) spherical tight framelets as well as their truncated systems and their fast spherical framelet transforms for the practical spherical signal/image processing. Thanks to the large spherical t-designs

and localization property of our spherical framelets, we are able to provide signal/image denoising using local thresholding techniques based on a fine-tuned spherical cap restriction. Many numerical experiments are conducted to demonstrate the efficiency and effectiveness of our spherical framelets, including Wendland function approximation, ETOPO data processing, and spherical image denoising.

On behavior of entropy and Fisher information of some solitons of nonlinear Schrödinger equation

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The shape (envelope profiles) of solitary waves contains intrinsic information, reflecting interaction effects in nonlinear dynamics. How can one quantify its content associated with the wave profile? No study so far has focused on the information aspect of the soliton solutions for nonlinear Schrödinger equations (NLSE). In the propagation of the solitary wave, the information changes over time and position. In this presentation, we show how Shannon entropy and Fisher information of soliton profiles (i.e., solution intensity) for the prototypical cubic NLSE change by numerical computation. We can obtain the analytical expressions for Fisher information for the bright and the dark solitons, whereas we must determine Shannon entropy numerically.

Our results show that the entropy of the bright soliton of sech-type increases monotonically as the dispersion coefficient increases when the nonlinear coefficient is large. We have also computed the two information contents for the solution intensity associated with the three primary solitons for the cubic NLSE in the context of nonlinear optics, i.e. Peregrine waves, Akhmediev breathers, and Kuznetzov-Ma solitons. These information contents have periodic structures, that is, the temporal patterns for Peregrine solitons and Akhmediev breathers show periodic peaks whose heights and intervals depend on the control parameter. Since Fisher information can capture a more detailed (gradient) change in the soliton profiles, it is more informative than Shannon entropy. We confirm this feature for the higher-order solitons of the Akhmediev-Peregrine breathers and the Kuznetzov-Ma solitons, whose profiles are more complex near the origin.

Well-conditioned mode matching method for applications in photonics

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To analyze photonics devices such as optical waveguides, resonant cavities and diffraction gratings, it is necessary to solve the Maxwell's equations numerically. Due to the complexity of the structure, conventional numerical methods, such as the finite difference and finite element methods, are not very efficient. Often, a photonic device consists of several simpler parts for which the dielectric function depends only on one spatial variable. The mode matching method and its many numerical variants have been widely used to analyze photonic devices with simple one-dimensional parts. Since the dielectric function is typically piecewise constant, numerical mode matching methods based on piecewise polynomials, such as the polynomial expansion mode matching method (PEMM) and the pseudo-spectral mode matching method (PSMM), are particularly efficient. However, the condition numbers associated with PEMM and PSMM are often very large, leading to limited accuracy and difficulty in convergence when iterative methods are used. In this paper, we develop a well-conditioned numerical mode matching method based on a spectral Galerkin scheme. We show that this method produces numerical modes with good orthogonality and significantly reduces the condition numbers of the final linear systems.

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