February 9, 2026 - Monday

Parallel Preconditioned Strategies for the Training of Neural Networks

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Training deep neural networks (NNs) gives rise to large-scale, highly nonconvex optimization problems, making optimizer performance sensitive to hyperparameter choice. We present the Additively Preconditioned Trust-Region Strategy (APTS), which is inspired by non-linear domain decomposition methods for the solution of PDEs. In addition, our strategy uses odeas from Trust-Region methods for global convergence control.

Based on a decomposition of the weights, we define local subdomain optimization problems, which provide local nonlinear corrections. We then combine these additively into a global preconditioned trial step. A subsequent global Trust-Region "post-smoothing"-step evaluates the full objective and updates the radius, providing stable progress and mitigating step-size sensitivity.

Building on APTS, we also introduce a non-monotone variant with a windowed acceptance rule that increases step acceptance by permitting controlled non-monotonicity over a recent window.

Numerical examples for the training of neural networks on common datasets as well as for the solution of PDEs with neural networks conclude our presentation.

Randomized Neural Networks for Solving PDEs

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Traditional numerical methods, supported by rigorous mathematical theory, high accuracy, and physical conservation, form the cornerstone of modern scientific computing. Nevertheless, they face intrinsic challenges, including mesh generation for complex geometries, limited ability to capture global structures, repeated reformulation under varying geometries or boundary conditions, the curse of dimensionality, and difficulties in integrating data and uncertainty. Neural-network-based methods have recently emerged as a promising alternative due to their strong expressive power, but conventional training-based approaches remain constrained by nonlinear and non-convex optimization, which limits both accuracy and efficiency.

To overcome these difficulties, we propose a family of Randomized Neural Network (RaNN) methods that integrate the mathematical rigor of classical numerical formulations with the flexibility of neural representations. The framework encompasses RaNN-Petrov-Galerkin (RaNN-PG), local RaNN-DG (LRaNN-DG), LRaNN-HDPG, and LRaNN-finite difference methods. We further introduce an Adaptive-Growth RaNN (AG-RaNN) strategy that uses prior and posterior information to identify informative features, adapt random parameter distributions, and dynamically refine the network architecture, substantially improving approximation accuracy. We also investigate RaNN-based acceleration of operator learning for parameterized PDEs.

Numerical experiments show that RaNN methods are mesh-free, structure-preserving, and highly expressive, achieving high accuracy with relatively few degrees of freedom and extending naturally

to high-dimensional and time-dependent problems. These results highlight RaNN as a promising direction for unifying traditional numerical methods with modern machine learning to enable efficient and accurate PDE solvers.

Hybrid Least Squares/Gradient Descent Methods for DeepONets

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We propose an efficient hybrid least squares/gradient descent method to accelerate DeepONet training. Since the output of DeepONet can be viewed as linear with respect to the last layer parameters of the branch network, these parameters can be optimized using a least squares (LS) solve, and the remaining hidden layer parameters are updated by means of gradient descent form. However, building the LS system for all possible combinations of branch and trunk inputs yields a prohibitively large linear problem that is infeasible to solve directly. To address this issue, our method decomposes the large LS system into two smaller, more manageable subproblems - one for the branch network and one for the trunk network - and solves them separately. This method is generalized to a broader type of L^2 loss with a regularization term for the last layer parameters, including the case of unsupervised learning with physics-informed loss.

From Laplace Regularization to Neural Solvers for Eikonal Equations

Jooyoung Hahn
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The eikonal equation is a fundamental model for distance and travel-time computation in complex geometries, but reliably approximating its viscosity solution on realistic and complex three-dimensional domains remains challenging. I will first present a Laplacian-regularized finite volume approach on polyhedral meshes, where the eikonal equation is interpreted through a vanishing-viscosity viewpoint and discretized by a cell-centered finite volume method with the Soner boundary condition ensuring the correct solution on non-convex domains. This algorithm numerically achieves second-order experimental convergence for smooth test cases, scales efficiently in parallel computing, and significantly reduces computational cost compared with time-relaxed formulations when the region of interest is far from the source set.

Building on this PDE-based foundation, I will then discuss three mesh-free deep learning methods that target the same viscosity solution without relying on a mesh. The first is a neural augmented Lagrangian method, which models the solution as an implicit neural representation and recasts the problem as a constrained optimization: it maximizes a geometric functional subject to a Lipschitz-type gradient constraint and a Soner-type boundary inequality, enforced robustly by an augmented Lagrangian formulation. The second is a viscosity-reduction variational approach for anisotropic eikonal equations, which derives an unconstrained variational problem from the vanishing-viscosity formulation and resolves both nonlinearity and small-viscosity instability via variable splitting and a normalized-output neural network architecture, enabling stable training on discontinuous anisotropic metrics and point-cloud geometry.

The third is a stochastic displacement-based method inspired by the Derivative-Free Loss Method:

instead of minimizing pointwise residuals, it learns local gradient-aligned transport using a Feynman-Kac type stochastic representation, yielding a transport-aware neural solver whose cost is essentially independent of the diffusion scale and which naturally adapts to non-convex domains with obstacles.

Efficient Deep Learning Methods for Very High Dimensional Quasilinear Parabolic PDEs and HJB Equations

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Solving high-dimensional PDEs with deep learning methods is often computationally and memory intensive, primarily due to the need for automatic differentiation to compute large Hessian matrices. We propose a deep random difference method (DRDM) that addresses these issues by approximating the convection-diffusion operator using first-order random differences, avoiding explicit Hessian computation. When incorporated into a Galerkin framework, the DRDM eliminates the need for pointwise evaluation of expectations, resulting in very efficient training procedure. Rigorous error estimates for DRDM are presented for linear PDEs. We further extend the approach to the Hamilton-Jacobi-Bellman (HJB) equations in stochastic optimal control. Numerical experiments demonstrate the efficiency of DRDM for solving quasilinear parabolic PDEs and HJB equations in dimensions up to 100000.

Nonlinear Preconditioning Algorithms with Learning Capability

Li Luo
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Nonlinear preconditioning algorithms have been applied successfully for solving some difficult nonlinear partial differential equations by identifying and balancing the nonlinearities in the system. One of the challenging tasks when applying the methods is to identify the unbalanced nonlinearities. We study some learning-based strategies that identify the bad behavior of a Newton solver from the slow residual subspace of a training problem. Numerical experiments show that the learning-based algorithms are more robust and efficient compared with existing nonlinear solvers.

Transformer: Structure-conforming Operator Learning

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The Transformer has emerged as one of the most advanced neural network architectures, with wide applications in large language models (LLMs), AI for Science, and image/video process. Despite its success, its mathematical foundations remain largely open. This research presents our recent progress toward addressing this gap, structured in two parts. First, we introduce a new perspective

based on Petrov-Galerkin projection and Fourier analysis to better interpret the attention mechanism. Building on this framework, we propose a modified Transformer architecture that admits a clearer mathematical interpretation and exhibits a frequency-bootstrapping property. Second, drawing inspiration from direct sampling methods (DSMs) for inverse problems, we develop a novel feature generation approach: data features are constructed by solving PDEs and then incorporated into the attention mechanism. By embedding a learnable nonlocal kernel, the DSM is naturally reformulated as such the modified attention mechanism. We demonstrate the proposed method on electrical impedance tomography (EIT), a prototypical severely ill-posed nonlinear inverse problem, which achieves superior accuracy over its predecessors and contemporary operator learners.

February 10, 2026 - Tuesday

Learning-accelerated Nonlinear Algebraic Solvers and Applications in Computational Biomechanics

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We consider the numerical simulations of blood flows in the human artery with the incompressible Navier-Stokes equations, and the focus is on the situations when the artery is abnormal due to the existence of stenosis and/or aneurysm. The problem is discretized with a fully implicit finite element method and solved by an inexact Newton based nonlinear solver which converges well when the solution is smooth but the convergence becomes unacceptably slow when abnormality of the artery is severe. For such difficult cases, we introduce a nonlinear preconditioning technique to reduce the stagnation and to speedup the convergence of the inexact Newton method based on an unsupervised learning.

Nonlinear Model Reduction and Scientific Machine Learning for Environmental and Urban Flows with Advection Dominated Features

Giovanni Stabile
The Biorobotics Institute, Sant'Anna School of Advanced Studies, Pisa, Italy

The proportion of the global population living in cities is rapidly increasing and is expected to reach 80% by 2050 . This trend highlights the urgent need for efficient and reliable models of the urban microclimate, which are essential tools for planners and policymakers striving to design more sustainable and comfortable cities. At the urban scale, pollutant dispersion is strongly influenced by daily weather conditions, requiring computational fluid dynamics (CFD) simulations with fine spatial and temporal resolution and repeated evaluations. These demands lead to very high memory and computational costs, making high-performance computing (HPC) indispensable. In addition, such problems exhibit complex solution manifolds with advection-dominated features, where standard linear compression techniques fail due to slow Kolmogorov n-width decay.

In this talk, I will review recent advances in physics-based nonlinear model order reduction (MOR) for problems characterized by these challenges. While purely datadriven methods - such as autoencoders and their variants - can learn nonlinear latent representations and provide accurate predictions where linear methods break down, they often lack interpretability, struggle outside the trainling regime, and fail to exploit the underlying physics during the predictive phase.

To address these limitations, I will present two variants of the nonlinear manifold projection approach previously introduced in other works [1,2], each employing distinct strategies for nonlinear dimensionality reduction and hyper-reduction. The methodology is validated across a range of increasingly complex test cases: from twodimensional nonlinear conservation laws and shallow water equations [3], to supersonic flow past a NACA airfoil with varying Mach number, and finally to incompressible turbulent flow around the Ahmed body with varying slant angle [4].

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Modified BDF Convolution Quadrature for Multi-singularity Problems Arising from Delay Fractional Diffusion-Wave Equations

Seak Weng Vong
University of Macau, Macau, China

In this talk, we focus on the pointwise-in-time error estimates for fractional diffusion-wave equations in the presence of time delay. The semi-discrete solution is derived through the convolution quadrature with the generating function given by κ-step BDF ($\kappa = 1, 2, 3$). For the sake of restoring the desired κ^{th}-order convergence accuracy of BDF_κ, the proper correction formula at the starting $\kappa - 1$ steps is developed. Theoretical result shows that the convergence order is $\min\{(k+1)\alpha, \kappa\}$ at $k\tau^+$, whereas it is α at 0^+, where $k \in N^+$, τ is the time delay, and $\alpha \in (1, 2)$ is the fractional order. Some numerical tests are given to justify the theoretical results. This talk is supported by the University of Macau (File no. MYRG-GRG2024-00100-FST-UMDF)

Optimal Preconditioners for Nonsymmetric Multilevel Toeplitz Systems with Application to Solving Non-local Evolutionary Partial Differential Equations

Siu Long Lei
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Preconditioning for multilevel Toeplitz systems has long been a focal point of research in numerical linear algebra. In this work, we develop a novel preconditioning method for a class of nonsymmetric multilevel Toeplitz systems, which includes the all-at-once systems that arise from evolutionary partial differential equations. These systems have recently garnered considerable attention in the literature. To further illustrate our proposed preconditioning strategy, we specifically consider the application of solving a wide range of non-local, time-dependent partial differential equations in a parallel-in-time manner. For these equations, we propose a symmetric positive definite multilevel τ preconditioner that is not only efficient to implement but can also be adapted as an optimal

preconditioner. In this context, the proposed preconditioner is optimal in the sense that it enables mesh-independent convergence when using the preconditioned generalized minimal residual method. Numerical examples are provided to critically analyze the results and underscore the effectiveness of our preconditioning strategy.

This is a joint work with Yuan-Yuan Huang, Sean Y. Hon, and Lot-Kei Chou, and the trip is supported by the research grant MYRG-GRG2024-00237-FST-UMDF from the University of Macau.

Efficient Nonlinear Preconditioning for Reservoir Simulation History Matching Using Random Features Learning

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Reservoir simulation plays a vital role in subsurface modeling, yet the computational cost of solving large nonlinear systems via Newton's method remains a significant bottleneck, especially in ensemble-based history matching workflows. To address this, machine learning (ML) techniques have been explored to accelerate simulations, with surrogate modeling and nonlinear preconditioning emerging as promising strategies. Building on recent advances in hybrid Newton's method, which integrate ML-based nonlinear preconditioners to improve initial guesses and solver convergence, this work incorporates the local hybrid Newton approach directly into the OPM reservoir simulator. We leverage ensemble-based history matching data to train neural network predictors, focusing on well event nonlinearities, without intrusive modifications to the physical model or solver logic. A key contribution is the application of the SWIM (Sample Where It Matters) method, which drastically reduces training time to under one second on CPU by employing random feature learning, making the overall accelerated history matching process computationally competitive with standard methods. We validate the approach on both the synthetic Drogon field and the Norne field, thus demonstrating improved nonlinear solver performance and runtime efficiency. Our results highlight the practicality and robustness of data-driven nonlinear preconditioning for accelerating reservoir simulations in real-world scenarios.

A High-dimensional Density Estimation Method and Its Application for Solving PDEs

Qifeng Liao
ShanghaiTech University, Shanghai, China

Probability density estimation remains an open challenging problem in computational science and engineering. By coupling the Knothe-Rosenblatt (KR) rearrangement and the flow-based generative model, we developed an invertible transport map, called KRnet, for high-dimensional density estimation. In this talk, we give an overview of KRnet and discuss its adaptive version for the Fokker-Planck equations and stochastic dynamic systems. KRnet for solving Bayesian inverse problems is also studied. This is joint work with Yani Feng, Junjie He, Kejun Tang and Xiaoliang Wan.

Enhancing Stability of Operator Learning for Solving Differential Equations

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Learning solution operators for differential equations with neural networks has shown great potential in scientific computing, but ensuring their stability under input perturbations remains a critical challenge. This paper presents a robust self-supervised neural operator framework that enhances stability through adversarial training while preserving accuracy. We formulate operator learning as a min-max optimization problem, where the model is trained against worst-case input perturbations to achieve consistent performance under both normal and adversarial conditions. We demonstrate that our method not only achieves good performance on standard inputs, but also maintains high fidelity under adversarial perturbed inputs. The results highlight the importance of stability-aware training in operator learning and provide a foundation for developing reliable neural PDE solvers in real-world applications, where input noise and uncertainties are inevitable.

Scientific Machine Learning Approaches to Cardiac Inverse Problems for Reconstructing Stimuli and Ischemia from Pseudo-ECG

Edoardo Centofanti
University of Pavia, Pavia, Italy

Inverse problems play a crucial role in computational cardiology, where the challenge is to infer hidden pathological or functional features from non-invasive measurements. In this work, we address the inverse reconstruction of ischemic regions and the localization of externally applied stimuli from pseudo-electrocardiographic (pseudo-ECG) signals, using the cardiac monodomain model [1] as the underlying physiological framework.

The forward problem maps spatial patterns of ischemia and initial stimulus configurations to body-surface pseudo-ECG signals. To accelerate this mapping, we employ Latent Dynamics Networks (LDNets) [2]| as efficient neural surrogates, enabling fast and accurate simulations. Our analysis spans both 2D square domains and anatomically realistic 3D geometries, including an ellipsoidal mesh that emulates a human cardiac ventricle.

This contribution highlights the growing synergy between deep learning and mechanistic models in tackling complex inverse problems in cardiac electrophysiology. Our work illustrates the promise of neural surrogates not only for accelerating simulations but also for enabling robust inverse reconstructions in potential clinically relevant scenarios. This is a joint work with Giovanni Ziarelli (Politecnico di Milano), Simone Scacchi (University of Milan) and Luca F. Pavarino (University of Pavia).

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February 12, 2026 - Tuesday

Neural Solvers for PDEs with Singularities

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The Chinese University of Hong Kong, Hong Kong, China

Over the last few years, there have been substantial progress and intensive studies on using neural networks for solving PDEs. However, these solvers remain challenging to apply to problems with nonsmooth / singular solutions. In this talk, we present novel neural solvers for PDEs with singularities, including singularity enriched neural networks for Poisson type equations and iterative deep Ritz method. We describe the methods, error analysis, and numerical experiments to illustrate the theory. We also briefly discuss the convergence issue related to the training of the neural networks.

On Second-order Solvers for Training Models in Scientific Machine Learning

Stefano Zampini
King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

In recent years, we have witnessed the emergence of scientific machine learning as a data-driven tool for the analysis, by means of deep-learning techniques, of data produced by computational science and engineering applications. At the core of these methods is the supervised training algorithm to learn the neural network realization, a highly non-convex optimization problem that is usually solved using stochastic gradient methods.

However, distinct from deep-learning practice, scientific machine learning training problems feature a much larger volume of smooth data and better characterizations of the empirical risk functions, which make them suited for conventional solvers for unconstrained optimization.

In this talk, we introduce PETScML, a lightweight software framework built on top of the Portable and Extensible Toolkit for Scientific computation (PETSc) to bridge the gap between deep-learning software and conventional solvers for unconstrained minimization.

Using PETScML, we empirically demonstrate the superior efficacy of a trust region method based on the Gauss-Newton approximation of the Hessian in improving the generalization errors arising from regression tasks when learning surrogate models for a wide range of scientific machine-learning techniques and test cases. All the conventional solvers tested, including L-BFGS and inexact Newton with line-search, compare favorably, either in terms of cost or accuracy, with the adaptive first-order methods used to validate the surrogate models.

Adaptivity in Physics-Informed Neural Networks

Alexander Heinlein
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Physics-informed neural networks (PINNs) are a powerful framework for solving partial differential equations (PDEs), but their accuracy is fundamentally limited by three sources of error: residual sampling, training, and neural network approximation error. In this talk, we focus on adaptive approaches for the first two, and on problems with complex spatial behavior, which pose challenges for standard PINN methods.

First, we show how residual sampling can be improved through adaptive collocation using the Point Adaptive Collocation Method for Artificial Neural Networks (PACMANN), which relocates training points toward regions of high residuals by following residual gradients. To improve the training dynamics and address spectral bias, we consider finite basis PINNs (FBPINNs) based on overlapping domain decomposition, which enable localized representations and improved learning of high-frequency features through an appropriate choice of the domain decomposition.

Computational Modeling of Brugada Syndrome with ST-Segment Elevation and Ventricular Arrhythmias

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Brugada syndrome (BrS) is characterized by coved-type ST-segment elevation in the right precordial leads and an increased risk of ventricular arrhythmias. The mechanisms underlying these ECG manifestations and arrhythmogenic vulnerability remain debated, with evidence implicating both repolarization and depolarization abnormalities. Accumulating observations suggest that BrS reflects an impaired conduction reserve in the right ventricular outflow tract (RVOT). The aim of the present study is to investigate the mechanistic basis of BrS ECG phenotypes and arrhythmia vulnerability using computational modeling. We develop a patient-specific biventricular model incorporating Purkinje-driven activation and a localized RVOT substrate with combined ionic and structural remodeling. Using a lead-field approach, we simulate ECGs for 120 BrS model configurations by sweeping the scaling factors of GNa, Gto, and ICaL, as well as the substrate size. Six representative cases are further examined using the programmed stimulation protocol to assess vulnerability to reentry. Our results show that: (1) coved-type ST-segment elevation with T-wave inversion occurs predominantly for the larger substrate ($R = 30$ mm), under the combined condition of strong Ito augmentation and reductions in ICaL and INa; (2) reducing the substrate size or limiting the extent of ionic remodeling attenuates the phenotype, shifting coved-type elevation toward saddleback-type or non-Brugada patterns; (3) sustained reentry is induced under conditions in which a pronounced inverted T wave is observed; and (4) reducing the substrate size or restoring normal conduction within the substrate suppresses reentry.

Multiscale Computational Modeling of Heterogeneous hiPSC-CM Cardiac Tissues

Sofia Botti
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Human induced pluripotent stem cell-derived cardiomyocytes (hiPSC-CMs) provide a powerful platform for investigating human cardiac electrophysiology and for supporting safety pharmacology studies. However, their intrinsic heterogeneity-typically involving mixtures of atrial-like and ventricular-like phenotypes-and the indirect nature of multielectrode array (MEA) [1] recordings make the interpretation of field potential (FP) biomarkers challenging. A quantitative understanding of how MEA derived metrics reflect the underlying action potential (AP) dynamics, which represent the gold standard, is still limited but essential for establishing robust and translatable *in-vitro* readouts [2]. In this work, we present a computational framework that couples the bidomain model with a detailed representation of MEA electrodes to perform an *in-silico* correlation study between FP- and AP-based electrophysiological biomarkers in heterogeneous hiPSC-CM tissues [3]. We first analyze a large set of 900 spatially distributed sampling points to explore the relationship between extracellular potentials - precursors of field potentials - and their corresponding cellular AP features across varying mixtures of atrial-like and ventricular-like cells. We then simulate a full MEA platform comprising 256 electrodes to assess how realistic subsampling, spatial organization, and tissue composition affect the extraction and interpretation of FP biomarkers. Across a broad panel of biomarkers, our results identify the FP metrics that most reliably reflect AP characteristics and demonstrate that the strength of FP-AP correlations increases as the tissue exhibits a more homogeneous ventricular-like phenotype. These findings not only clarify the mechanistic basis of MEA readouts in hiPSC-CM systems but also highlight the predictive potential of our computational tool: by integrating tissue composition, spatial sampling, and electrophysiological modeling, the framework can serve as a virtual platform to anticipate biomarker behavior, optimize MEA-based experimental designs, and ultimately strengthen the translational value of hiPSC-CM assays in preclinical research.

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Adaptive BDDC for Unstructured Ventricular Meshes

Ngoc Monica Mai Huynh
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Accurately simulating the heart's electrical activity requires solving large, complex systems of equations on detailed, patient-specific geometries. In this talk, I will present adaptive Balancing

Domain Decomposition by Constraints (BDDC) preconditioners developed for the Bidomain model of cardiac electrophysiology - a mathematical model describing how electrical signals propagate through the heart. These adaptive methods improve on standard BDDC techniques by enriching the coarse problem through localized eigenvalue problems, leading to faster and more robust solvers. Using unstructured finite element meshes of the human left ventricle with realistic fiber data, it is possible to show how these preconditioners achieve scalability and efficiency on modern high-performance computing systems, enabling more realistic and computationally feasible heart simulations [1].

This is a joint work with T. Abdelhamid (Menoufya University), S. Scacchi (Università degli Studi di Milano), L.F. Pavarino (Università degli Studi di Pavia), S. Zampini (King Abdullah University of Science and Technology) and R. Chen (Shenzhen Institute of Advanced Technology).

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Structure-guided Gauss-Newton and Newton Methods for Non-Convex Optimization Problems Arising from ReLU Neural Network Approximation

Zhiqiang Cai
Great Bay University / Purdue University, Dongguan, China / West Lafayette, USA

This talk will present our recent work on structure-guided Gauss-Newton and Newton methods for iteratively solving non-convex optimization problems. Those nonlinear problems are resulted in discretization of the physics-preserved neural network (P^2NN) methods for PDEs, whose solution is non-smooth and/or discontinuous. The modified Gauss-Newton and Newton methods exploit ReLU neural network algebraic structure and geometrical and physical meanings of neural network parameters.

This presentation will use some materials from joint work with J. Chen, J. Choi, T. Ding, A. Doktorova, R. Falgout, C. Herrera, M. Liu, X. Liu, and J. Xia.

Adaptive Feature Capture Method for Solving Partial Differential Equations with Near Singular Solutions

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We propose the Adaptive Feature Capture Method (AFCM), a novel machine learning framework that adaptively redistributes neurons and collocation points in high-gradient regions to enhance local expressive power. Inspired by adaptive moving mesh techniques, AFCM employs the gradient norm of an approximate solution as a monitor function to guide the reinitialization of feature function parameters. This ensures that partition hyperplanes and collocation points cluster where they are

most needed, achieving higher resolution without increasing computational over- head. The AFCM extends the capabilities of RFM to handle PDEs with near-singular solutions while preserving its mesh-free efficiency. Numerical experiments demonstrate the method's effectiveness in accurately resolving near-singular problems, even in complex geometries. By bridging the gap between adaptive mesh refinement and randomized neural networks, AFCM offers a robust and scalable approach for solving challenging PDEs in scientific and engineering applications.