Saturday, February 21

8:30–9:00	**Registration**		
9:00–9:10	**Welcome remarks**		
9:10–9:50	IT	**Ming-Jun Lai** University of Georgia	Multivariate splines and their classic and modern applications
9:50–10:30	IT	**Marco Tezzele** Emory University	Predictive digital twins based on graphical models: From infrastructure management to on-orbit operations
10:30–10:50	**Coffee**		
10:50–11:30	**Poster Blitz**		
11:30–12:30	**Poster Session**		
12:30–14:00	**Lunch**		
14:00–14:40	IT	**Helen Xu** Georgia Tech, CSE	Optimizing data movement in sparse computations via cache-friendly layouts
14:40–15:20	IT	**Chi-Kuang Yeh** Georgia State University	Single and multi-objective optimal designs for group testing experiments
15:20–15:40	**Coffee**		
15:40–16:20	IT	**Haomin Zhou** Georgia Tech, Math	A parameterized Wasserstein Hamiltonian flow approach for solving the Schrödinger equation

Abstracts of Plenary Talks

Multivariate Splines and Their Classic and Modern Applications

Ming-Jun Lai (University of Georgia)

I will begin with the Weierstrass theorem and the well-known Runge example to motivate the introduction of spline functions. Alongside the finite element method, I will explain multivariate spline functions, which are smooth piecewise polynomial functions over triangulation, tetrahedralization, spherical triangulation, and polygonal partitions. I will then discuss classic applications, such as scattered data interpolation and fitting, numerical solutions of linear and nonlinear PDEs, and smooth curve and surface construction. Finally, I will cover modern applications including image compression, image and data denoising, the construction of multivariate orthogonal polynomials, and analyzing tooth surfaces.

Predictive digital twins based on graphical models: from infrastructure management to on-orbit operations

Marco Tezzele (Emory University)

A digital twin (DT) is a virtualization of a physical asset built upon a set of computational models that dynamically update to persistently mirror a unique asset of interest throughout its operational lifespan, enabling informed decisions that realize value. This talk presents a progressive view of re-

cent advancements in predictive DTs, emphasizing the integration of probabilistic graphical models, Bayesian inference, and risk-aware optimal control spanning applications from civil infrastructure to aerospace systems.

The first part of the talk introduces a DT framework for civil engineering structures, where the asset-twin system is formalized via a dynamic Bayesian network. Reduced order models and deep learning are leveraged to assimilate structural health data from sensors and support condition-based maintenance and lifecycle optimization [1, 2]. Then we propose a modular DT architecture for multi-spacecraft on-orbit servicing missions, supporting decentralized state estimation, subsystem-level health monitoring, and coordinated control. The framework handles uncertainties in the kinematic states as well as the health of the propulsion subsystem and demonstrates the generation of mission-robust policies through simulation of rendezvous scenarios involving partially degraded assets [3]. We conclude with pgmtwin, a new Python library for DTs based on graphical models [4]. This progression highlights the scalability and adaptability of probabilistic DTs across domains with stringent performance and reliability requirements.

References:

[1] M. Torzoni, M. Tezzele, S. Mariani, A. Manzoni, and K. E. Willcox, "A digital twin framework for civil engineering structures," *Computer Methods in Applied Mechanics and Engineering*, vol. 418, p. 116584, 2024. doi: 10.1016/j.cma.2023.116584.

[2] E. Varetti, M. Torzoni, M. Tezzele, S. Mariani, and A. Manzoni, "Adaptive digital twins for predictive decision-making: Online Bayesian learning of transition dynamics," 2025. arXiv:2512.13919.

[3] S. Henao-Garcia, M. Kapteyn, K. E. Willcox, M. Tezzele, et al., "Digital-twin-enabled multi-spacecraft on-orbit operations," in *AIAA SCITECH 2025 Forum*, American Institute of Aeronautics and Astronautics, Inc., 2025. doi: 10.2514/6.2025-1432.

[4] pgmtwin — A Python library for Digital Twins based on Probabilistic Graphical Models. Available at: `https://github.com/pgmtwin/pgmtwin`

Optimizing data movement in sparse computations via cache-friendly layouts

Helen Xu (Georgia Institute of Technology, CSE)

Sparse matrix and graph computations are foundational to modern workloads spanning scientific computing, machine learning, and network analytics. They are bottlenecked by irregular memory access and excessive data movement. This talk presents two examples of how to optimize data layouts and mitigate memory bottlenecks in sparse computations: 1) compression and 2) reordering. Specifically, we cover two recent advances: the Compressed Packed Memory Array (CPMA) for dynamic graphs [Wheatman, Burns, Buluc, and Xu, PPoPP '24] and hierarchical reordering for sparse matrix-sparse matrix multiplication (SpGEMM) [Islam, Xu, Dai, and Buluc, SC '25]. The CPMA is a compressed, pointer-free dynamic structure that preserves ordering while enabling efficient batch-parallel updates, reducing indirection and improving cache utilization in sparse set and graph representations. In contrast, recent work on SpGEMM demonstrates how hierarchical row reordering and cluster-wise computation can significantly improve reuse of matrix data, achieving

up to 1.39× speedup by aligning computation with locality in the memory hierarchy . Together, these works illustrate the potential for efficient data layouts to improve the performance of sparse computations.

Single and multi-objective optimal designs for group testing experiments

Chi-Kuang Ye (Georgia State University)

Group testing, or pooled-sample testing, is widely used in large-scale screening and resource-constrained studies, yet principled design methodology for precise parameter estimation remains limited. This talk presents an optimal design framework for group testing that targets efficient estimation of key model parameters while accounting for cost constraints. Beyond classical criteria such as D-, D_s-, and A-optimality, a central novelty is the introduction of maximin design principles, including potentially non-differentiable criteria, into group testing procedures. These nondifferentiable criteria have not previously been explored in this context and yield designs with strong worst-case guarantees and improved robustness. The framework accommodates both large-sample settings through optimal approximate designs and small-sample studies through exact optimal designs, enabling systematic assessment of robustness to changes in criteria, statistical models, and cost structures. We demonstrate the practical impact of this approach through an application to Chlamydia screening using imperfect assays under budget constraints, and show that precise parameter estimation via optimal design is a foundational step that directly enables efficient and reliable sequential group-testing procedures.

This talk will be mainly based on the paper that is in revision, https://arxiv.org/abs/2508.08445, and the other paper that is under review.

A parameterized Wasserstein Hamiltonian flow approach for solving the Schrödinger equation

Haomin Zhou (Georgia Institute of Technology, Math)

I will present a reformulation of Schrödinger using a generative model and an associated computational method to solve it in higher dimensions. The reformulation stems from a parameterization approach that can be used to design algorithms simulating geometric flows on the Wasserstein manifold, the probability density space equipped with the optimal transport metric. The approach leverages the theory of optimal transport and the Machine Learning techniques like push-forward operators and neural networks, leading to a system of ODEs for the parameters of neural networks. The resulting methods are meshless, basisless, sample-based schemes that scale well to higher-dimensional problems. The strategy works on the Wasserstein Hamiltonian flows, including the Schrödinger equation. This presentation is based on joint work with Shu Liu (Florida State), Hao Wu (Wells Fargo), and Xiaojing Ye (Georgia State).

List of Poster Titles

Massively parallel random phase approximation correlation energy via Lanczos quadrature

Abir Haque, *Georgia Institute of Technology*

Impact of stochasticity on dynamic entrainment in a neuronal spiking model
Aidan Tillman, *Georgia State University*

Rate-selective synchronization in switching networks: when timing meets structure
Angelo Kwaku Boateng, *Georgia State University*

Randomized hybrid projection methods with recycling for inverse problems
Ansley Bentley, *Emory University*

Physics-enhanced deep surrogates for the phonon Boltzmann transport equation
Antonio Varagnolo, *Georgia Institute of Technology*

Infinite-dimensional Stein variational inference with derivative-informed neural operators
Ben Burns, *Georgia Institute of Technology*

Shocks without shock capturing; compressible flow at 1 quadrillion degrees of freedom without loss of accuracy
Ben Wilfong, *Georgia Institute of Technology*

Flight stability of cones and wedges
Chloe Maitrejean, *Georgia State University*

Highly-parallel fluid-solid interactions for compressible flows
Daniel Vickers, *Georgia Institute of Technology*

ELMs with space-time collocation for the numerical resolution of parabolic PDEs
Davide Elia De Falco, *Scuola Superiore Meridionale/Emory University*

Comparative analysis of β-adrenergic stimulation of myocyte contraction by different agonists
Dilmini Warnakulasooriya, *Georgia State University*

Computational methods for hyperparameter estimation with applications to separable nonlinear inverse problems
Elle Buser, *Emory University*

Transform method for modeling erosion analysis with cylindrical bodies in channel flow
Emeka Mazi, *Georgia State University*

High-performance tensor contractions in computational chemistry
Eric Fowler, *Georgia Institute of Technology*

Modeling and control of highly pathogenic avian influenza in poultry using network disease dynamics
Hamed Karami, *Georgia State University*

Understanding denoising autoencoders through the manifold hypothesis: a geometric perspective
Haoran Yan, *Georgia Institute of Technology*

Test double descent with color intermittent diffusion (DD-CID) with challenges in different disciplines
Jiuru Lyu, *Emory University*

Network model of tissue engineering scaffolds
Justyna Sokolik, *Georgia State University*

Autoregressive multifidelity neural surrogate modeling under scarce data regimes
Kashvi Mundra, *Georgia Institute of Technology*

Manifold-aware perturbations for constrained generative modeling
Katherine Keegan, *Emory University*

Dynamic entrainment for optimal pulse timing in Morris-Lecar model
Lawan Wijayasooriya, *Georgia State University*

Aperiodic 1/f fingerprints of excitation–inhibition balance in human epilepsy
Marrium Shamshad, *Georgia State University*

Latent twins: learning physical systems from data
Max Collins, *Emory University*

What makes a good preconditioner for data science?
Mitchell Scott, *Emory University*

Variable projected augmented Lagrangian methods for generalized Lasso problems
Riley Yizhou Chen, *Emory University*

PDPO: parametric density path optimization
Sebastian Gutierrez Herandez, *Georgia Institute of Technology*

The evolutionary games of leader-follower tumor ecology and treatment optimization
Somiya Rauf, *Georgia State University*

Kronecker approximations of covariance matrices for solving inverse problems
Srijon Sarkar, *Emory University*

Commitment issues in motoneurons: how ionic currents enable bistability
Tommy Stell, *Georgia State University*

Statistical meta-analysis to investigate the association of SNP (rs4680) in COMT gene with multiple cancers
Umma Hafsah Himu, *Georgia State University*

Multifidelity operator inference: non-intrusive reduced order modeling from scarce data
Vivian Zhang, *Georgia Institute of Technology*

Data efficiency of surrogate models: learning physics data from full field data vs. inductive bias from approximate PDE solvers
Xian Hadia, *Georgia Institute of Technology*

Neural operator accelerated evolutionary strategies for PDE-constraint optimization
Xiangming Huang, *Georgia Institute of Technology*

A primal-dual price-optimization method for computing equilibrium prices in mean-field games models
Xu (Melissa) Wang, *Emory University*

Nationwide epidemiologic and cost burden analysis of chemotherapy-induced neurological disorders
Yiran Xu, *Georgia State University*

Understanding in-context learning on structured manifolds: bridging attention to kernel methods
Zhaiming Shen, *Georgia Institute of Technology*

Towards understanding generalization in DP-GD: a case study in training two-layer CNNs
Zhongjie Shi, *Georgia Institute of Technology*