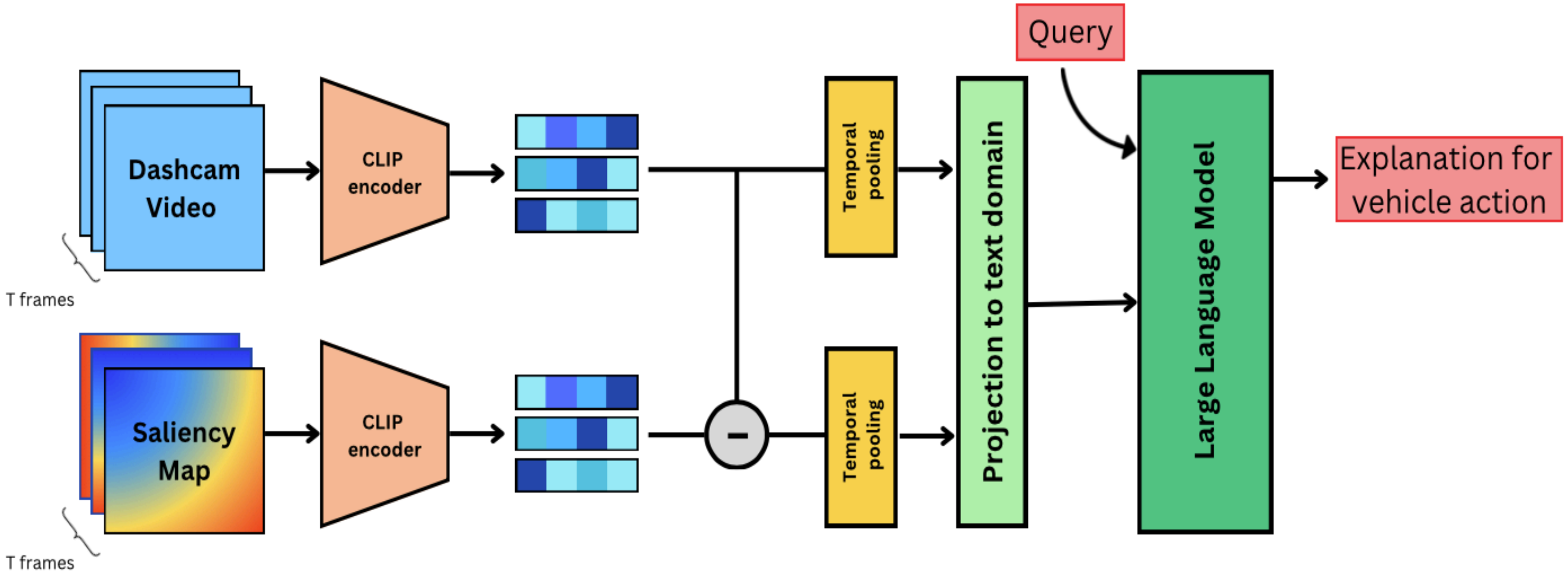
UConn's AI & Quantum Innovation Ecosystem

Sanguthevar Rajasekaran

Integrating LLMs into System Automation (Bi)



- We provide a Transformer-based encoder (CLIP) to extract features from the video footage as well as network saliency map
- We merge the extracted features from each frame of the video using temporal pooling to come up the final visual representation
- This pooling layer also projects the visual representation into the text domain
- An LLM (e.g., ChatGPT) can provide users with an accurate explanation for the decisions of the automated system

Quantum Techniques for Speeding Up Computations (Sanguthevar Rajasekaran, Walter Krawec, Bing Wang)

- A computational problem can be challenging for various reasons: the problem might involve the processing of voluminous data, or the problem might be inherently difficult (e.g., NP-hard).
- Traditional Parallel Computing helps.
- If P is the number of processors used, the maximum speedup we can get is P.
- There are problems (e.g., training LLMs) that require massive parallelism.
- Quantum Computing offers the promise of exponential (in the number of qubits) speedups!

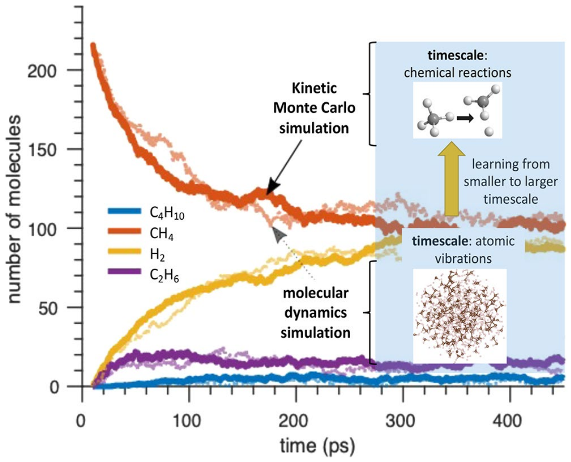
Quantum Techniques
(Sanguthevar Rajasekaran, Walter Krawec, Bing Wang)

- Quantum mechanics allows a qubit to be in a superposition of multiple states at the same time.
- If we have a system of n qubits, then there are a total of 2^n possible joint states for the system. This quantum system will be in a superposition of all of these possible states simultaneously.
- Many of the problems involved in materials discovery, health care, and human performance are very complex and intractable.
- We propose to create novel quantum algorithms for solving these challenging problems.
- In our recent work we have created the state-of-the-art quantum algorithms for particle simulations.

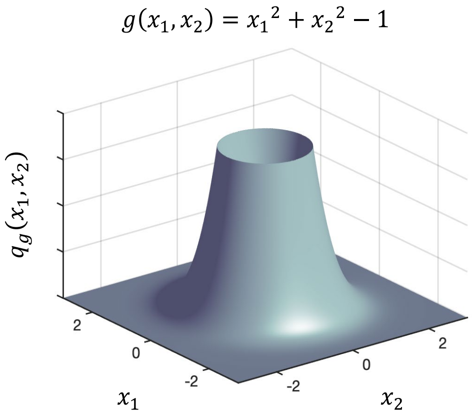
UCONN
UNIVERSITY OF CONNECTICUT

Scientific & Computational Machine Learning Laboratory (Yang)

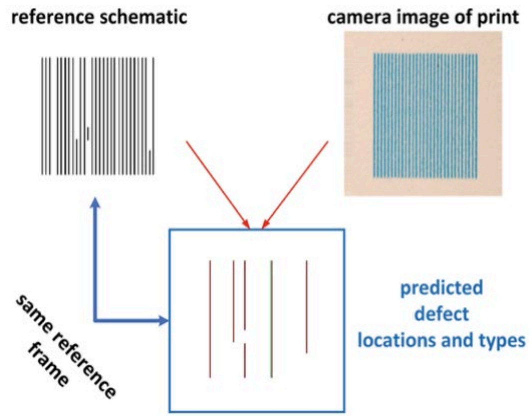
A



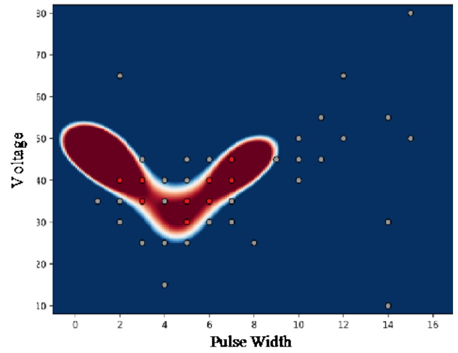
B



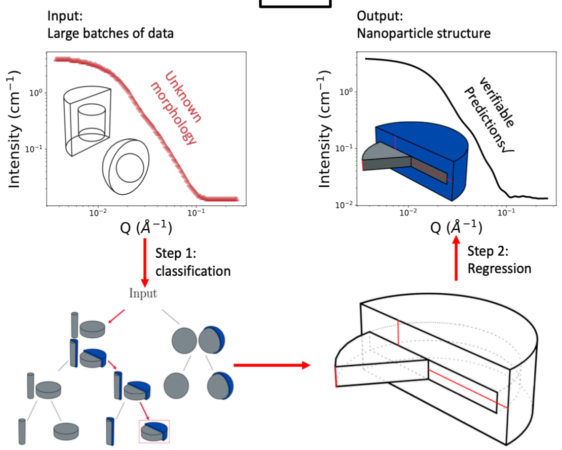
C



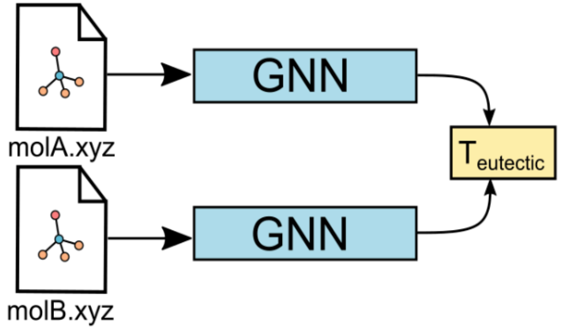
D



E



F



Selected work from **Qian Yang's lab**: (A) data-driven learning and model reduction of chemical reaction networks from molecular dynamics simulations. Figure from Clark, A., et al., ACS Cent. Sci. 7, 8, 1271-1287 (2021); (B) symbolic regression using a probabilistic framework to learn implicit relationships from small, noisy data. Figure from Roberts, G., et al., GECCO (2024); (C) Semi-Siamese neural network for robust, data-efficient defect detection for 3D printing. Figure from Niu, Y., et al., ICVS (2023); (D) active machine learning for 3D printing with novel model selection approach. Figure adapted from Pardakhti, M., et al., 3D Printing & Additive Manufacturing (2023); (E) machine learning framework for inverse analysis of small angle scattering data. Figure from Roberts, G., et al., ChemRxiv (2024); (F) Siamese graph neural networks for predicting melting temperatures of molten salt eutectics. Figure from Mandal, N., et al., in preparation.

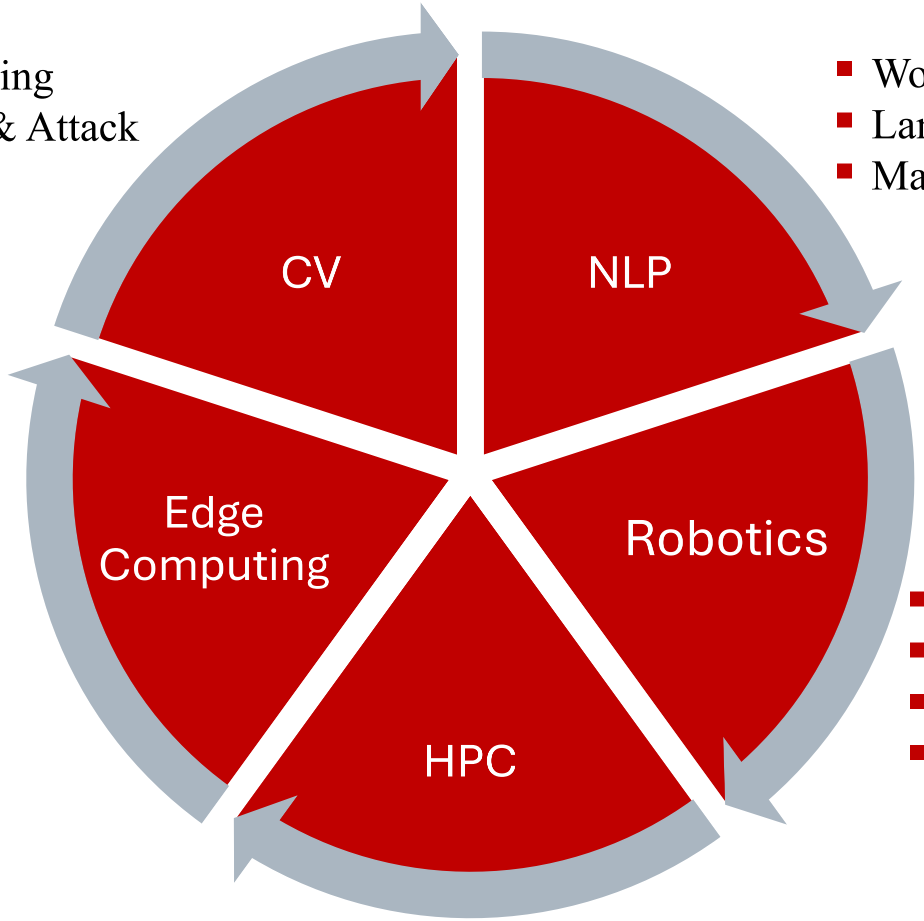
Key Questions in **ML for Manufacturing & Materials**: *small data*; *interpretability*; *extrapolation*

Intelligent Systems Lab (Ji)

Bring Intelligence to Robotic Systems and Make them Accurate, Efficient, and Secure

- Self-supervised Learning
- Adversarial Defense & Attack
- Energy-based Models
- Explainable AI
- Point-cloud Analysis

- Word Embedding
- Language Modeling
- Machine Translation



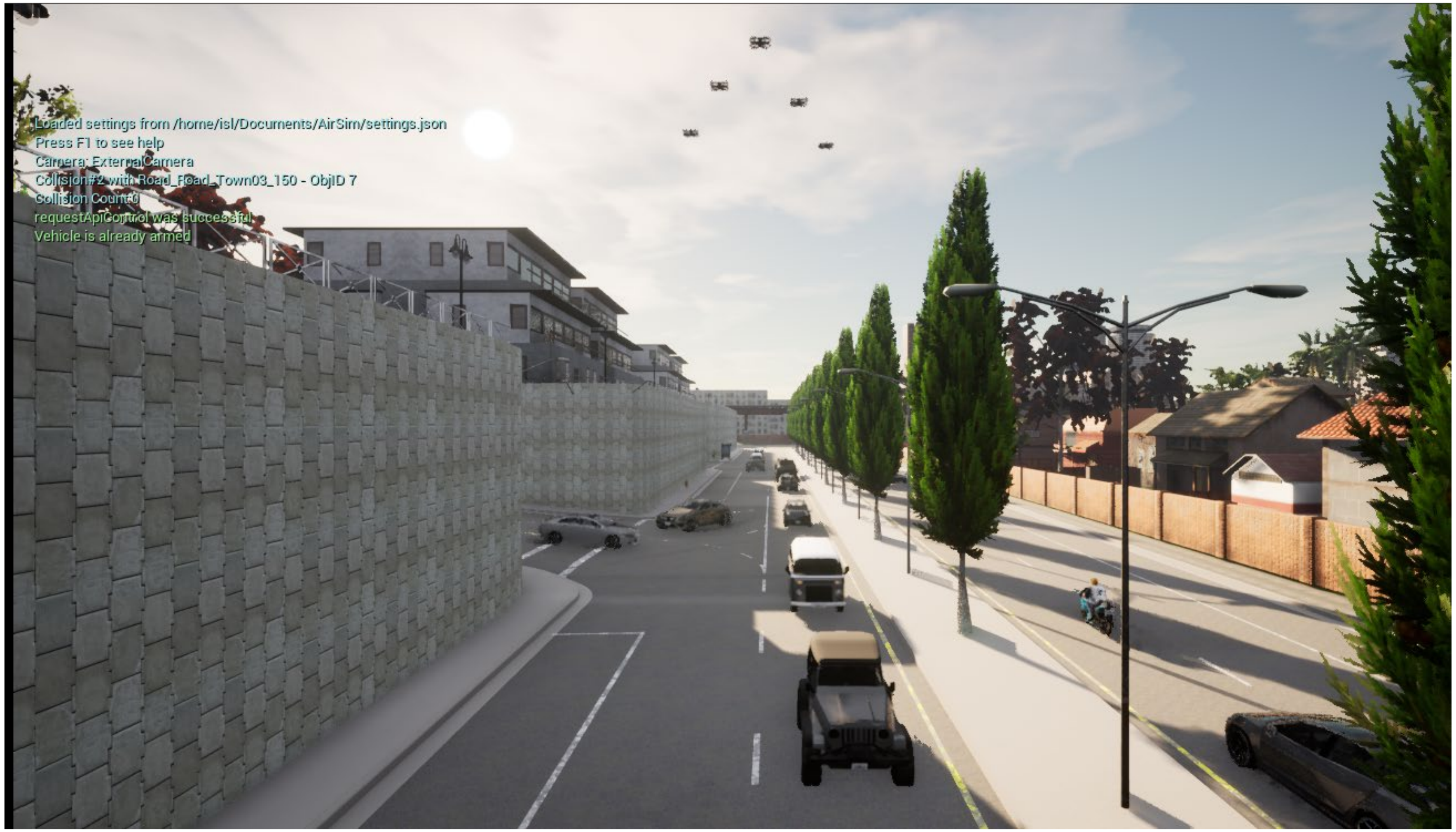
- Model Compression
- FPGA, NVidia Jetson

- LLMs/VLMs for Robotics
- Object Navigation
- 3D Object Detection
- 3D Scene Representation

- Parallel and Distributed Computing on CPU and GPU Clusters

Example Research Demo

- Networked Drones for 3D Perception

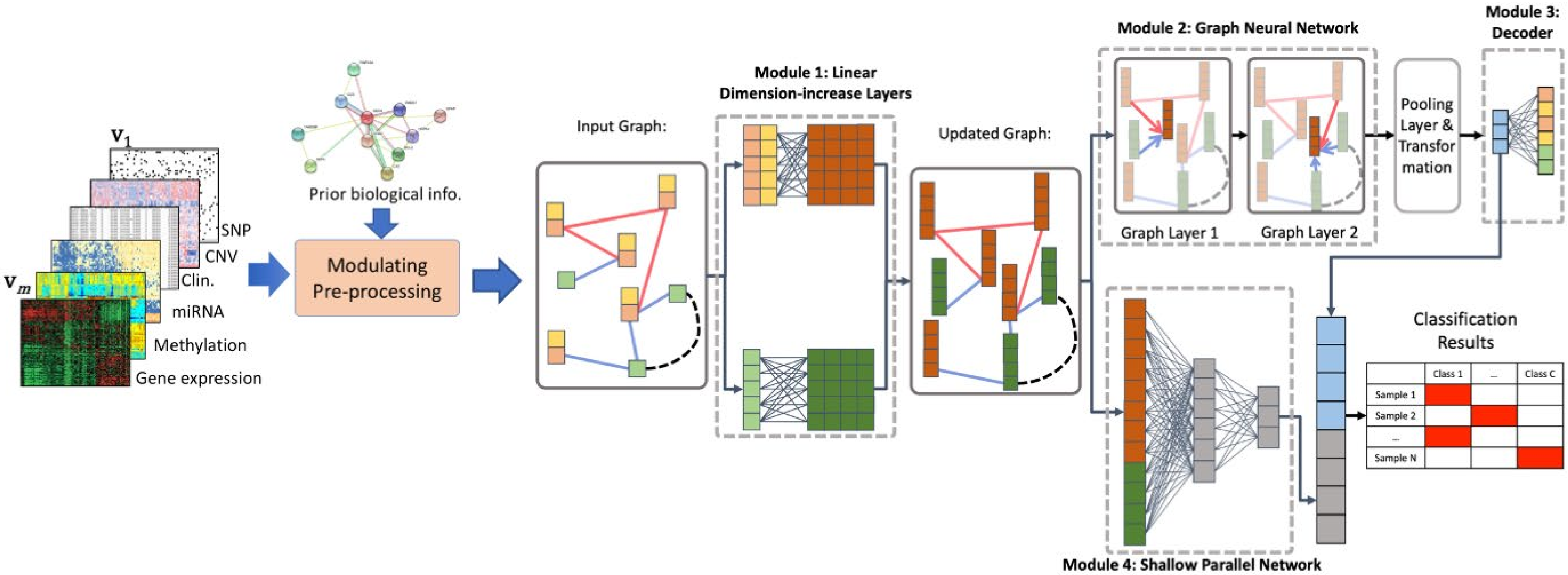


Demo website: https://huiyegit.github.io/UAV3D_Benchmark/

Bioinformatics and Biotechnology

- Understanding the evolution of various biological entities (Mukul Bansal)
- Single-cell analysis, metagenomics, and genomics-guided cancer immunotherapy (Ion Mandoiu)
- Biomedical Data Mining (Dong-Guk Shin, S. Rajasekaran)
- Machine Learning and Traditional Algorithmic Techniques for the Detection of Aspiration (Pramod Bonde – Yale, S. Rajasekaran)

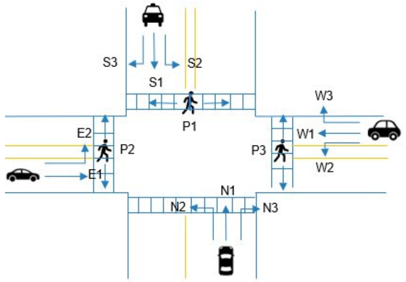
Integrating genomic data to identify candidate biomarkers and building phenotypic predictive models for cancer studies (Sheida Nabavi)



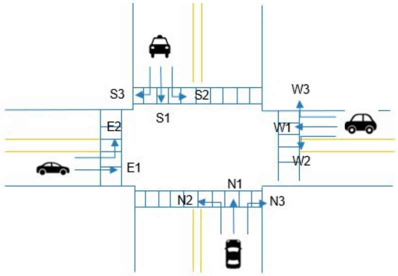
AI-based Video Analytics for Intersection Safety and Operations (Kai Wang)

The major goal of this research is to investigate and develop computing algorithms to analyze camera and video data for intersections in CT, using modern AI and computer vision technologies. The project focuses on analyzing both traffic operation information and traffic safety metrics, to help CTDOT better optimize the signal phasing to maximize capacity and minimize delay and identify driver behavior issues and improve safety for intersections.

AI-based Traffic Safety Analysis



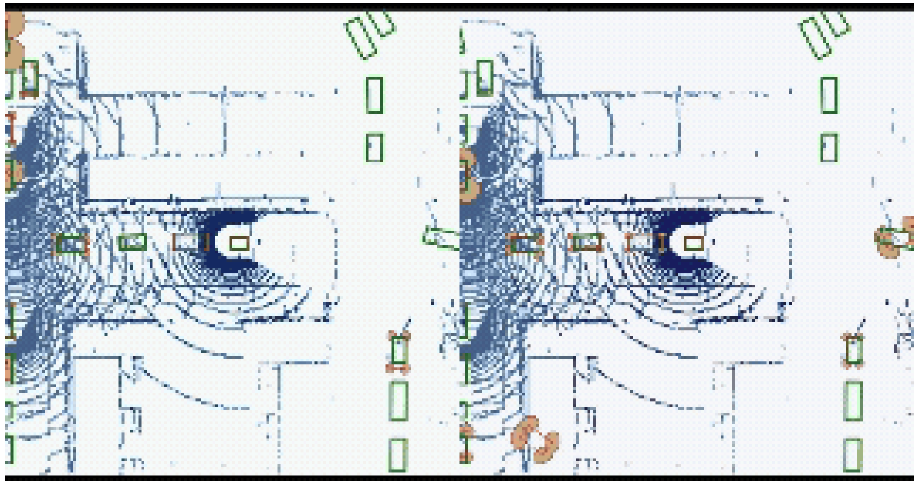
Conflict Type	TTC		PET	
	≤ 2s	(2s – 5s]	≤ 3s	(3s – 6s]
S3 vs. P1	13	7	20	7
W3 vs. P1	13	22	8	16
E2 vs. P1	0	0	1	4
N2 vs. P2	0	0	0	2
S3 vs. P2	0	1	1	0
N3 VS. P3	0	0	0	0
S2 vs. P3	0	0	0	0
W3 vs. P3	0	0	0	0



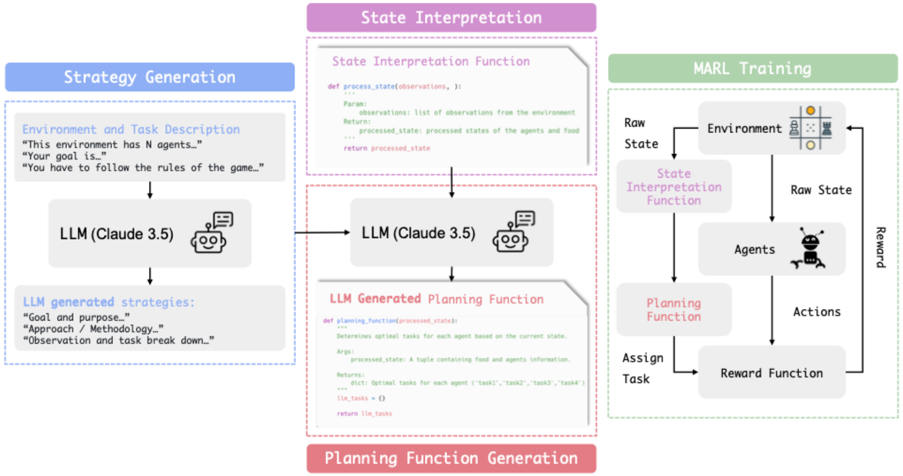
Conflict Type	TTC		PET	
	≤ 2s	(2s – 5s]	≤ 3s	(3s – 6s]
S1 vs. S1	11	41	79	40
S1 vs. N2	10	11	23	17
S2 vs. N3	17	28	47	47
S2 vs. N1	28	50	40	67
N2 vs. S3	1	0	19	13
W2 vs. S3	14	13	11	19
N1 vs. W3	13	13	11	4
N3 vs. E1	10	41	34	55
E1 vs. W2	44	34	34	43
E2 vs. W3	10	14	19	29
E2 vs. W1	52	88	43	55

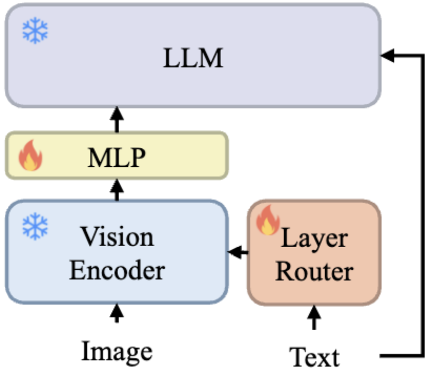
Learning and Optimization for Safety, Efficiency, and Robustness of AI Systems

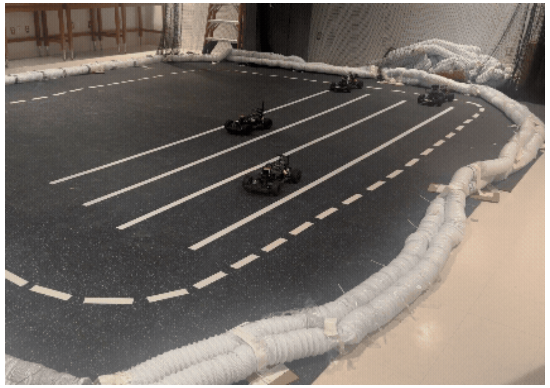
Fei Miao, Uconn School of Computing, Pratt & Whitney Associate Professor, fei.miao@uconn.edu,
https://www.linkedin.com/in/fei-miao-76964727/, www.feimiao.org, https://scholar.google.com/citations?user=fH2YF6YAAAAJ&hl=en



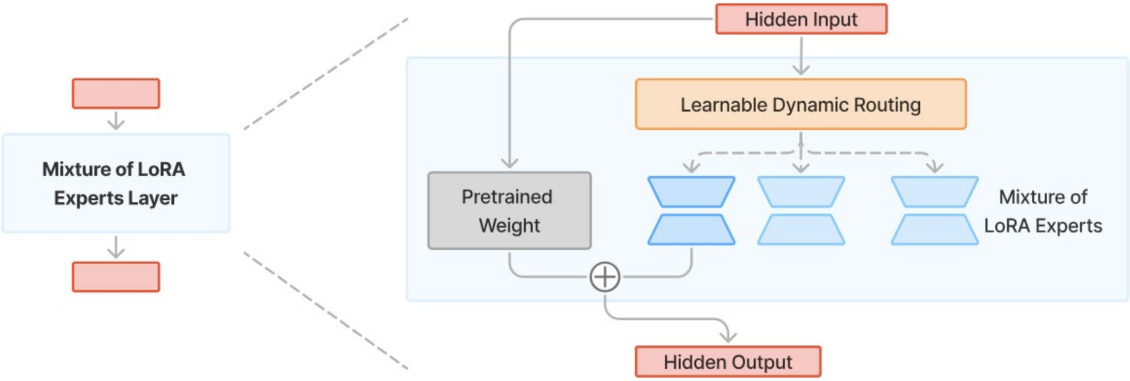
Computer vision (2D and 3D, object detection and tracking) and uncertainty quantification: improve accuracy and reduce uncertainty.







Reinforcement learning (Multi-Agent), Safe RL, Robust RL:
First open-source robust multi-agent RL on robots--theory, algorithm design, and **hardware demonstration**; improved safety, system efficiency, and resiliency, validated on hardware.



LLM, VLM (Vision-Language Foundation Model) and AI Agent:
LLM for multi-agent coordination; vision-language-action model (VLA);
Efficient fine tune algorithms for LLM, VLM, VLA (2~8 GPU)—with open-source pretrained model (Llava, Qwen), fine tune AI agent with local/customizable datasets according to specific user needs.

Sponsor: NSF, DOT, DOE, Nvidia, Qualcomm, etc.

ACS ES&T Water

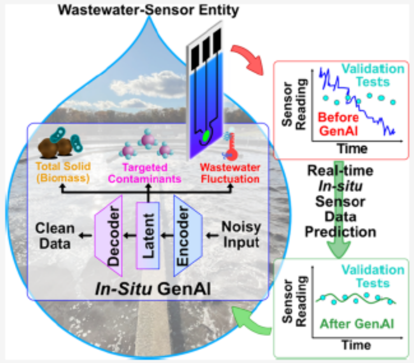
pubs.acs.org/estwater | Article

Deciphering Sensor Reading Noises in Complex Wastewater Environments Using Real-Time *In Situ* Hybrid GenAI Wastewater-Sensor Entity

Xingyu Wang, Zhiyuan Zhao, Samuel Rothfarb, Shan Lu, Lucy Temple, Yutong Yang, and Baikun Li*

Cite This: https://doi.org/10.1021/acsestwater.5c00510 | Read Online

ABSTRACT: Current wastewater monitoring relies on generic sensor denoising, lacking the ability to distinguish noise types arising from wastewater complexity. Decoding this complexity demands identifying, quantifying, and separating noise sources within raw sensor data sets, underscoring the need to shift from sensor-focused denoising to an integrated wastewater–sensor framework. With NH_4^+ ion selective membrane (ISM) sensors as the target, we defined wastewater complexity comprising solids, targeted contaminants, and physical fluctuations, processing sensor noises as the electrochemical fingerprints for distinct wastewater complexity groups. We developed an innovative tridomain (time, frequency, and independent component) data processing approach to decompose monodimensional raw noisy sensor readings into multidimensional sensor data consisting of noise-free sensor readings and three-component noises (sensor reading drifting, impulse, and background noises). Furthermore, we achieved *in situ* predictive noise categorization through a variational autoencoder (VAE)-based generative artificial intelligence (GenAI). Our VAE-based GenAI wastewater-sensor entity reduced wastewater-induced drift, impulse, and background noises from 9.33, 0.34, and 0.08 mg/L to 2.8, 0.13, and 0.0003 mg/L,



ELSEVIER

Environmental Research
Volume 275, 15 June 2025, 121401

Multi-agent large language model frameworks: Unlocking new possibilities for optimizing wastewater treatment operation

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Arash Zaghi

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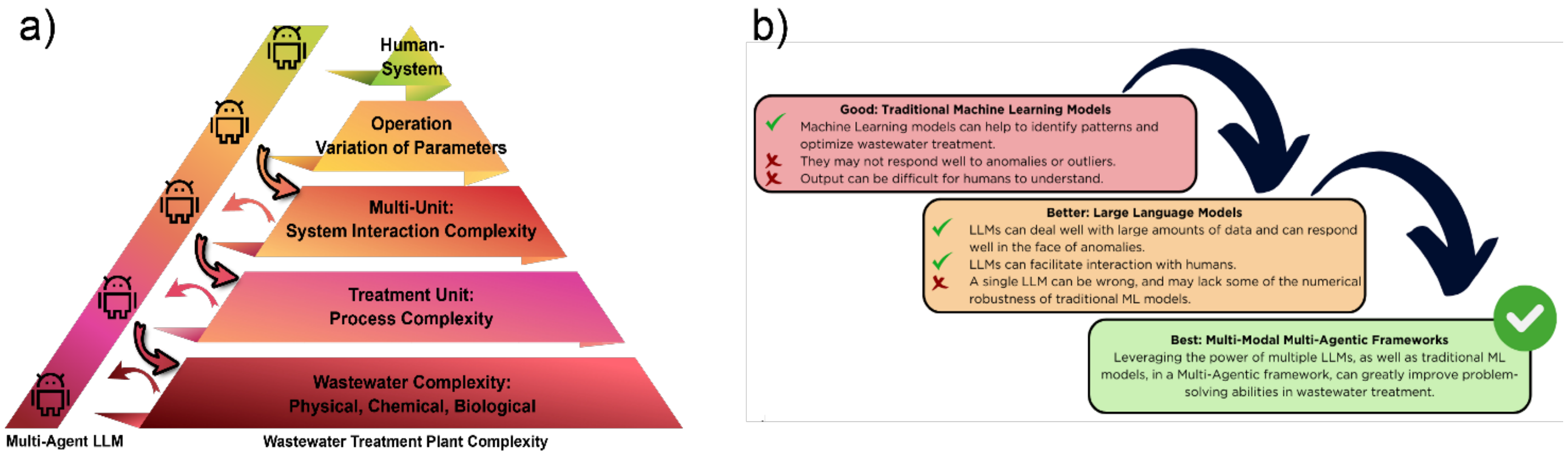
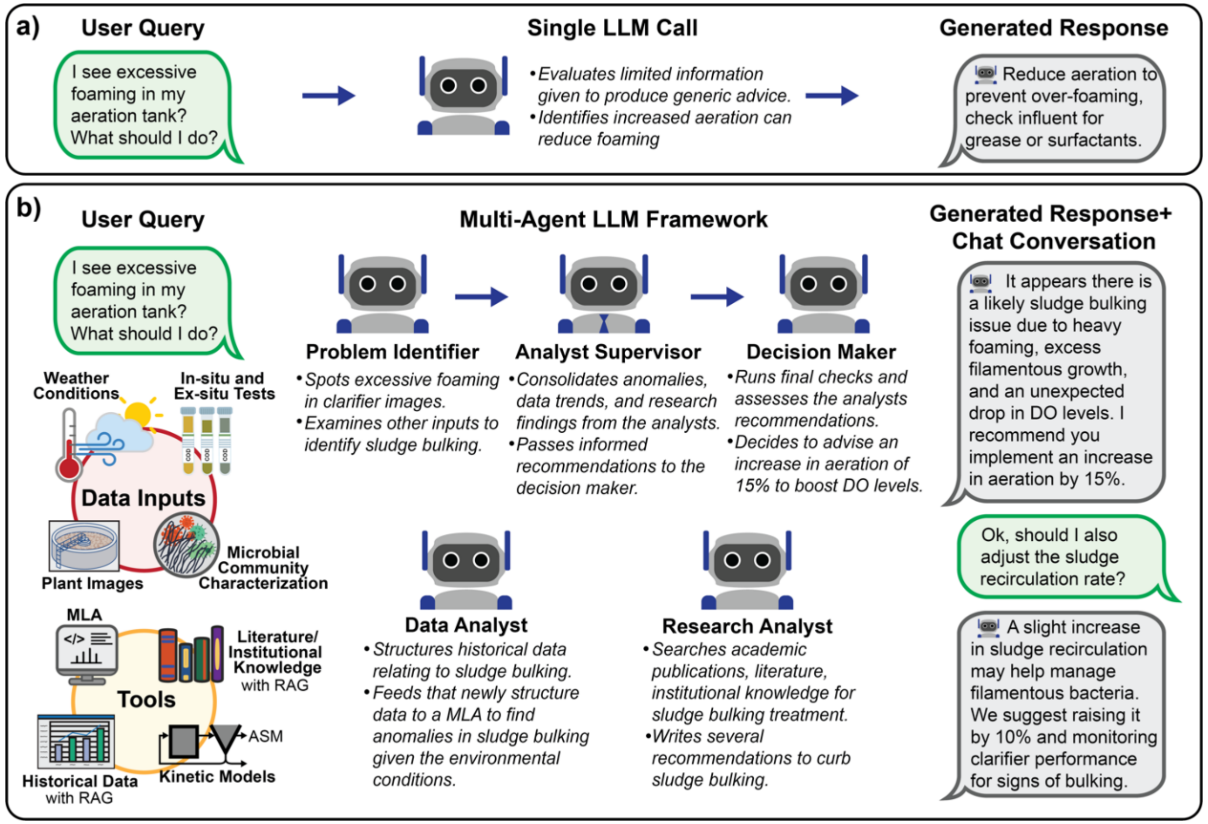


Figure 1. (a) Complexity of WWTPs at each stage. (b) Comparison between existing algorisms and multimodal, multi-agentic LLM frameworks in the context of complex environmental systems.



Chemical and Biomolecular Engineering

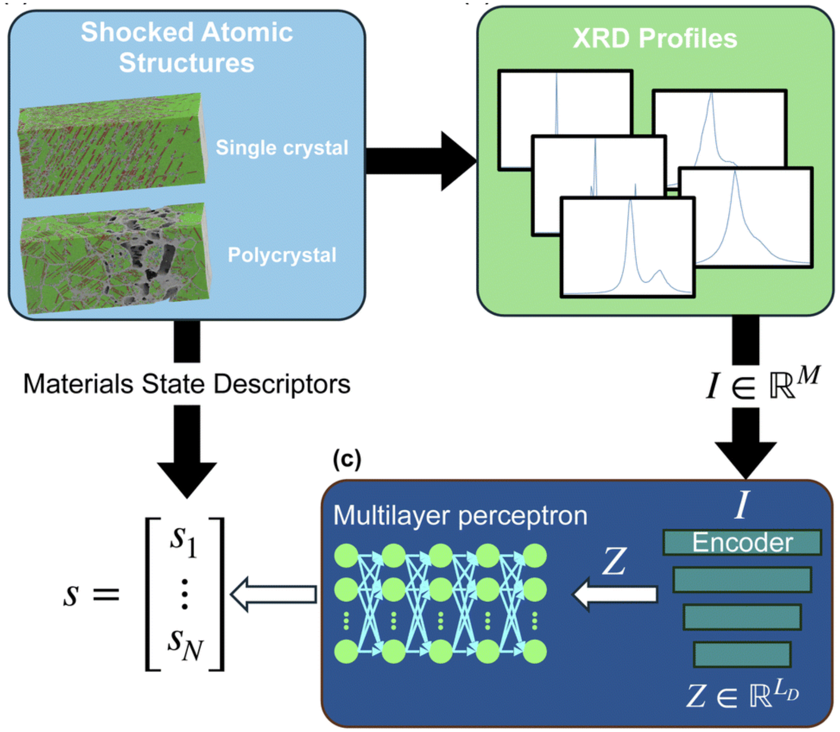
- Matthew D. Stuber: ML models for optimization and decision-making applications such as control systems.
- Dan Burkey: LLMs and PLMs for scalable qualitative data analysis for assessment of student textual/narrative responses.
- Brian Willis: Quantum – Nanofabrication strategies for single photon sources.
- Anson Ma: Autonomous optimization of inkjet printing through machine learning (with Qian Yang)

Materials Databases and Informatics

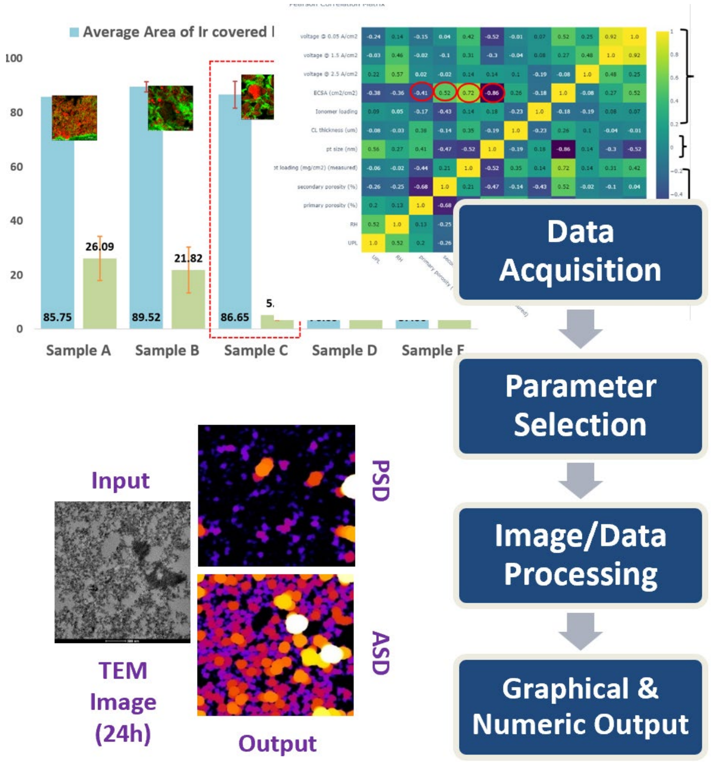
AI-based analysis of microstructure using X-ray diffraction data

AI-based image/data processing for microscopy analysis

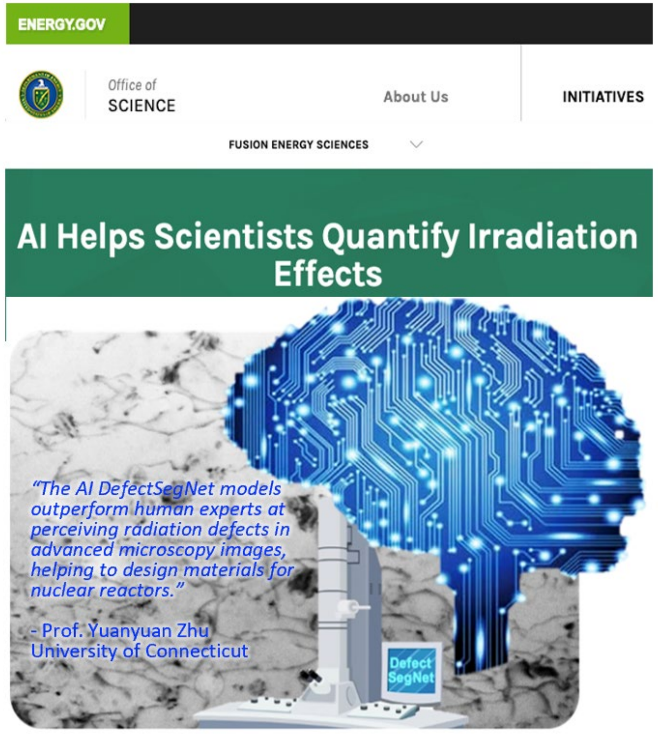
Computer Vision for High-throughput Analysis



Dongare Research Group



Jankovic Research Group



Zhu Research Group

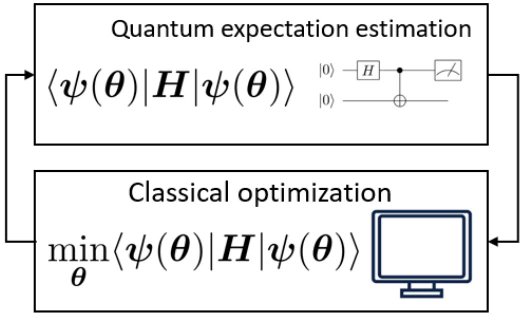
School of Business

- **Wei Chen:** Generative AI for Business
- **Sudip Bhattacharjee:** AI/ML, data-driven operations, policy analytics
- **Chen Liang:** Algorithmic bias, AI and future of work
- **Karen Xie:** AI in marketplaces (e.g. Airbnb, Zillow)
- **Ramesh Shankar:** Big Data analytics & social media AI
- **Debanjan Mitra:** AI's impact on marketing, innovation, strategy
- **David Bergman:** Constraint Programming; Quantum annealing and combinatorial optimization
- **Carlos Cardonha:** Quantum optimization and machine learning
- **Curriculum and Talent Pipeline; Partnerships and Applied Projects; Ecosystem and Engagement Opportunities**

Benchmark quantum algorithms for fluid dynamics problems

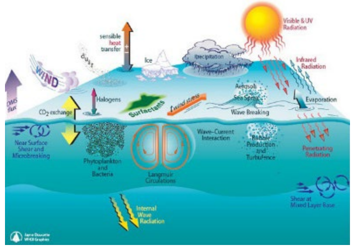
Quantum encoding of tridiagonal matrices

$$A_n := I \otimes A_{n-1} + (X \otimes I^{\otimes(n-1)}) \left[\frac{1}{2^{n-1}} \sum_{t=0}^{\lfloor n/2 \rfloor} (-1)^t \sum_{\pi} S_\pi (X^{\otimes(n-2t)} \otimes Y^{\otimes 2t}) \right] (X \otimes I^{\otimes(n-1)})$$



Variational quantum eigensolver

Applications: Aerospace, Chip Cooling, Oceanography



Supported by UConn Quantum Innovation Seed Grants,
NASA Connecticut Space Grant Consortium, IBM quantum credits

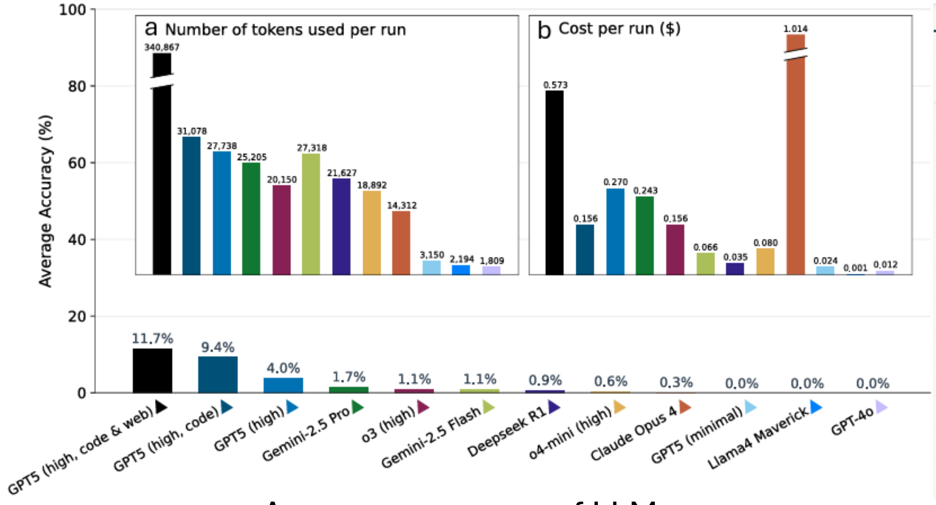
Dr. Chang Liu
chang_liu@uconn.edu

Research Areas:
Fluid Dynamics; Control; Turbulence; AI; Quantum

Probing the Critical Point of AI Reasoning:

Benchmarking LLMs at the Frontier of Physics

Collaboration with Argonne National Laboratory and UIUC



Average accuracy of LLMs

Model Outputs | Expert Solution

Model Name	Challenge	Checkpoint 1	Checkpoint 2 Self Carryover	Checkpoint 2 Oracle Carryover	Checkpoint 3 Self Carryover	Checkpoint 3 Oracle Carryover
GPT-5 (high, code & web)	2/5	5/5	5/5	5/5	3/5	3/5
GPT-5 (high, code)	4/5	5/5	5/5	5/5	5/5	4/5
GPT-5 (high)	0/5	5/5	5/5	5/5	0/5	0/5
Gemini-2.5 Pro	0/5	3/5	3/5	1/5	0/5	0/5
o3 (high)	0/5	5/5	2/5	2/5	0/5	0/5
DeepSeek R1	0/5	3/5	3/5	2/5	0/5	0/5
o4-mini (high)	0/5	5/5	1/5	0/5	0/5	0/5
Gemini-2.5 Flash	0/5	2/5	0/5	0/5	0/5	0/5
Claude Opus 4	0/5	0/5	0/5	0/5	0/5	0/5
GPT-5 (minimal)	0/5	0/5	0/5	0/5	0/5	0/5
Llama-4 Maverick	0/5	0/5	0/5	0/5	0/5	0/5
GPT-4o	0/5	0/5	0/5	0/5	0/5	0/5

Example benchmark results

71 composite research challenges.
Created by 50+ physics researchers.
Cover broadly the physics research areas.

Technical Report:
(https://arxiv.org/abs/2509.26574)

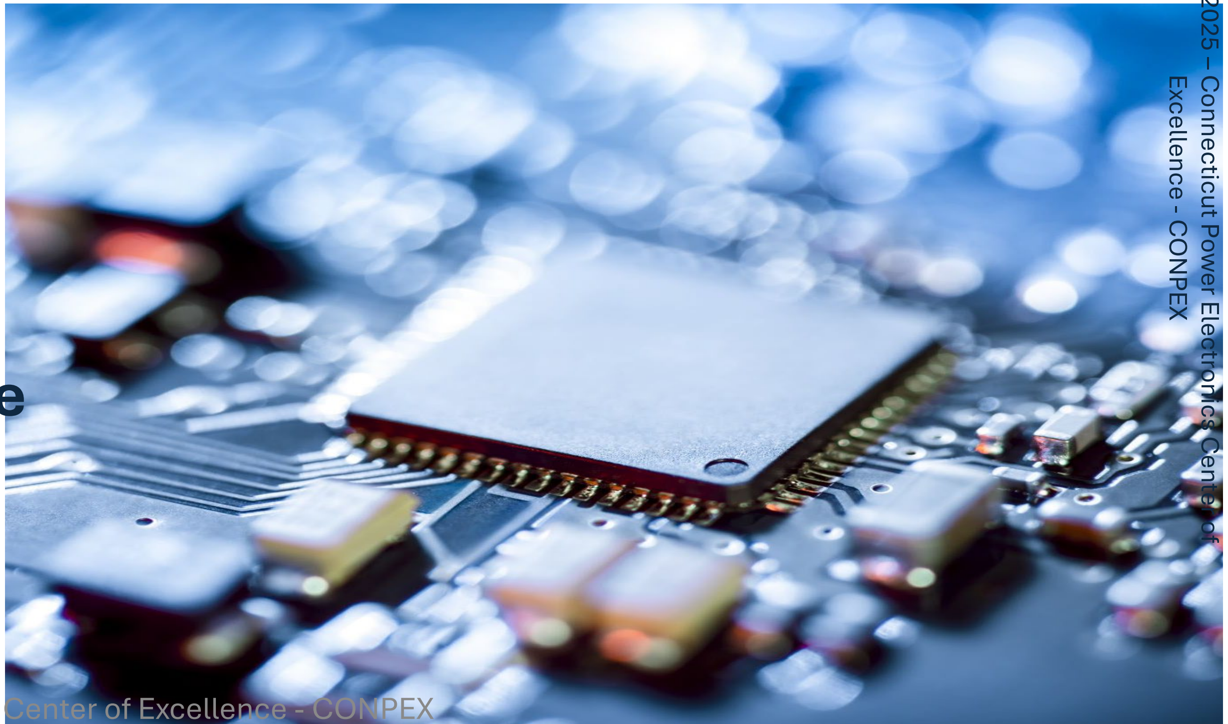
Website: https://critpt.com/

AI/AE Assisted Semiconductor Identification

UConn Team

Ali Bazzi	Electrical & Computer Engineering
Necmi Biyikli	Electrical & Computer Engineering
Georges Pavlidis	School of Mechanical, Aerospace & Manufacturing Engineering
Qian Yang	School of Computing
Yuanyuan Zhu	Materials Science & Engineering
Mehdi Anwar	Electrical & Computer Engineering

UConn in partnership with industry, federal laboratories and other universities is leading an effort in Artificial Intelligence (AI/ML) assisted material identification and autonomous experimentation (AE) targeting semiconductors. The application specific identification of semiconductors, targets reduction in concept to market time to 3-years or less.



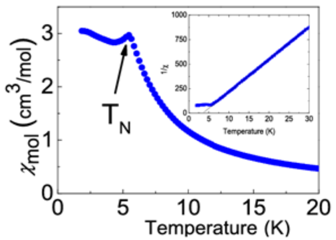
Contact: Mehdi Anwar
Electrical and Computer Engineering, UConn
Email: a.anwar@uconn.edu

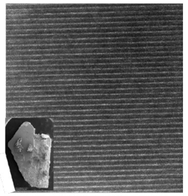
Physics Department

- **Richard Jones:** AI to advance state-of-the-art simulations of particle interactions from high-energy collisions.
- **Andrew Puckett:** AI/ML to improve the charged-particle track reconstruction in the environment of nuclear accelerator-based experiments.
- **Tom Blum:** ML to predict parts of QCD correlation functions from different parts to dramatically reduce the cost of numerical simulations.
- **Cara Battersby:** ML to measure the 3-D structure of our Galaxy's center and to understand the mechanisms that control the star formation, black hole feeding, etc.
- **Xian Wu: T**raining a GPT model to generate isomorphic multiple-choice questions for intro physics courses.
- **Pavel Volkov:** Quantum materials and devices, focusing on superconductivity and superconducting devices.
- **Simone Colombo:** Uses ultracold atoms and light to probe the fundamental limits of quantum mechanics
- **Gerald Dunne:** Studies quantum entanglement entropy in quantum field theory, in particular studying how thermal entropy can be converted into entanglement entropy.
- **Kyungseon Joo:** Studies quantum entanglement entropy in quantum field theory, in particular studying how thermal entropy can be converted into entanglement entropy.
- **Jason Hancock:** Leads the development of a UConn Quantum certificate

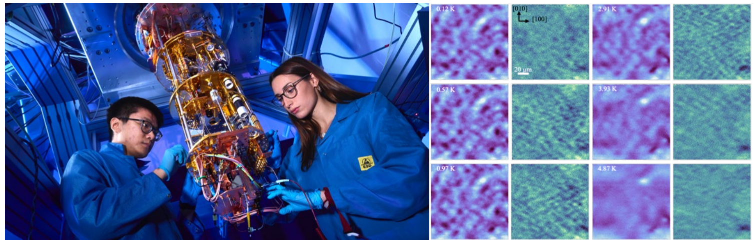
Quantum CT and UConn Physics
Quantum Materials

M. Jain – multiferroics+ magnetism,
Synthesis, bulk magnetic and magnetotransport
measurements (2-400 K, up to 9 T)



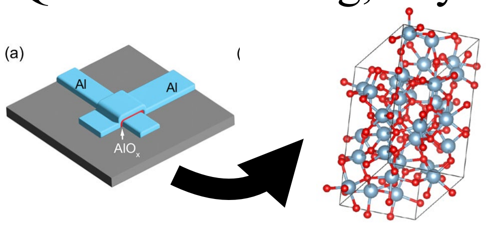


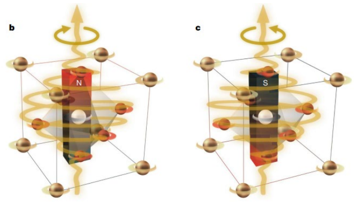
I.Sochnikov– quantum sensing, magnetism, Femtotes
DC magnetometers,
Single-microwave-photon



Phys. Rev. B 112, 104430 (2025)

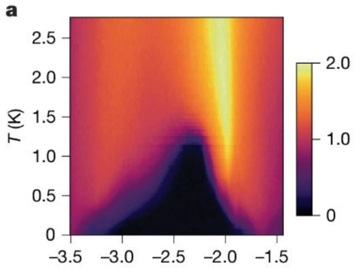
A. Balatsky – dynamics multiferroics, superconductivity,
Quantum Printing, Physics of Qubits

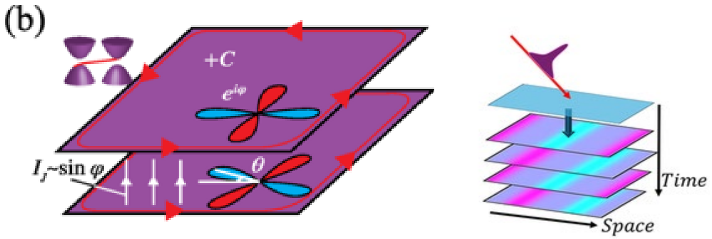




Nature 628, 534–539 (2024).

P. Volkov– 2D and Moire Materials, Unconventional
and high-TC SC, Light-induced phase transitions





Banerjee, Nature (2025), Volkov et al., PRL (2023), Kaplan et al. PRL (2025)

UConn Health Center: Quantum

- Nuclear magnetic resonance (NMR) spectroscopy utilizes the quantum-mechanical properties of nuclear spin systems in molecules to probe their structure, dynamics, and interactions.
- UConn is the lead institution for a $40M NSF mid-scale grant for building a national Network for Advanced NMR, democratizing access to high magnetic field instruments for applications in biomedicine, chemistry, and materials science.
- Advances in quantum sensing are needed to address the most challenging applications of NMR.
- Research at UConn Health is exploring stochastic NMR that exploits parallel excitation of quantum mechanical coherence transfer pathways, a potential approach for accelerating quantum algorithms.

UConn Health Center: AI/ML

- UConn Health hosts the National Center for Biomolecular NMR Data Processing and Analysis, an NIH Biomedical Technology Research Resource.

- The NMRbox platform developed by the Center provides AI/ML resources to the US biomolecular NMR community:
  - ➢ High performance computing resources tailored for ML (e.g. Nvidia Grace Hopper)
  - ➢ Provides access to ML software
  - ➢ Hosts local instances of AlphaFold and DeepSeek on HPC hardware
  - ➢ Provides training resources for ML
  - ➢ Is holding an "NMR AI/ML Boot Camp" in summer 2026