

Al and High-Performance Computing: Accelerating the Future of Mobility

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About me

- Lead of Data and AI Section 50 researchers and engineers
- Research in intelligent agents, machine learning, swarming technology, genetic algorithms, deep learning on high performance, quantum, and neuromorphic computers.
- 160+ research papers, 19 patents, 4 R&D 100 awards, **3** Gordon Bell Finalists
- Married 36 years, a son in the US Navy, and a daughter who works at ORNL
- Love/Hate relationship with my 1966 GTO (since 1980)









Machine Learning and AI – It's a wild ride

- Al is everywhere, everyone is an expert
- Great opportunities with huge challenges
- A pivotal time for Al in mobility



Brief History of AI – The Perceptron – Model the Brain

1943 - The Perceptron – a simple neuron and synapse system

1958 - Perceptron machine created

Start of the first AI revolution

Could not do XOR, the Perceptron is dead



Perceptron

McCulloch, W; Pitts, W (1943). <u>"A Logical</u> <u>Calculus of Ideas Immanent in Nervous</u> <u>Activity</u>". Bulletin of Mathematical Biophysics. 5: 115–133



Rosenblatt, Frank (1957). "The Perceptron—a perceiving and recognizing automaton". Report 85-460-1. Cornell Aeronautical Laboratory.



Expert System – Follow the rules

Represent knowledge in graphs and rules

With enough knowledge and rules a computer should be able to think?

Define a representation and rules for an employee?





The Perceptron and GPUs







- Train on examples (people's faces)
- Predict based on new data
- Revolutionary results, new Al revolution



Deep Learning Network





AI/ML Background



New Al Trends



•What word comes next?





Learning from graphsDoes this person fit in my soc

•Does this person fit in my social network?

Brain Inspired ComputingNative AI at very low power

Vaswani, A., "Attention Is All You Need", arXiv e-prints, 2017. Kwei-Herng Lai, et al. 2020. Policy-GNN: Aggregation Optimization for Graph Neural Networks.(KDD '20). Catherine Schuman



Example: Representing an employee



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Example: Using the network



Is this person a fit for SMMC?

What sessions would be of interest?

Who should they meet?



Nine Yards – Material Science



In the title salt, $C_{10}H_{i1}N_4O_2^+\cdot I^-$, the asymmetric unit consists of a pyridinium cation bearning a (1-methyl-5-nitro-1*H*imidazol-2-yl)methyl group at the N position and an iodide anion. The imidazole ring is quasiplanar, with a maxiumum deviation of 0.0032 (16) Å, and forms a dihedral angle of 67.39 (6)° with the plane of the pyridinium ring. The crystal packing can be described as alternating zigzag layers of cations parallel to the (001) plane, which are sandwiched by the iodide ions. The structure features two types of hydrogen bonds (C-H···O and C-H···I), viz. cation-anion and cation-cation, which lead to the form ation of a three-dimensional network.

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Generative AI and Knowledge Graph



Will this material produce a better batteries?

Under what conditions can this battery operate?

Can it be used to power a vehicle?



Neuromorphic Computing: Back to the perceptron in hardware -Engine Control for Fuel Efficiency



International Conference on Green and Sustainable Computing 2020. Accepted.

Neuromorphic Engine Control for Fuel Efficiency





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Objective

- Develop <u>a prediction model</u> for estimation of future system state and utility → removes computation load from the RL engine and can be used as a low-cost, low fidelity model to improve RL efficiency.
- Develop <u>a reinforcement learning-based control system</u> for traffic signal timing.
- Partial Observability Issue: limited sensor coverage \rightarrow use Graph Neural Network (GNN) to estimate.
- <u>Scalability</u>: RL agent is trained in a decentralized way: all controllers to have an independently trained with neighbor data -> allow rapid real world deployment.
- Coupled Transportation Digital Twins and AI-empowered Control





Performance of the prediction model (GNN + LSTM)

16

Performance of RL agent: traffic volume

Neuromorphic Computing: Energy Efficient AI for the Edge

- Open research questions:
 - 1. How do we design Al for edge computing?
 - 2. What are the technological barriers to development and deployment of AI to the edge?
 - How effective can Al leverage multi-sensor data (e.g., camera, LIDAR, Radar, GPS, IMUs)?



From small scale Test & Development



To full scale Test & Development





Driving Innovation: The Strength of ORNL

8	Award-Winning Al Research:	Recognized Excellence: Our groundbreaking AI research has garnered prestigious awards, pushing the boundaries of artificial intelligence and its transformative potential.
₹ .	National Transportation Research Center:	Pioneering Mobility Solutions: At the forefront of national transportation research, we are shaping the future of mobility through cutting-edge technologies and sustainable practices.
	World's Fastest Computer:	Powering Possibilities: Unleashing unprecedented computational capabilities, our institution is home to the world's fastest computer, driving advancements across diverse fields and propelling us into the digital frontier.

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Questions?



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