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Artificial Intelligence Strategy and Implementation

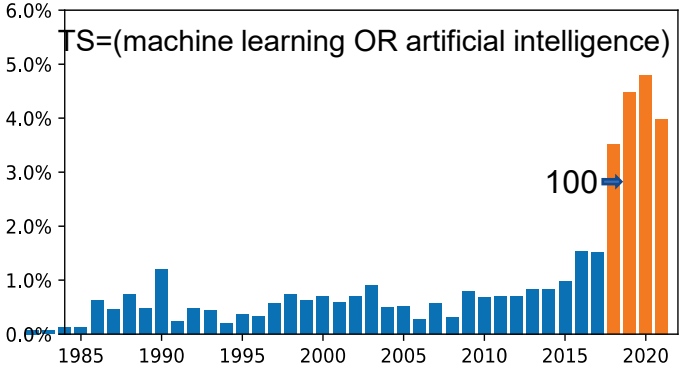
Aric Hagberg
Computer, Computational, and Statistical Sciences Division

March 7, 2022

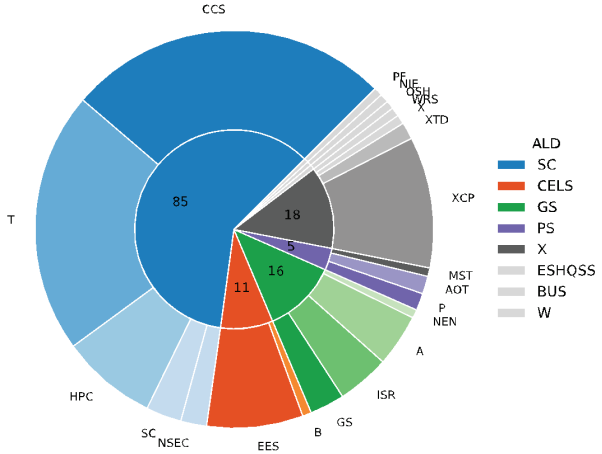
Artificial Intelligence at Los Alamos

- R&D in AI and Machine Learning has expanded rapidly with combination of fundamental and mission applications
- Leveraging historical strengths in computational physics – “physics-informed ML”
- **Focus on integration of AI with modeling and simulation**
- Investing with LDRD program to develop capability and teams
- Increasing portfolio of SC, LDRD, DOE Applied Energy, NNSA, and Global Security projects – total scope > $30M and growing
- Access to latest ML hardware and partnerships with hardware vendors
- Engaging community through LANL-led workshops and conferences
- Developing pipeline with structured student research internships

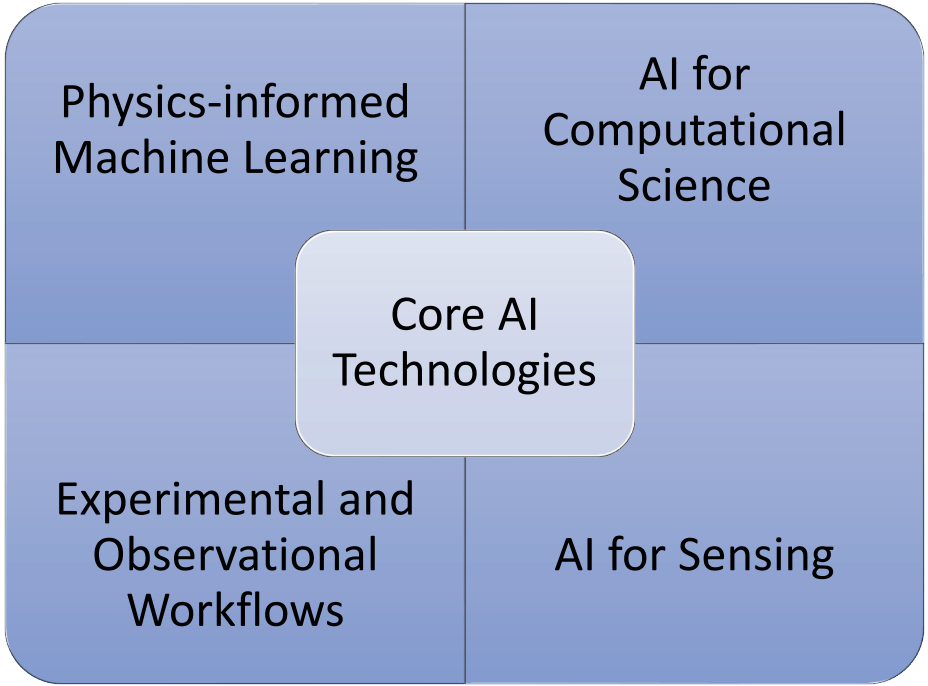
AI Papers/All Papers at LANL



AI workforce spans laboratory > 250



AI Capability Themes at Los Alamos

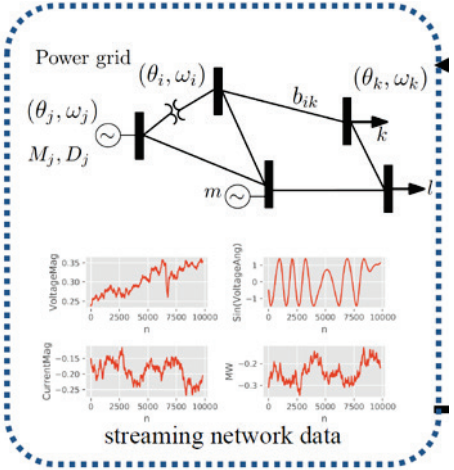


AI is part of multiple Capability Pillars

ENGINEERING	MATERIALS FOR THE FUTURE	Defects and Interfaces Extreme Environments Emergent Phenomena
	NUCLEAR AND PARTICLE FUTURES	Accelerator Science & Technology Applied Nuclear Science & Engineering High Energy Density Plasmas & Fluids Nuclear, Particle, Astrophysics & Cosmology
	INTEGRATING INFORMATION, SCIENCE, AND TECHNOLOGY FOR PREDICTION	Computing Platforms Computational Methods Data Science
	SCIENCE OF SIGNATURES	Nuclear Detonation Nuclear Processing, Movement, Weaponization Natural and Anthropogenic Phenomena
	COMPLEX NATURAL AND ENGINEERED SYSTEMS	Human–Natural System Interactions: Nuclear Engineered Systems Human–Natural System Interactions: Non-Nuclear
	WEAPONS SYSTEMS	Design Manufacturing Analysis

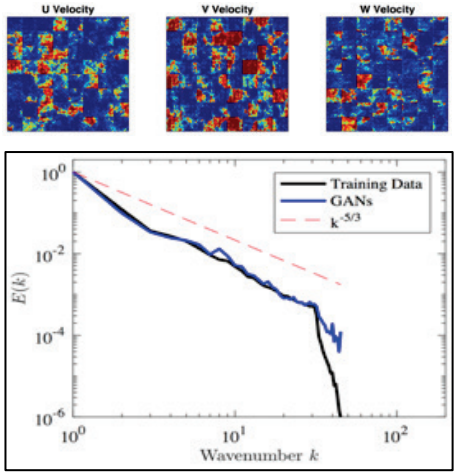
Physics-informed Machine Learning

Anomaly Detection in Energy Systems



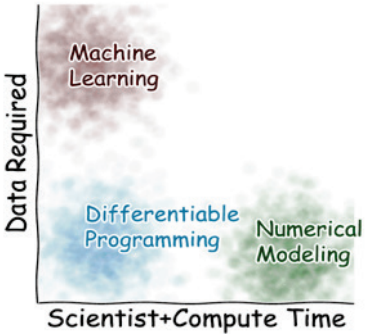
Incorporate known physics of electrical circuits

Machine Learning for Turbulence



Add physics constraints to black-box ML for turbulence emulators

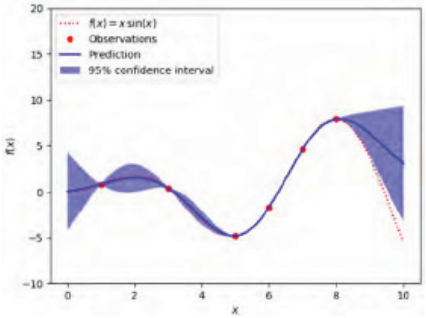
Differentiable Programming: Bridging the Gap between Numerical and Machine Learning Models



Combine trustworthy numerical modeling with ML to produce fast models

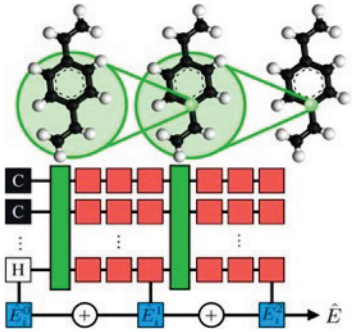
AI for Computational Science

Enabling Predictive Scale-Bridging Simulations through Active Learning



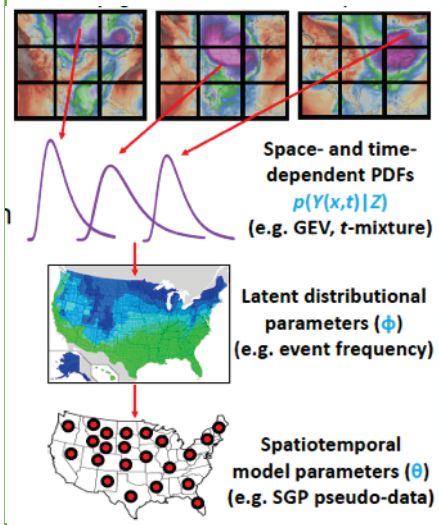
Neural networks predict upscaled parameters and uncertainties in multiscale systems. Materials damage.

Quantum Chemistry and Molecular Dynamics



ML constructs potentials based upon large datasets of quantum calculations. Materials properties, aging.

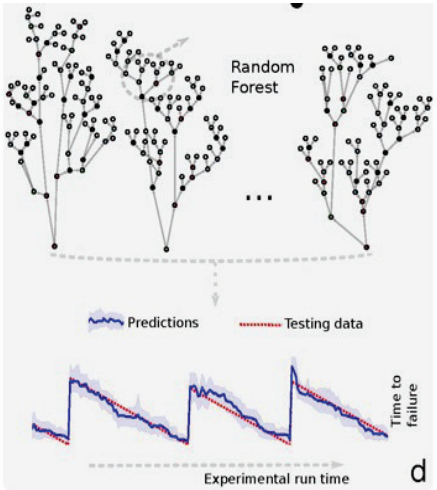
In-situ Inference



Bringing advanced data science into exascale simulations. Climate, space weather.

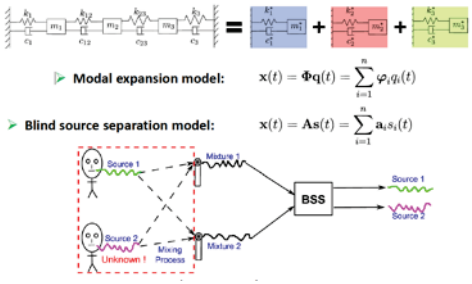
AI for Sensing

Earthquakes



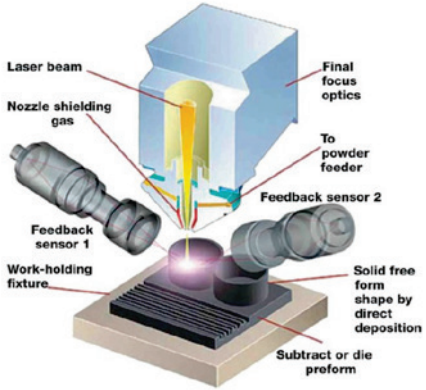
ML to probe fault physics and assess earthquake hazard

Structural Health Monitoring



Remote measurement of high-resolution full-field spatio-temporal dynamics

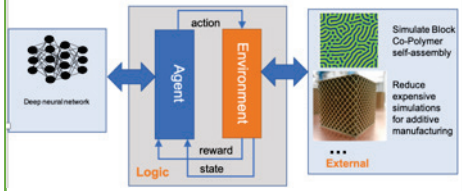
Manufacturing



Monitor formation of pores using acoustic emissions data + machine learning methods

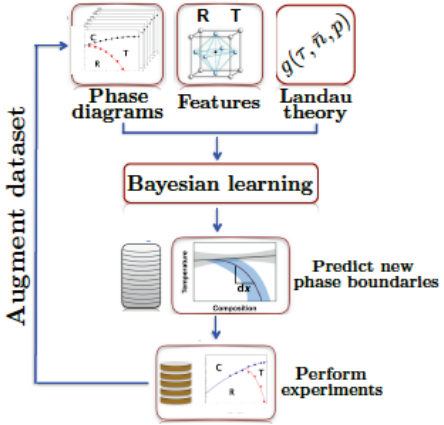
Experimental and Observational Workflows

Reinforcement Learning for Scientific Environments

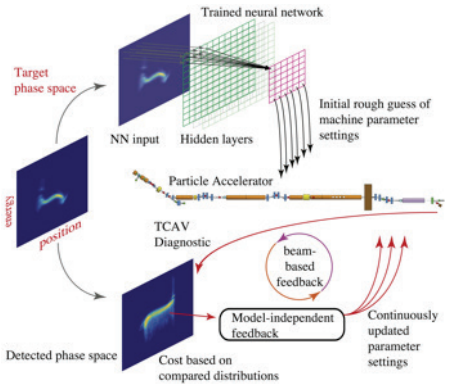


ExaRL:" Developed as part of the Exascale Computing Project ExaLearn

Real-time Adaptive Acceleration of Dynamic Experimental Science

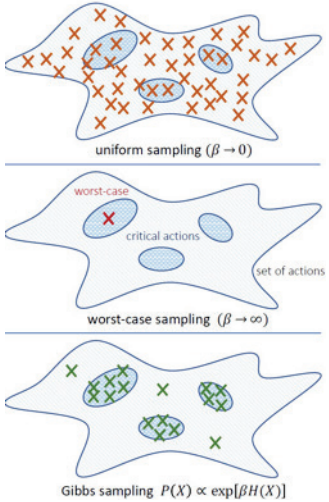


Adaptive Machine Learning for Closely Spaced Ultra-Short Intense Accelerator Beams



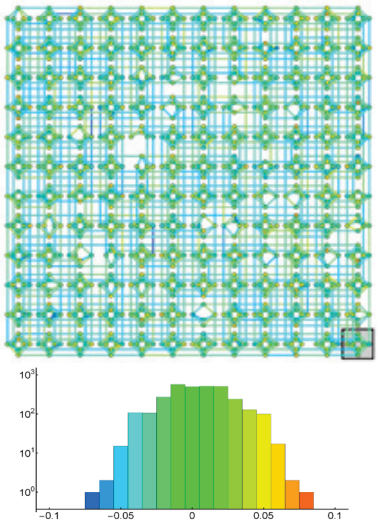
Core AI Technologies

Optimization of ML
Constrained, robust, tractable, learning methods



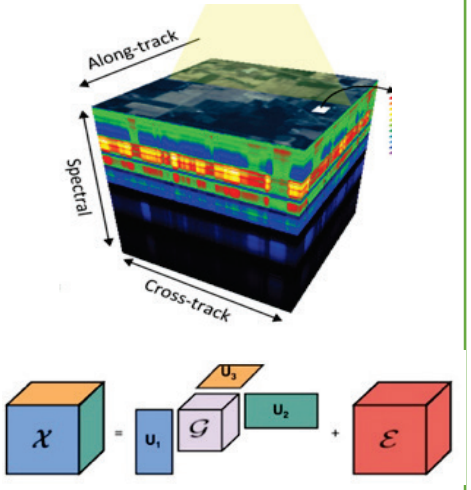
Anomaly detection in energy systems

Graphical models
Probabilistic machine learning methods



Calibrating the D-Wave quantum annealer

Tensor factorization
Extraction of explainable hidden features in data



Applications in cancer, earthquakes, ~100TB data

LANL Strategic Activities for AI

Goal: Accelerate development of AI-enabled capabilities for science and security

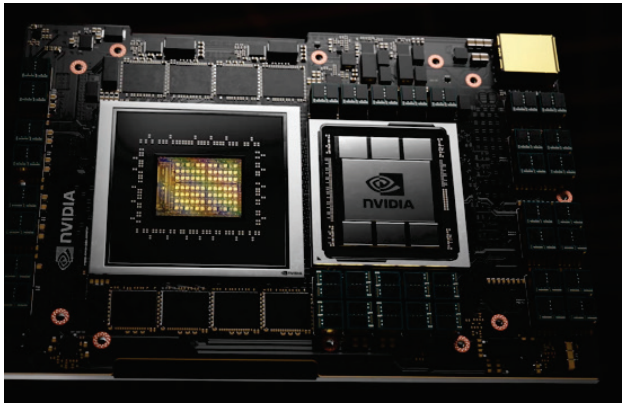
- Develop mission-relevant core AI technologies (and apply them)
- Create AI workforce pipeline and training opportunities
- Build AI partnerships and community (lead, and participate in broader fora)

Technology: LDRD Program is Investing in Core AI R&D (~$15M/year)

	DOE ASCR Scientific ML Priority Research Directions	LANL LDRD Research Projects
Scientific Machine Learning: **Foundations**	**Domain-Aware:** Leverages & respects scientific domain knowledge. Physics principles, symmetries, constraints, uncertainties & structure-exploiting models	Differentiable Programming: Bridging the Gap between Numerical Models and Machine Learning Models, Dan O'Malley Topological Relation-Based Image Analysis using Graphs, Diane Oyen
	Interpretable: Explainable and understandable results. Model selection, exploiting structure in high-dimensional data, use of uncertainty quantification with machine learning	Uncertainty Quantification for Robust Machine Learning, Diane Oyen Deep Learning in a Noisy World: Algorithms for robust training and predictive uncertainty, Sunil Thulasidasan Trustworthy Artificial Intelligence, Juston Moore
	Robust: Stable, well-posed & reliable formulations. Probabilistic modeling in ML, quantifying well-posedness, reliable hyperparameter estimation	The Optimization of Machine Learning: Imposing Requirements on Artificial Intelligence, Russell Bent
Scientific Machine Learning: **Capabilities**	**Data-Intensive SciML:** Scientific inference & data analysis. ML methods for multimodal data, in situ data analysis & optimally guide data acquisition	Machine Learning for Realizing Next-Generation Quantum Hardware, Michael Martin Tensor Networks: Robust Unsupervised Machine Learning for Big-Data Analytics, Boian Alexandrov
	Machine Learning-Enhanced Simulations: ML hybrid algorithms & models for predictive scientific computing. ML-enabled adaptive algorithms, parameter tuning & multiscale surrogate models	Sampling the unknown: Robust modeling of atomic potentials, Kipton Barros In-Situ Inference: Bringing Advanced Data Science into Exascale Simulations, Earl Lawrencee Enabling Predictive Scale-Bridging Simulations through Active Learning, Tim German Machine Learning for Turbulence, Daniel Livescu
	Intelligent Automation and Decision Support: Adaptivity, automation, resilience, control. Exploration of decision space with ML, ML-based resource management, optimal decisions for complex systems	AI@Sensing, Satish Karra, Aric Hagberg

Partnerships: Advanced ML Computing Resources

- SambaNova ML hardware and tools
  - Showing ~3x speed up over Nvidia GPU
- Groq-ML accelerators
- LANL partnership with NVIDIA will bring in a large CPU-GPU system in 2023 – Venado.



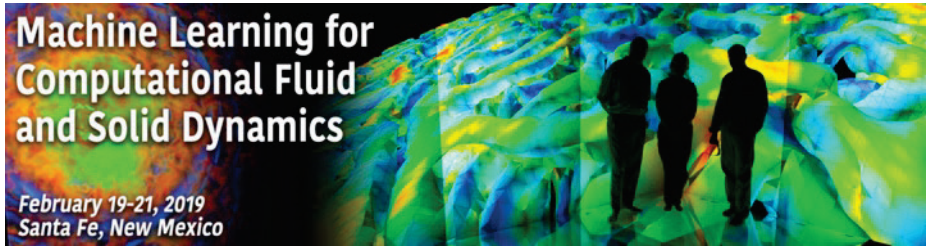
NVIDIA®

Community: Convening Workshops and Conferences

- Physics Informed Machine Learning
  - 2016,2018,2020,2022
- Machine Learning in Solid Earth Geoscience
  - 2018,2019,~~2020~~, 2022
- Conference on Data Analysis
  - 2012,2014,2016,2018,2020, ~~2022,~~ 2023
- Machine Learning for Computational Fluid and Solid Dynamics
  - 2019, ongoing international seminars

PHYSICS INFORMED MACHINE LEARNING

April 5-7, 2022 | Santa Fe, New Mexico
Exploring Data-Focused Research across the Department of Energy

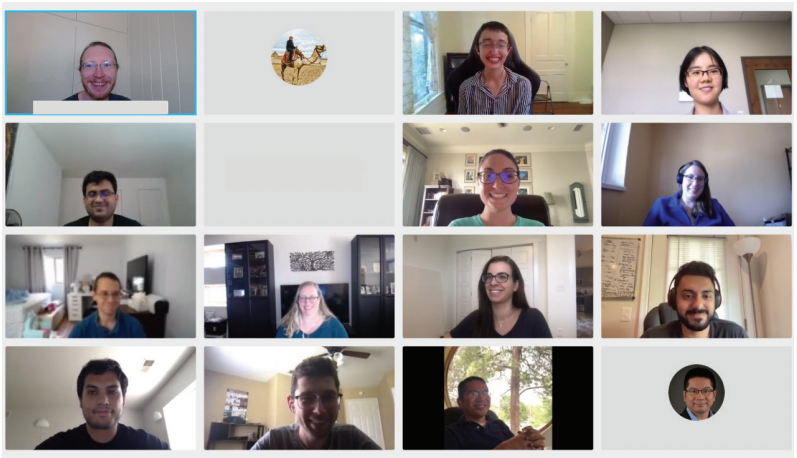


Pipeline: Machine Learning

ISTI Applied Machine Learning Summer Research Internship

- Collective advertising helps recruit a large applicant pool with highly-qualified students
- Students come from various disciplines (mostly not computer science)
- Team Science: Students work on our research projects in small teams with teams of mentors – provides typical lab team science experience

AML 2021
Virtual



6th year of program

- 2017 Class 12 students
- 2018 Class 24 students
- 2019 Class 15 students
- 2020 Class 16 students
- 2021 Class 12 students

Typically about 10x applicants.

We track outcomes and have former students returned as graduate students, postdocs, and staff