Advancing Machine Learning for Mission-Critical Applications

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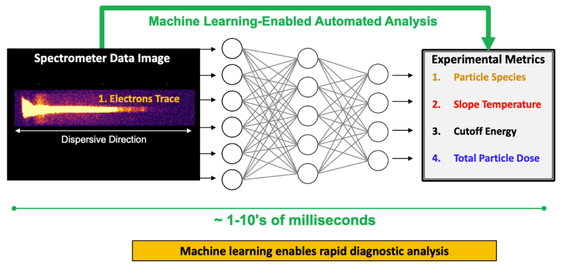
Our primary goal is to make fundamental advances in four critical machine learning (ML) research areas to tackle challenging mission-critical problems. We believe this can be best achieved through a synergistic partnership between ML, HPC, and the programs.

1 PHYSICS-INFORMED ML

Advancing data-driven methods for scientific impact requires the integration of domain knowledge with ML solutions.

INNOVATIONS:
- Domain-aware ML architectures
- Science-preserving generative models
- Smart, high dimensional sample design
- Customized loss functions

IMPACTS:
- Cognitive simulation efforts in ICF/Plasma physics
- Traumatic brain Injury studies
- Pilot2 cancer modeling

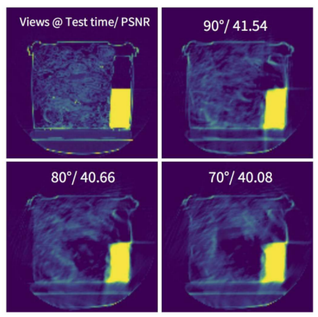


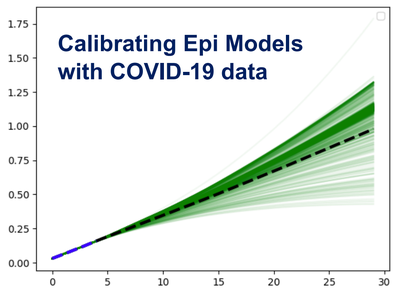
2 INVERSE PROBLEMS

Solving ill-posed inverse problems using ML through novel data-based and model-based priors.

INNOVATIONS:
- Breakthrough in limited angle CT imaging
- Accurate posterior estimation
- Generative priors for inverse problems
- Unsupervised source separation

IMPACTS:
- Accurate CT imaging in security/healthcare
- History matching with complex simulation codes
- Calibrating epidemiological codes for COVID-19 studies





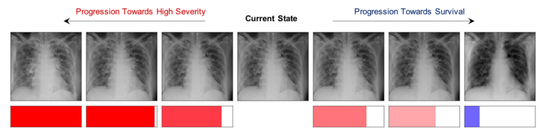
Build ML solutions that cater to unique challenges in real-world scientific problems

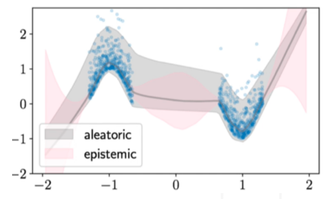
3 UQ & INTERPRETABILITY

Uncertainty quantification and interpretable ML are critical to creating trust and enabling users to gain insights into models and data.

INNOVATIONS:
- Pioneering UQ for scientific ML
- New explainability and counterfactual reasoning methods
- State-of-the-art in active learning

IMPACTS:
- Reliable diagnosis in healthcare
- Causal attribution in neuroscience problems
- Interpretable material design



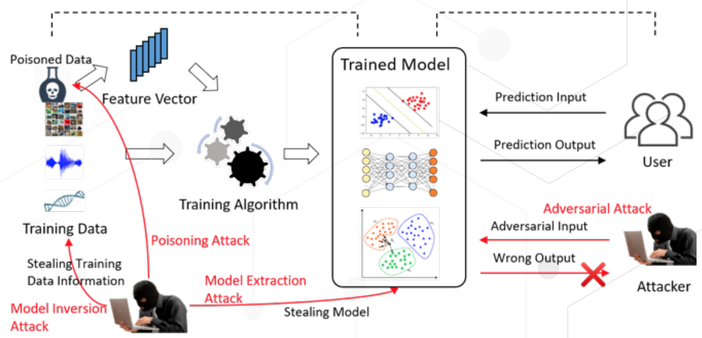


4 SECURITY & PRIVACY

Certifiably robust and privacy-preserving ML solutions for safety-critical applications.

INNOVATIONS:
- Developed automated tools for certified training and robustness verification.

IMPACTS:
- Tools can fundamentally transform the state-of-practice in deep learning for cyber-physical security, power grid, and sciences.
- Critical in healthcare system design



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