SAND2016-13540

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Using Machine Learning to Detect and Reduce Uncertainty in Turbulent Flow Simulations

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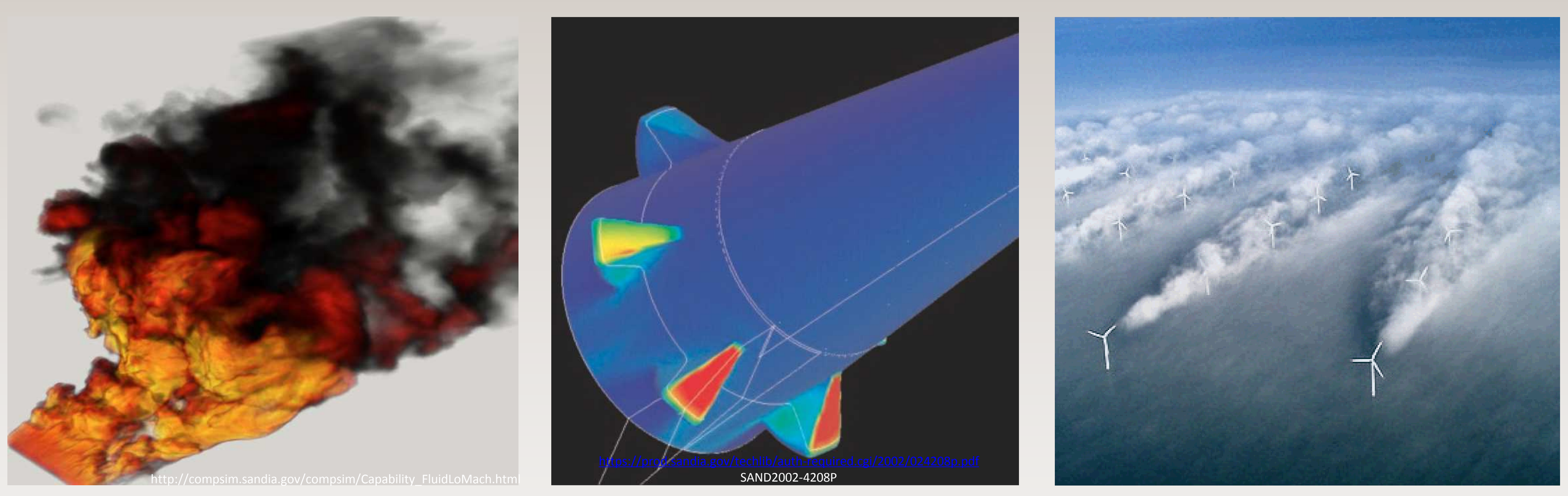
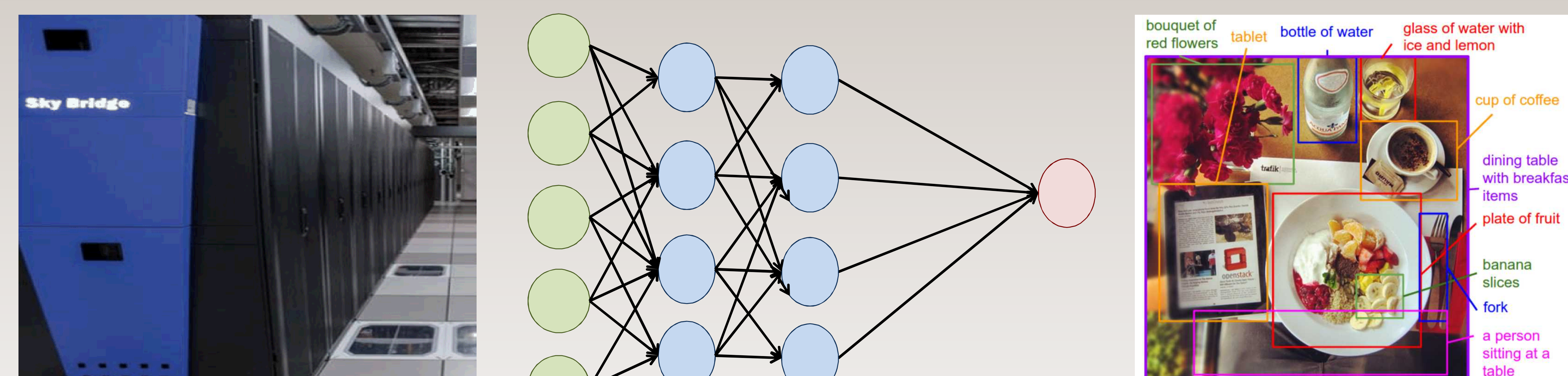
Thermal/Fluids Science and Engineering (8253)

Turbulence Simulations



- Turbulent flows occur in many applications of interest at Sandia
- High fidelity direct numerical simulations are computationally expensive—not feasible for many flows of interest
- Approximate empirical models are used to simulate these flows in a computationally tractable way
  - It is critical to assess the uncertainty of these models

Machine Learning



Karpathy, Andrej, and Li Fei-Fei. Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition. 2015

- Set of data-driven algorithms for regression, classification, clustering
- *E.g.*: Neural networks for deep learning of image classification
- Have been broadly applied in finance, software engineering, retail
- Applying these algorithms to physical systems presents unique challenges and opportunities

Major Innovations

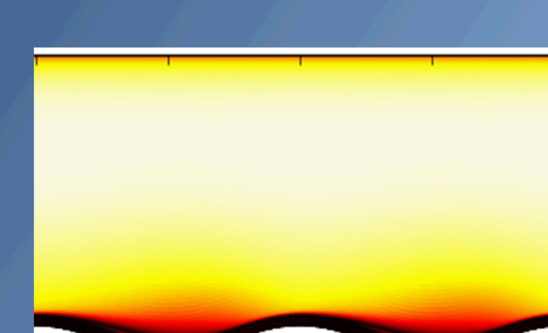
- Defined strategy for embedding physical symmetries into machine learning models
- Applied machine learning to detect regions of high uncertainty in turbulence simulations
- Developed framework for data-driven adaptive physics modeling
- Extracted physical intuition from complex machine learning models

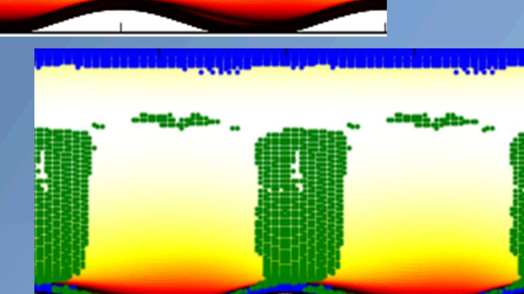
Embed Physical Symmetries into Machine Learning Models

- Many physical systems have known invariance properties
- Applied concepts from group theory and representation theory to embed invariance properties into machine learning models without loss of information
- Demonstrated 100 X gain in computational efficiency versus brute force approach that did not embed symmetry
- Applied to cases in turbulence modeling and crystal elasticity

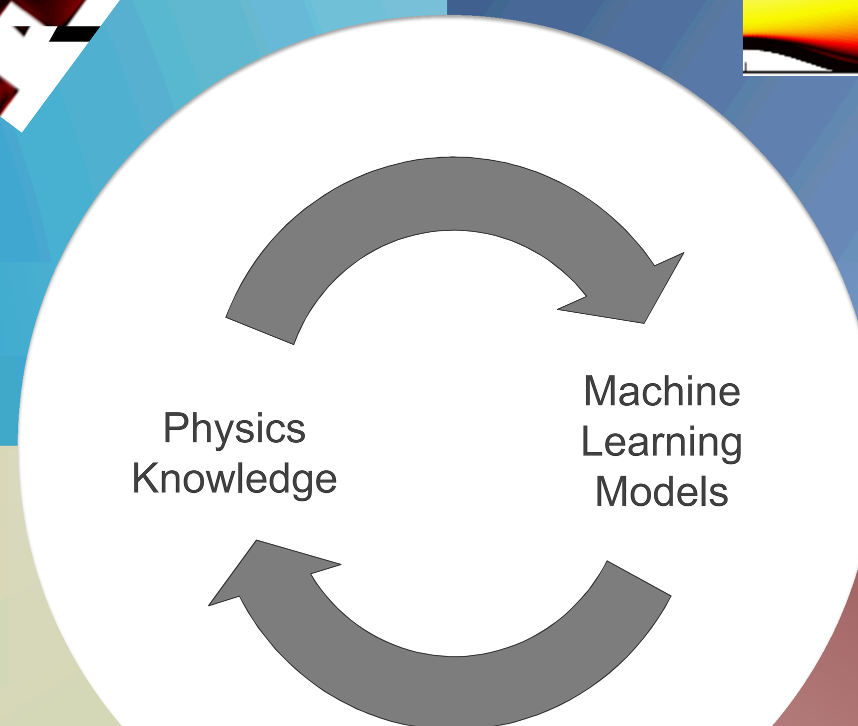
Detect Regions of High Uncertainty

- Developed machine learning methods to detect when empirical turbulence model assumptions are violated
- Leveraged big data from high fidelity simulations of canonical flows to train model
- Achieved 3 X more accurate error detection than previous state-of-the-art





Blue: Isotropy assumption violated
Green: Linearity assumption violated

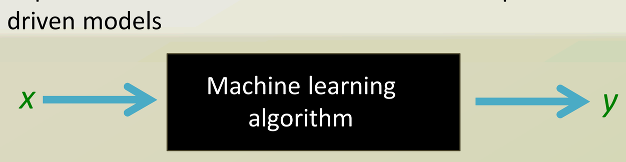


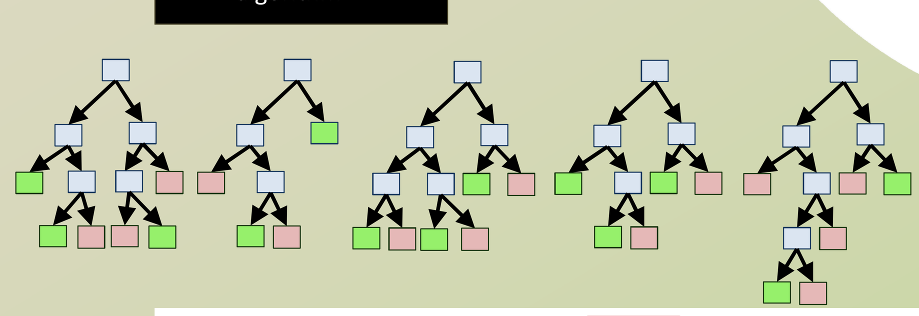
Impact Areas

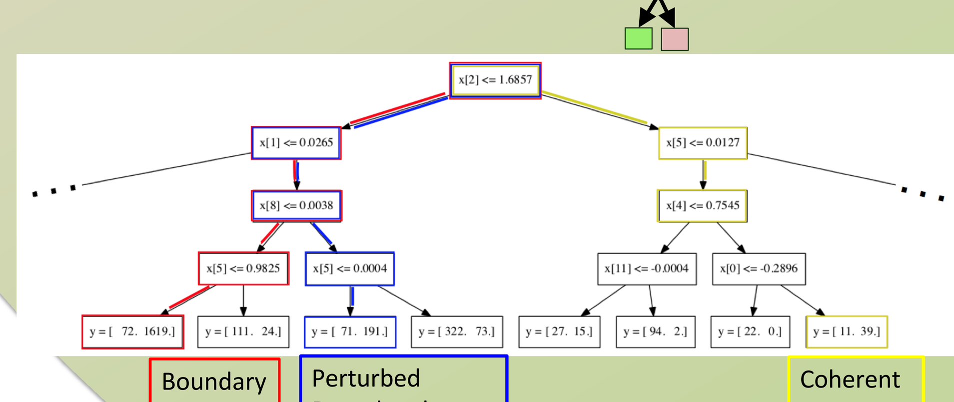
- Robust uncertainty quantification for turbulence simulations
- Efficient methods for improving predictive accuracy
- Novel strategies for model development
- Applications in:
  - Nuclear safety: abnormal thermal environments
  - Re-entry flows
  - Captive carry
  - Engine combustion
  - Renewable energy: wind farms

Rule Extraction

- Machine learning models are often treated as "black boxes"
- Used rule extraction to regain physical intuition for improved turbulence models from these complex data-driven models

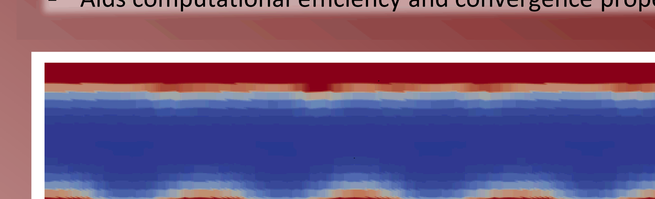


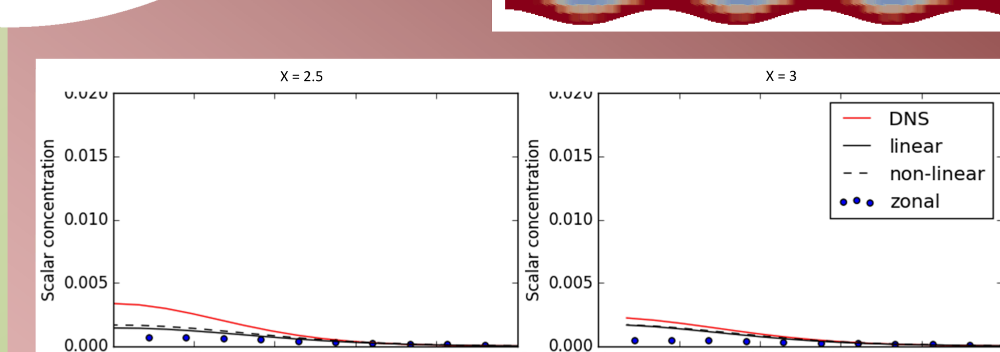




Enable Adaptive Physics Modeling

- Use machine learning classifiers to trigger model corrections on the fly
- Apply the correction term where it's needed, when it's needed
- Aids computational efficiency and convergence properties





Cross-Cutting Themes

- Computational Mechanics
- Machine Learning
- Uncertainty Quantification
- Big Data

Publications

- J. Ling and J. Templeton, "Evaluation of machine learning algorithms for prediction of regions of high Reynolds averaged Navier Stokes uncertainty," Physics of Fluids, (2015).
- J. Ling, "Using Machine Learning to Understand and Mitigate Model Form Uncertainty in Turbulence Models," IEEE ICMLA, (2015).
- J. Ling, A. Ruiz, G. Lacaze, and J. Oefelein, "Uncertainty analysis and data-driven model advances for a Jet-in-Crossflow," ASME Tubo Expo 2016, *accepted.*
- J. Ling, R. Jones, and J. Templeton, "Machine Learning Strategies for Systems with Invariance Properties," Journal of Computational Physics, *submitted.*

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NNSA National Nuclear Security Administration

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Many thanks to my technical mentor Jeremy Templeton and my manager Amanda Dodd