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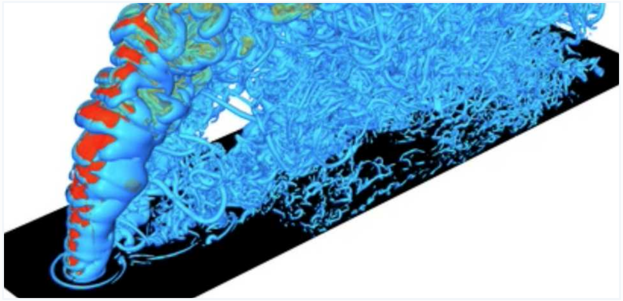

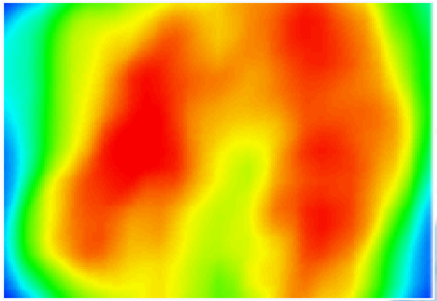

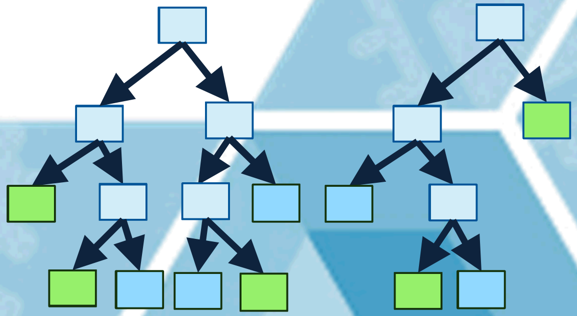

Machine Learning for Turbulence Modeling

Julia Ling

November 2016

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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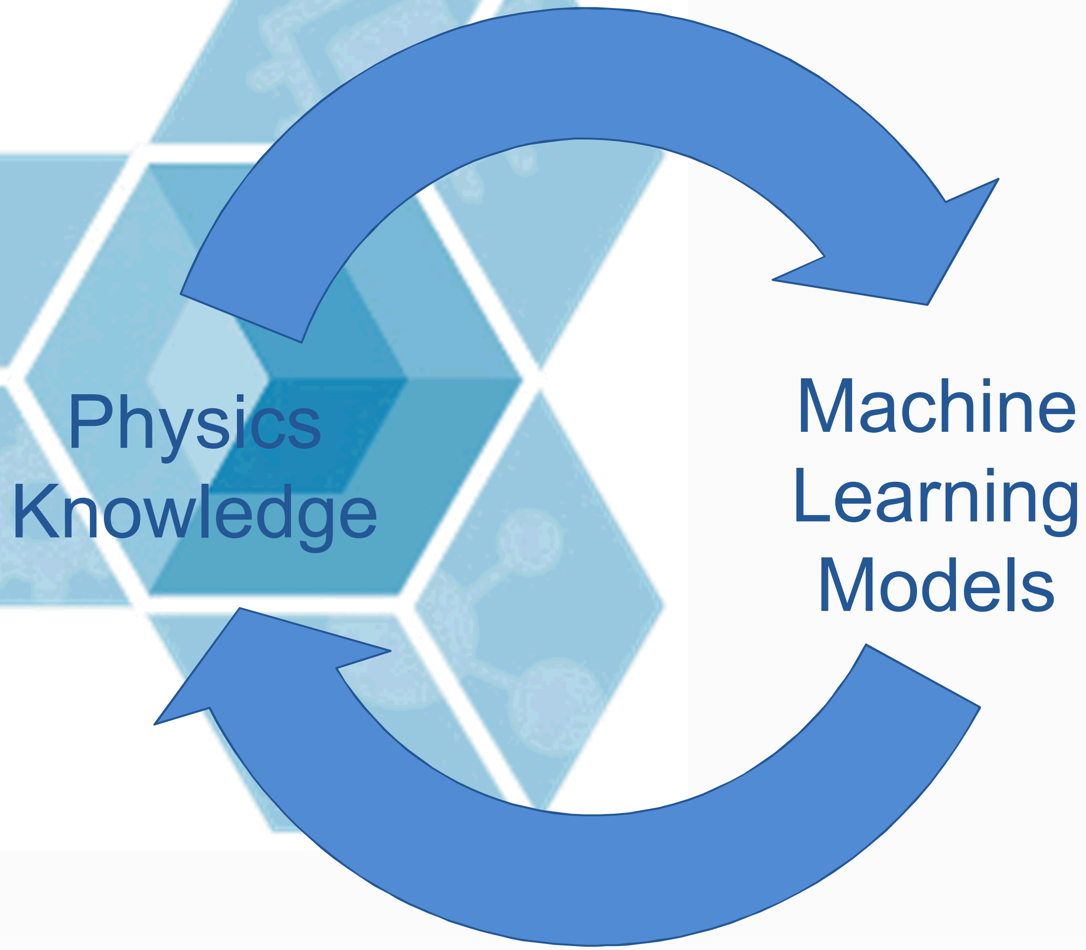
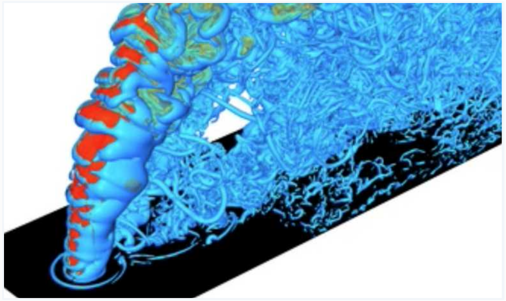
Machine Learning on Engineering Systems

- How should scientific domain knowledge interact with data-driven models?





Outline

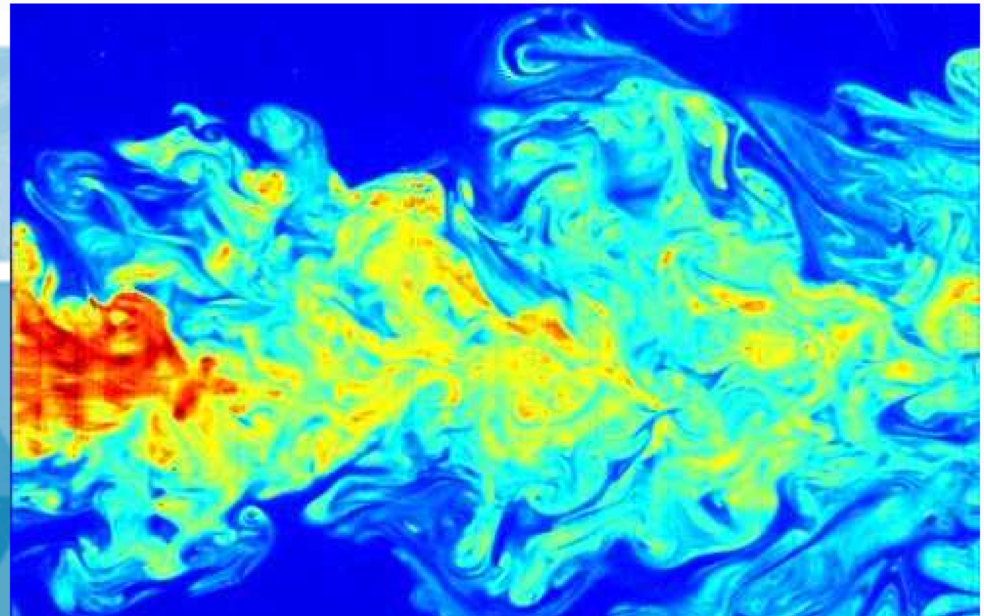
1) Machine learning for turbulence uncertainty quantification

1) Rule extraction to gain physical intuition

1) Deep learning with embedded invariances

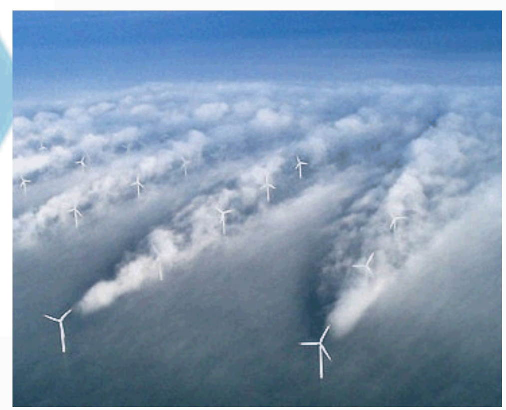
Turbulence

Chaotic 3-D fluid motion at a continuum of scales



Fukushima et al.

Hokusai (c 1830)

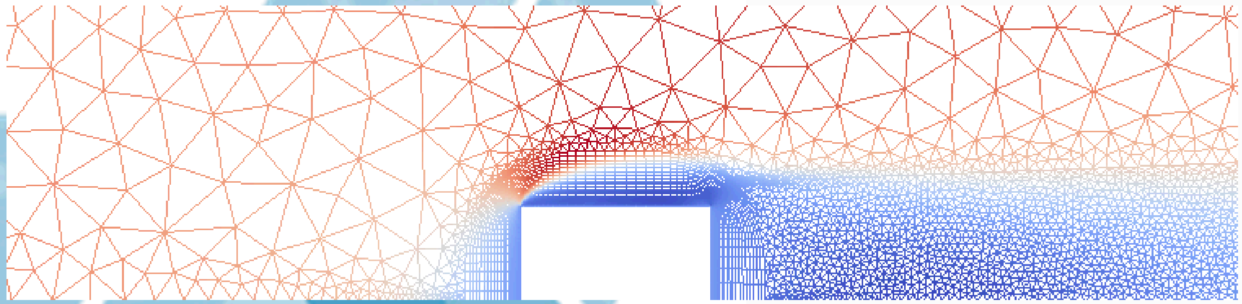


http://www.windturbinesyndrome.com/2011/wind-turbine-turbulence-what-are-the-micro-climate-effects/

https://brilliant.org/wiki/rocket-physics/

Turbulence Simulations

"When I die and go to heaven there are two matters on which I hope for enlightenment. One is quantum electrodynamics, and the other is the turbulent motion of fluids. And about the former I am rather optimistic." –Horace Lamb



Direct Numerical Simulation (DNS)

- Hundreds of millions of core hours for even simple flows
- Exact

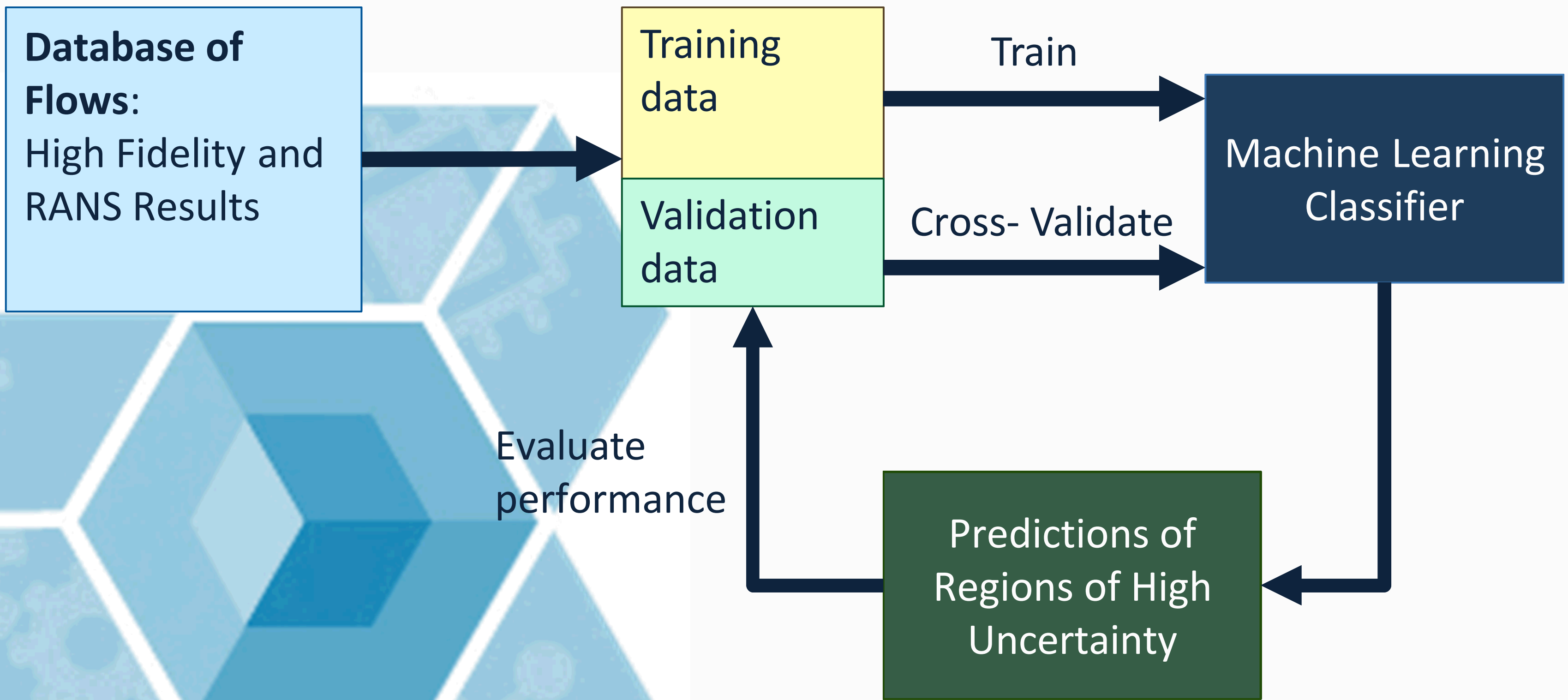
Reynolds Averaged Navier Stokes (RANS)

- Orders of magnitude less computationally expensive
- Approximate

Machine Learning Problem Set-Up

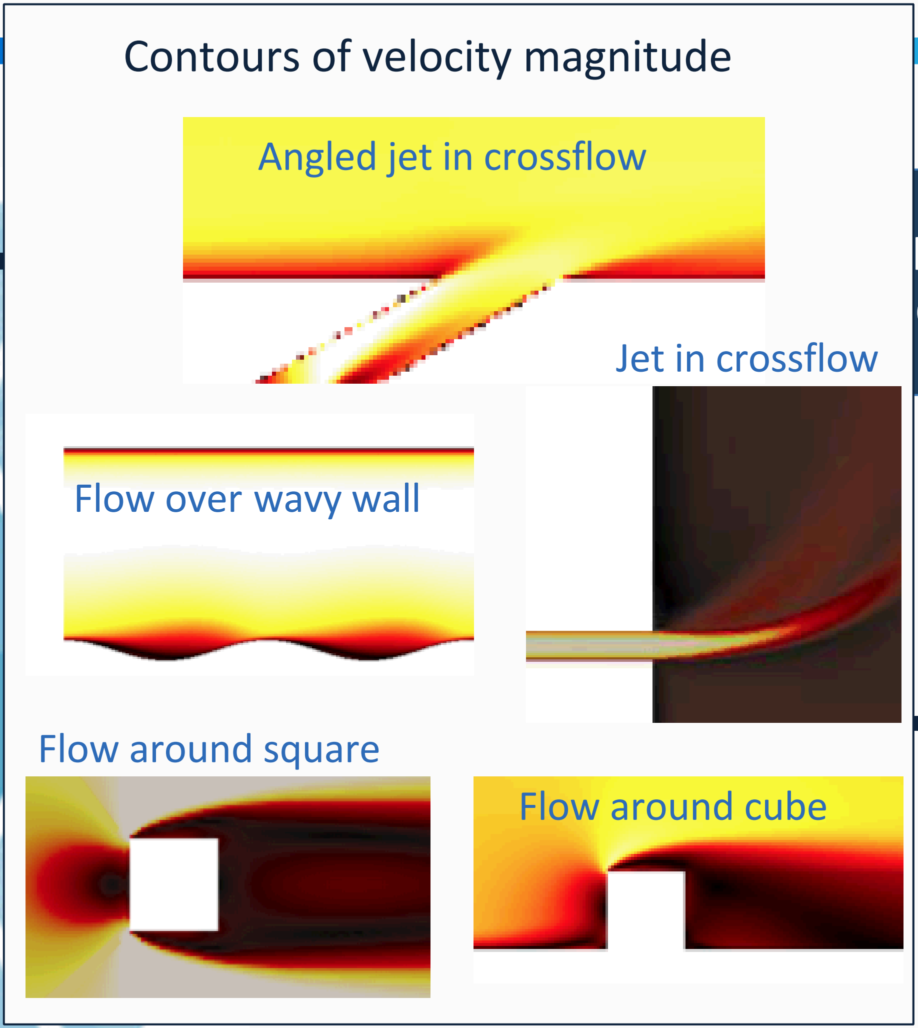
- Assemble a database of flows for which both DNS and RANS results are available
- Use the DNS as “truth” data for supervised machine learning
- Build a binary classifier to predict when RANS has high uncertainty based on when specific model assumptions are violated
- Inputs are local flow variables from RANS (velocity, pressure, density, …)
    - Each point in the mesh represents a separate data point

Classifier Development



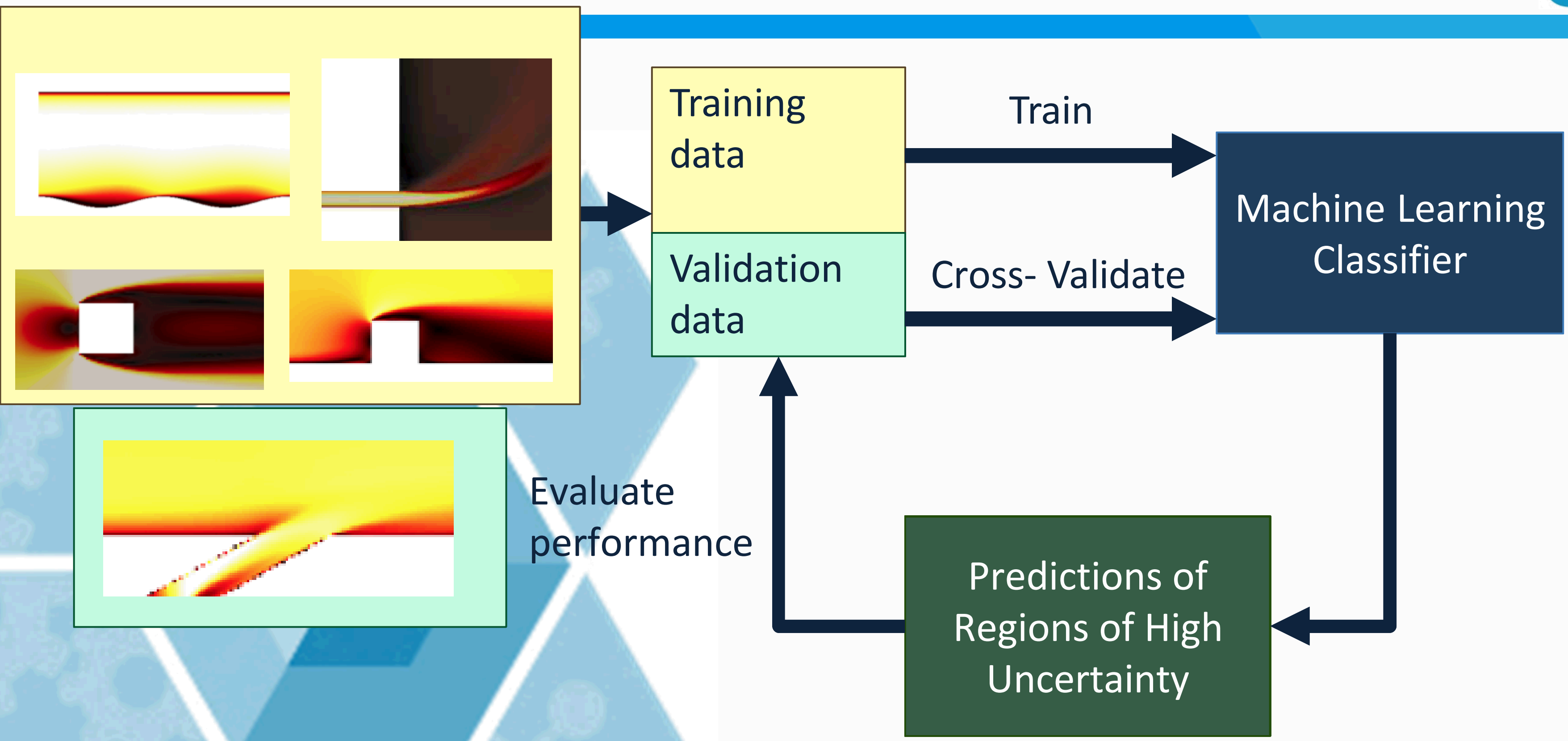
Classifier Development

Database of Flows:
High Fidelity and RANS Results

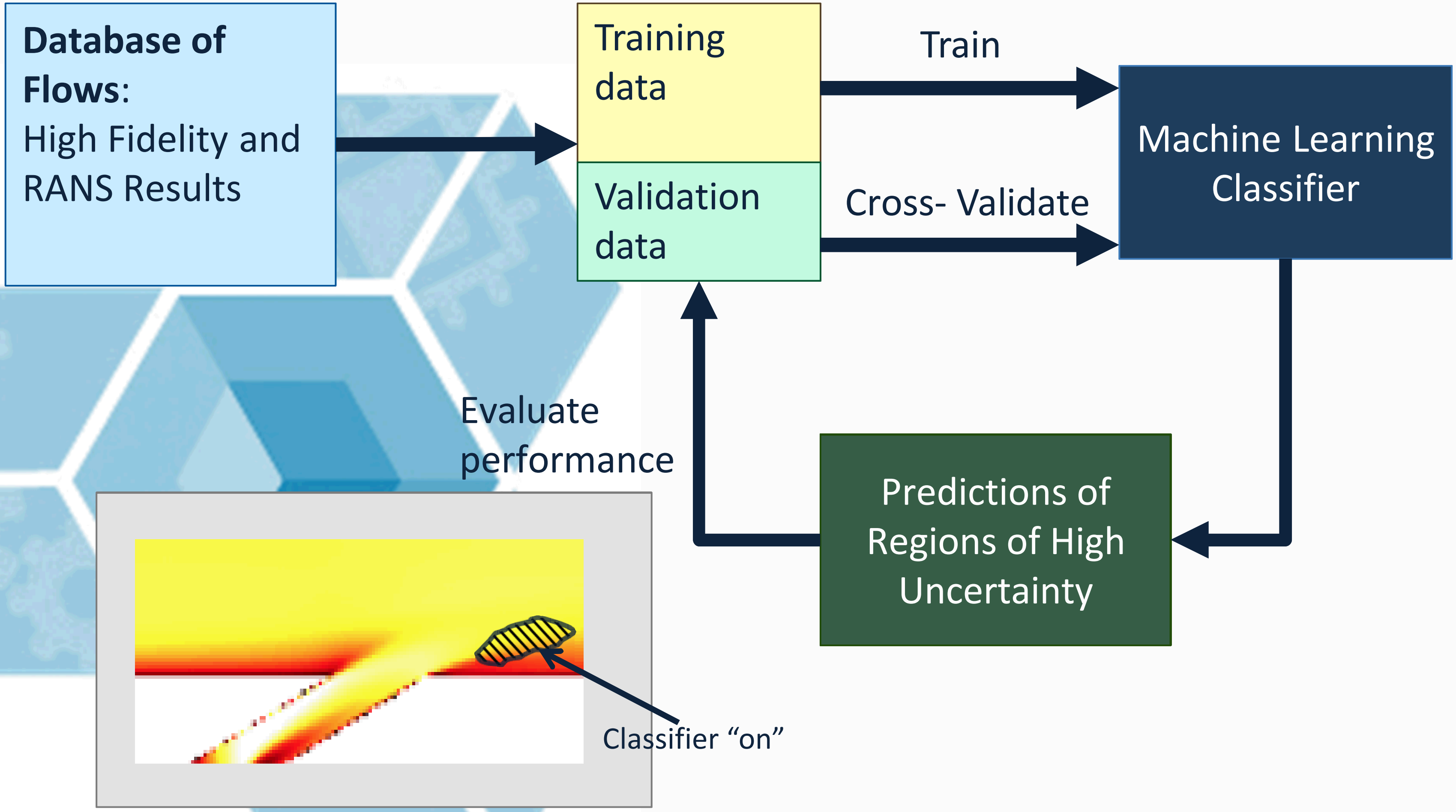


hine Learning
Classifier

Classifier Development

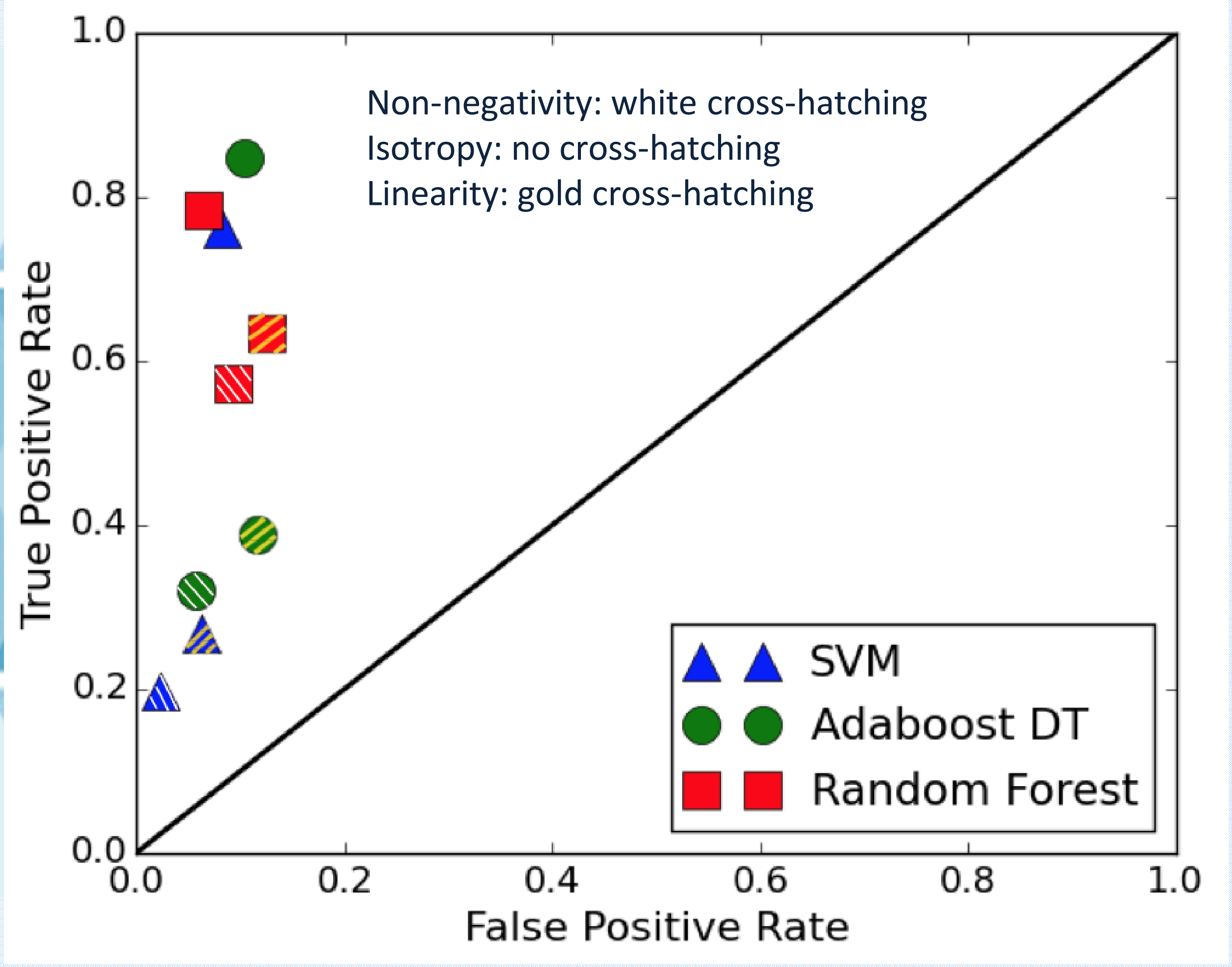


Classifier Development

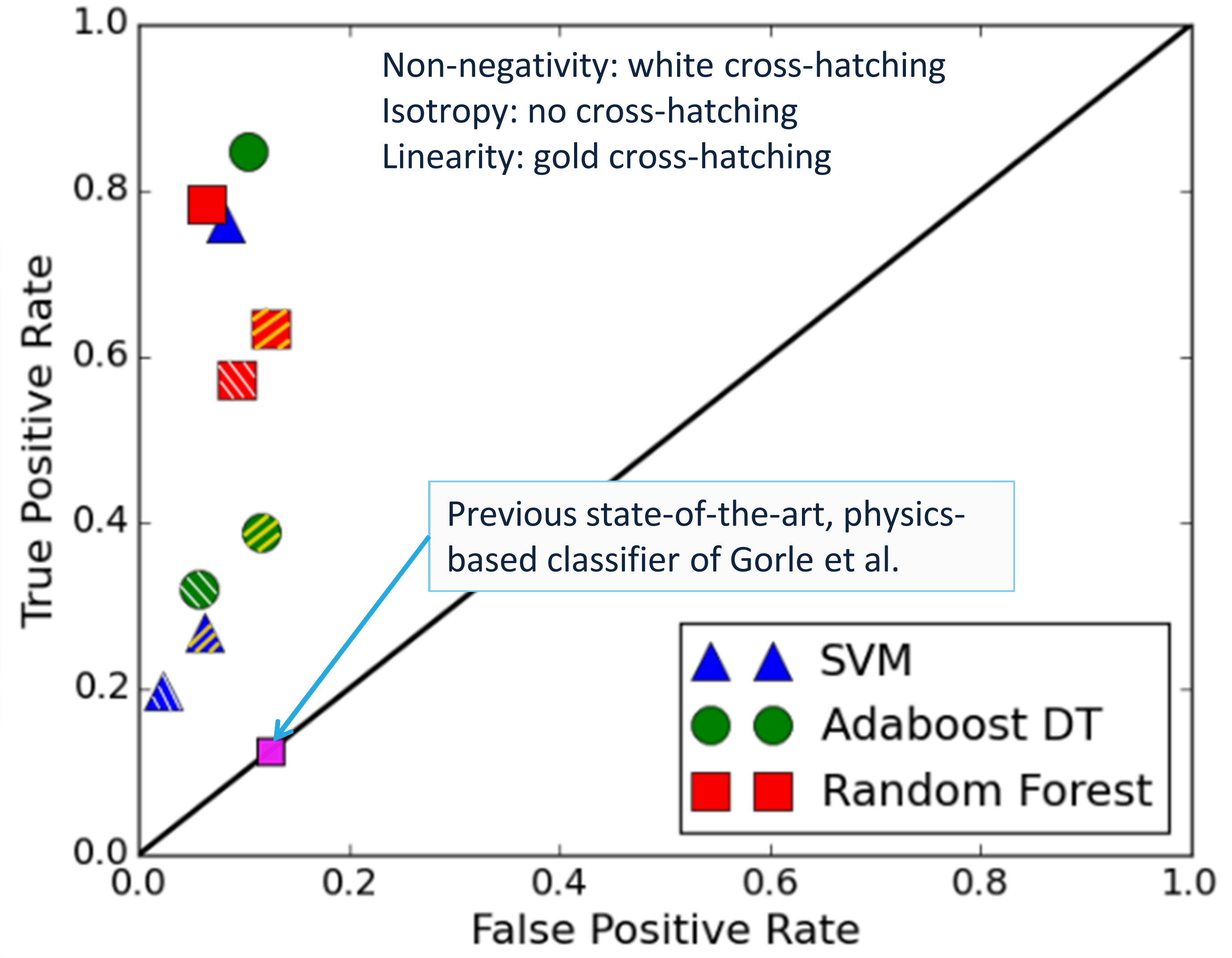


- Use classifier to make predictions on validation set
- Evaluate classifier by comparing to high fidelity results
- Leave-one-out cross-validation

Classifier Performance



Classifier Performance



Outline

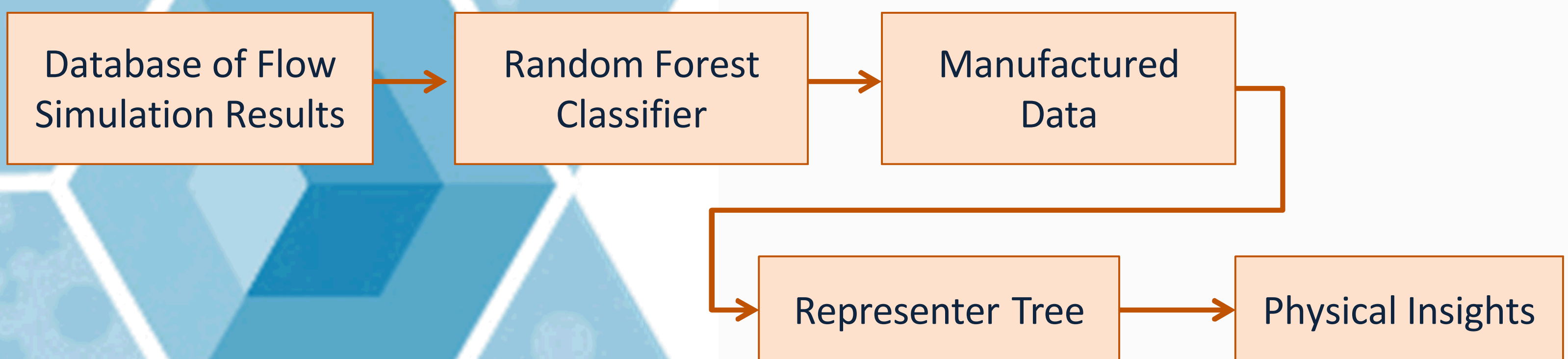
1) Machine learning for turbulence model form uncertainty quantification
   - Achieved 3X more accurate error detection than previous state of the art

2) Rule extraction to gain physical intuition

1) Deep learning with embedded invariances

Rule Extraction

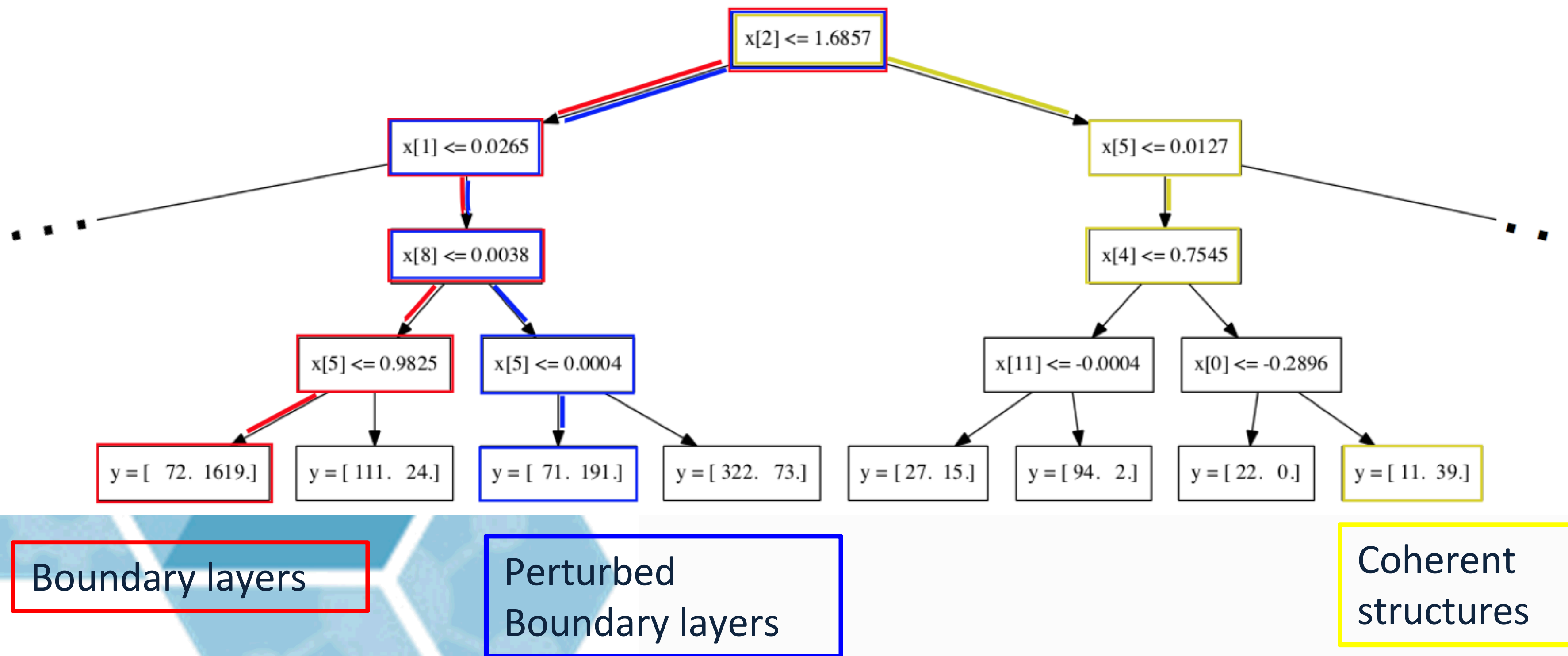
- Random Forests are much more robust and high-performance than single decision trees, but what have we lost?
  - Clarity—how can we understand these machine learned models?
- Representer Trees



- Trained a representer decision tree based on Random Forest that predicted when the RANS isotropy assumption was invalid

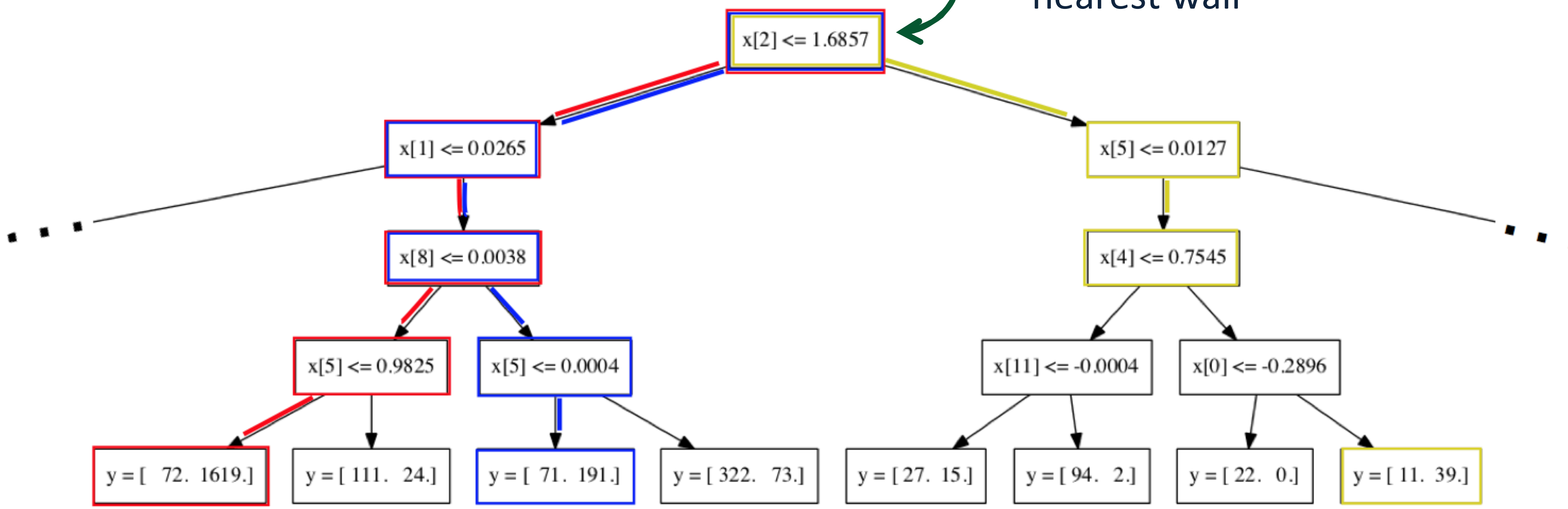
Analyzing the Representer Tree

- Look for consistent branches



Analyzing the Representer Tree

First split is on x[2], which is non-dimensional distance to the nearest wall

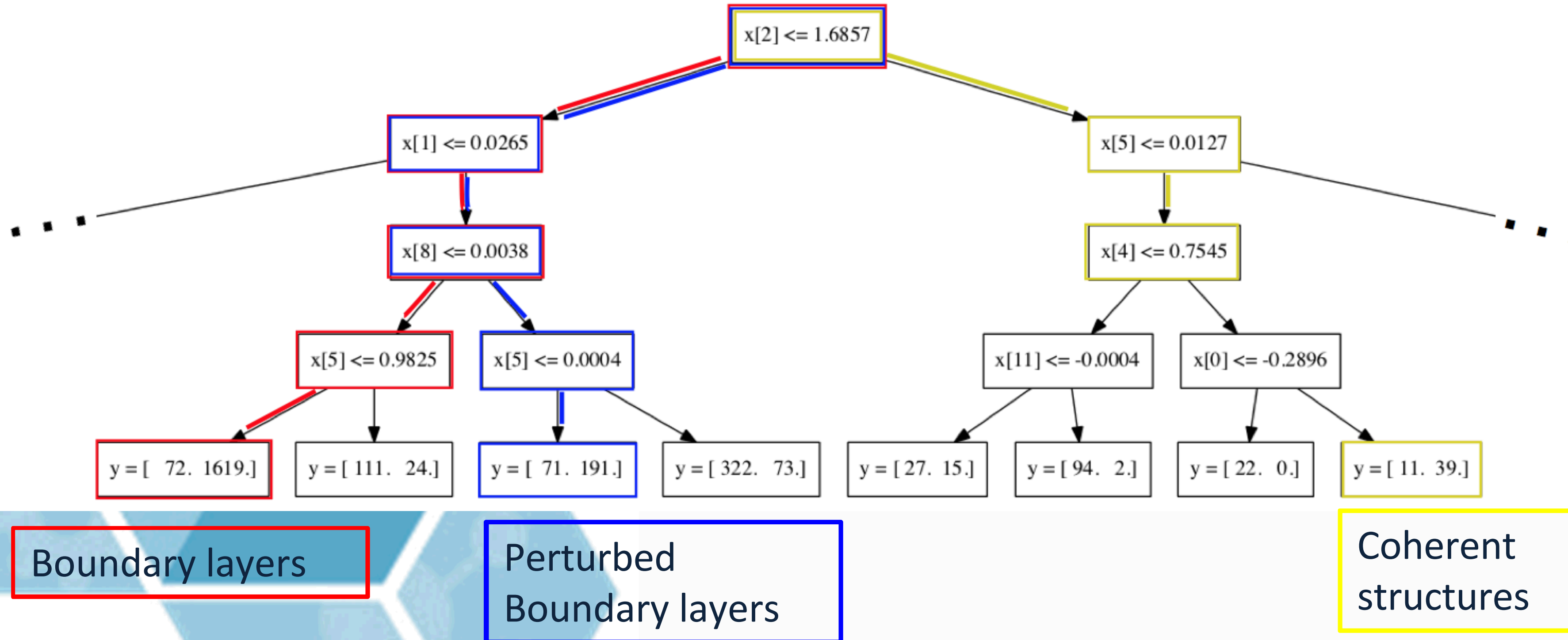


Boundary layers

Perturbed Boundary layers

Coherent structures

Analyzing the Representer Tree



- Can determine physical regimes where assumptions are violated
- Can see that different mechanisms cause assumption to break down in near wall region than in free stream

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2) Rule extraction to gain physical intuition
   - Used rule extraction to understand how the complex machine learning algorithm was making its predictions
   - Increases confidence in ML predictions
   - Provides feedback to turbulence modeler

3) Deep learning with embedded invariances

Deep Learning for Turbulence Modeling

- RANS simulations rely on empirical models to model the turbulence transport
- These models were proposed based on theory + sparse experimental data
- We want to use a deep neural network to model the turbulence transport

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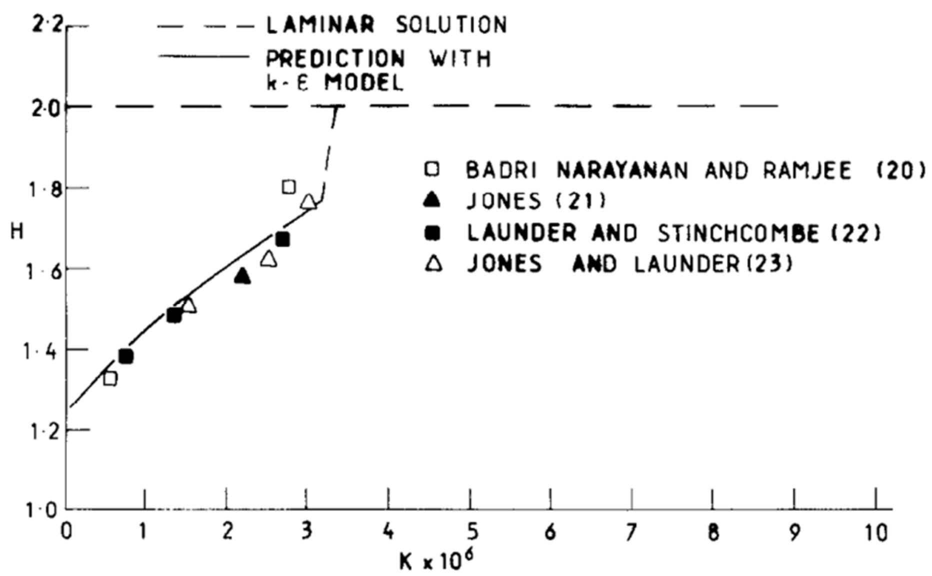


FIG. 2. Sink flow turbulent boundary layers.

Deep Learning for Turbulence Modeling

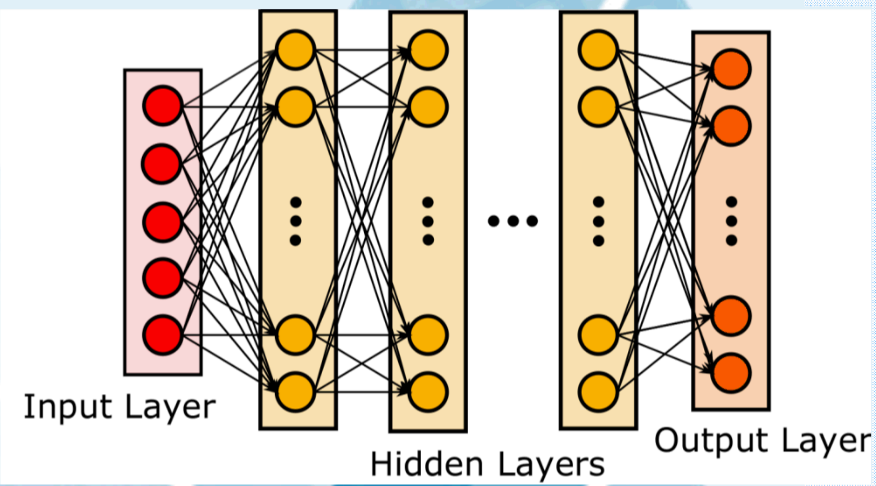
- Inputs: Tensors **x**, **y**
- Output: Tensor **b**

- Would like to enforce Galilean invariance
  - Invariance to inertial coordinate frame transformations
  - Borrow some ideas from group theory, representation theory
  - All Galilean invariant tensors that are a function of **x** and **y** lie on a tensor basis: the *integrity basis* of **x** and **y** for the orthogonal group

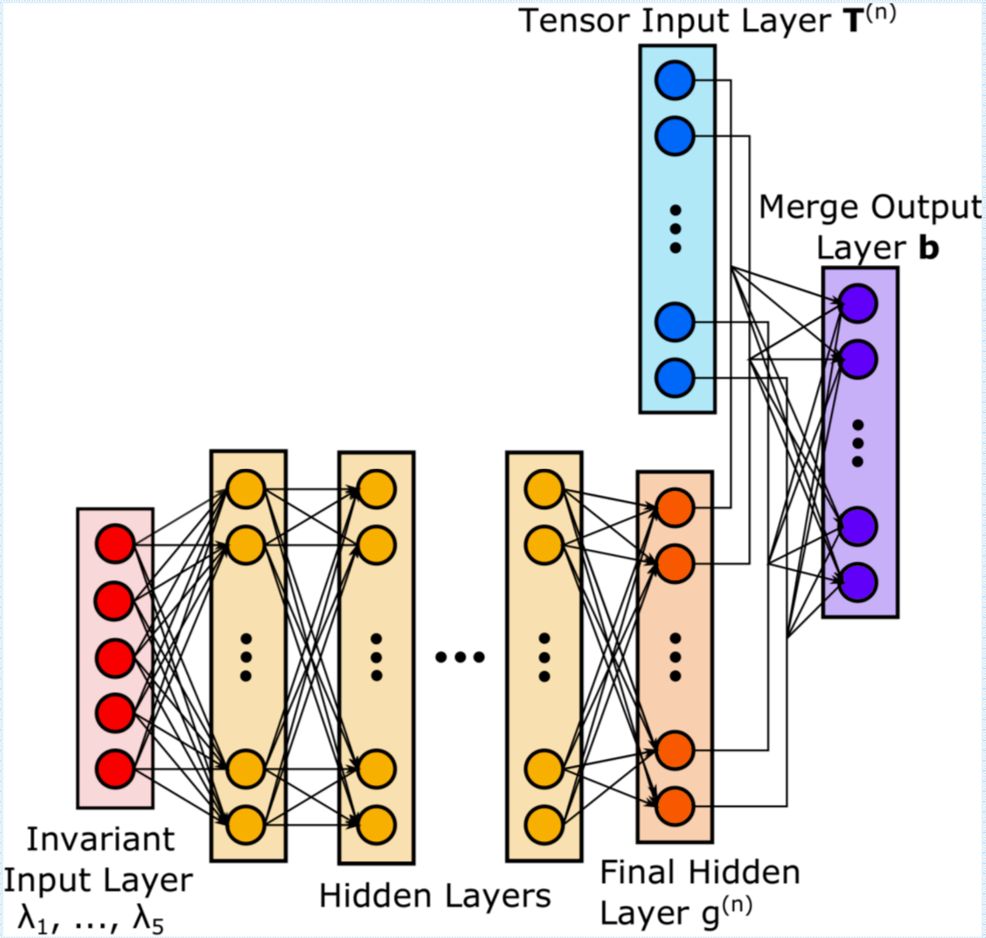
$$\boldsymbol{b} = \sum_{n=1}^{10} g^{(n)}(\lambda_1, ..., \lambda_5)\boldsymbol{T}^{(n)}$$

Embedding Galilean Invariance

Generic MLP

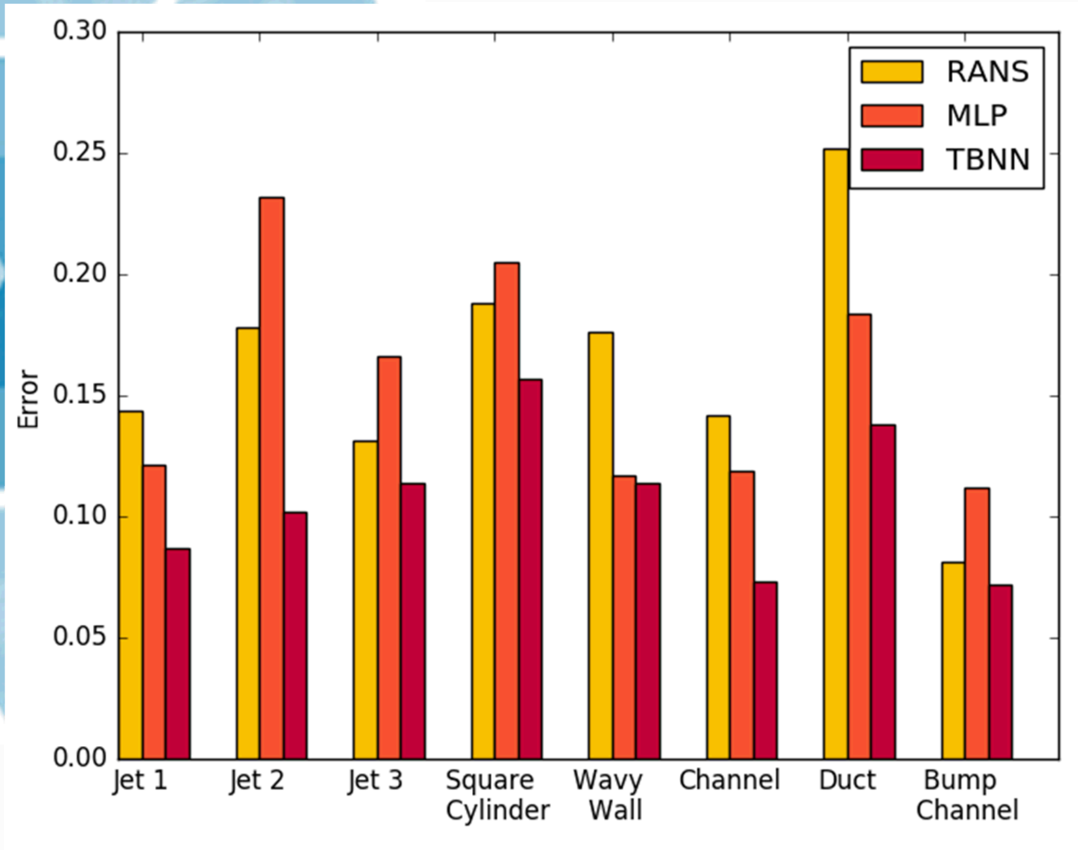


Tensor Basis Neural Network



Deep Learning for Turbulence Modeling

- Deep neural networks implemented using the Lasagne library: built on Theano
- Bayesian optimization used to tune the network hyper-parameters
- Trained an ensemble of networks to provide regularization



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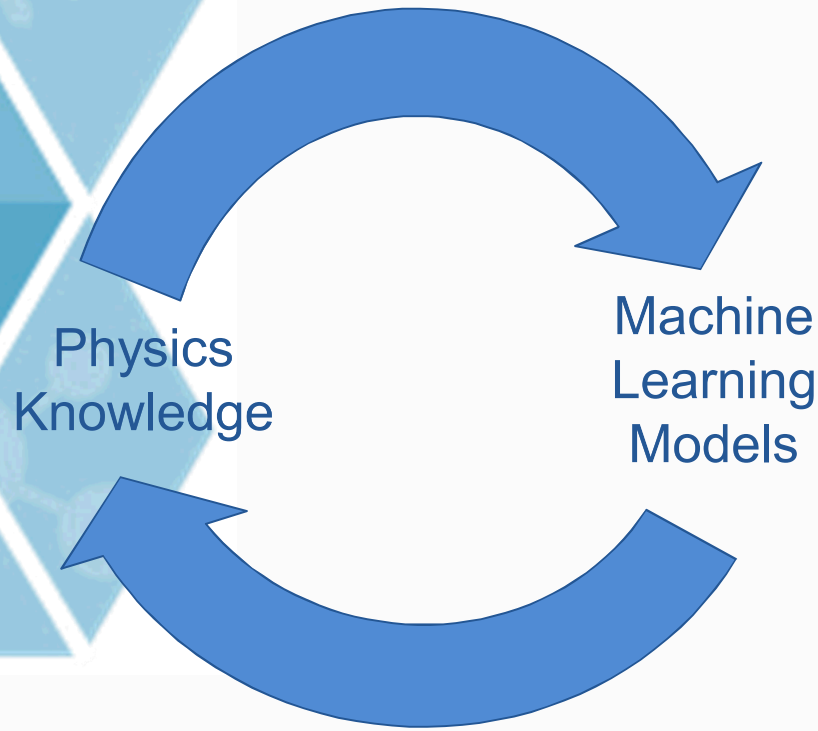
3) Deep learning with embedded invariances
   - Embedded known invariance property into network architecture
   - Achieved significantly improved Reynolds stress anisotropy predictions
   - First application of deep learning to turbulence modeling

Big Picture

- Directly embedding scientific domain knowledge into machine learning models can give improved performance
- Rule extraction on machine learning models can give improved physical understanding



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Questions