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Machine Learning for Uncertainty Quantification in Turbulent Flow Simulations

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NNSA National Nuclear Security Administration

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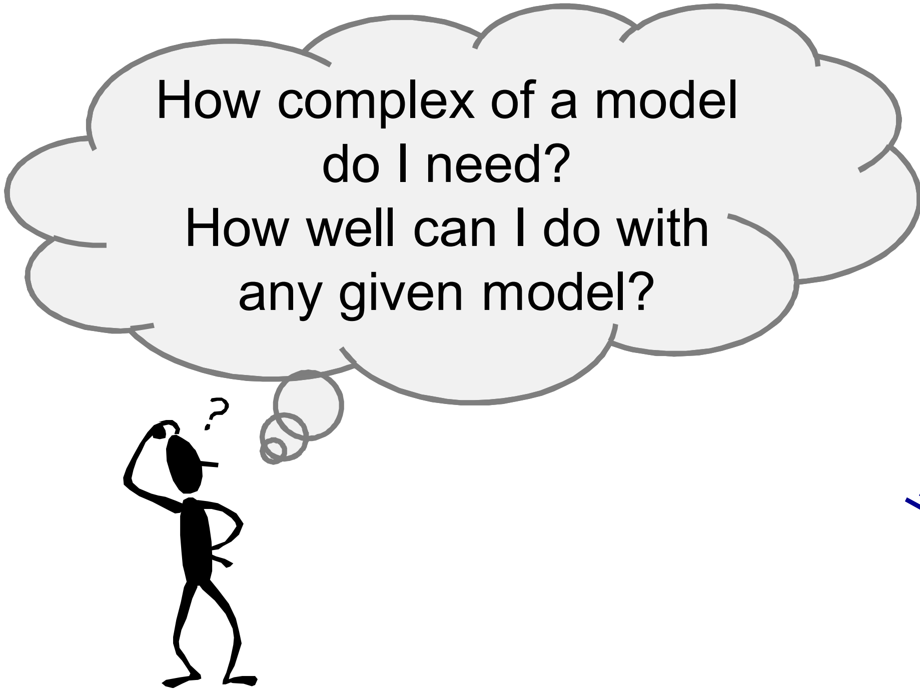
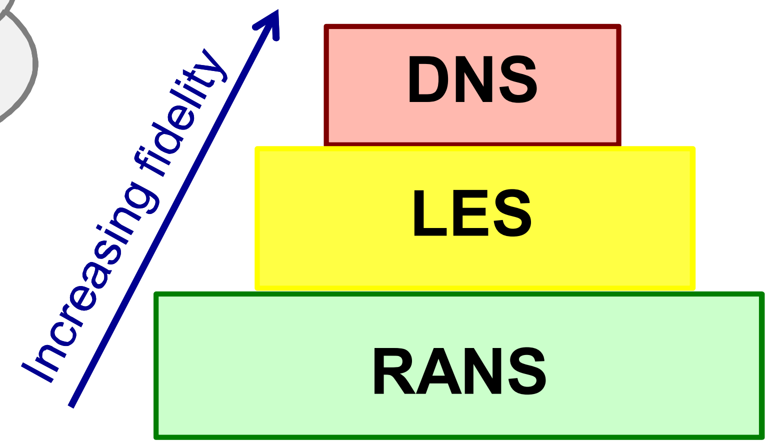
Turbulence Simulations



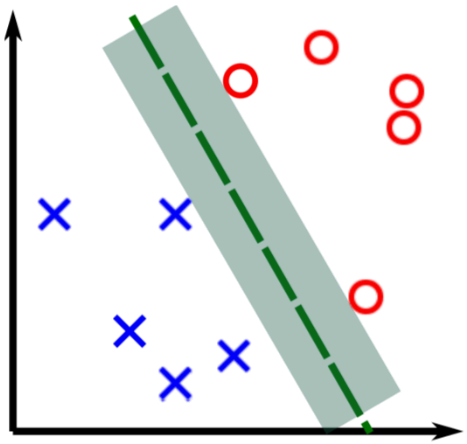


RANS

- Most widely used turbulence model
- Relies on modeling assumptions→ Model form uncertainty
- Sometimes accurate, sometimes inaccurate
  - Very difficult to assess model form uncertainty
- **Idea: Use machine learning to detect regions of high uncertainty based on when specific model assumptions are violated**

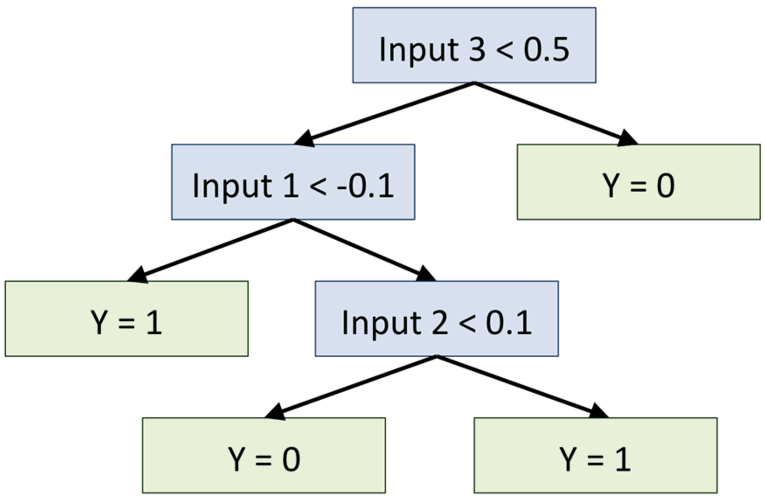
Machine Learning

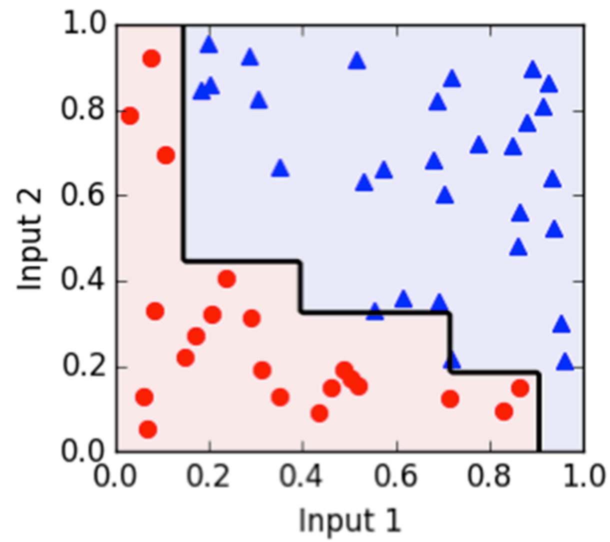
- Set of data-driven algorithms for regression, classification, clustering
- *E.g.*: linear regression, support vector machines, neural networks
- Have been broadly applied in finance, software engineering, retail
- Challenge: how to incorporate domain knowledge into machine learning algorithms
  - These techniques have a range of physics applications
- **For this application: use binary classifier to flag regions of high RANS uncertainty on a point-by-point basis**



Random Forests

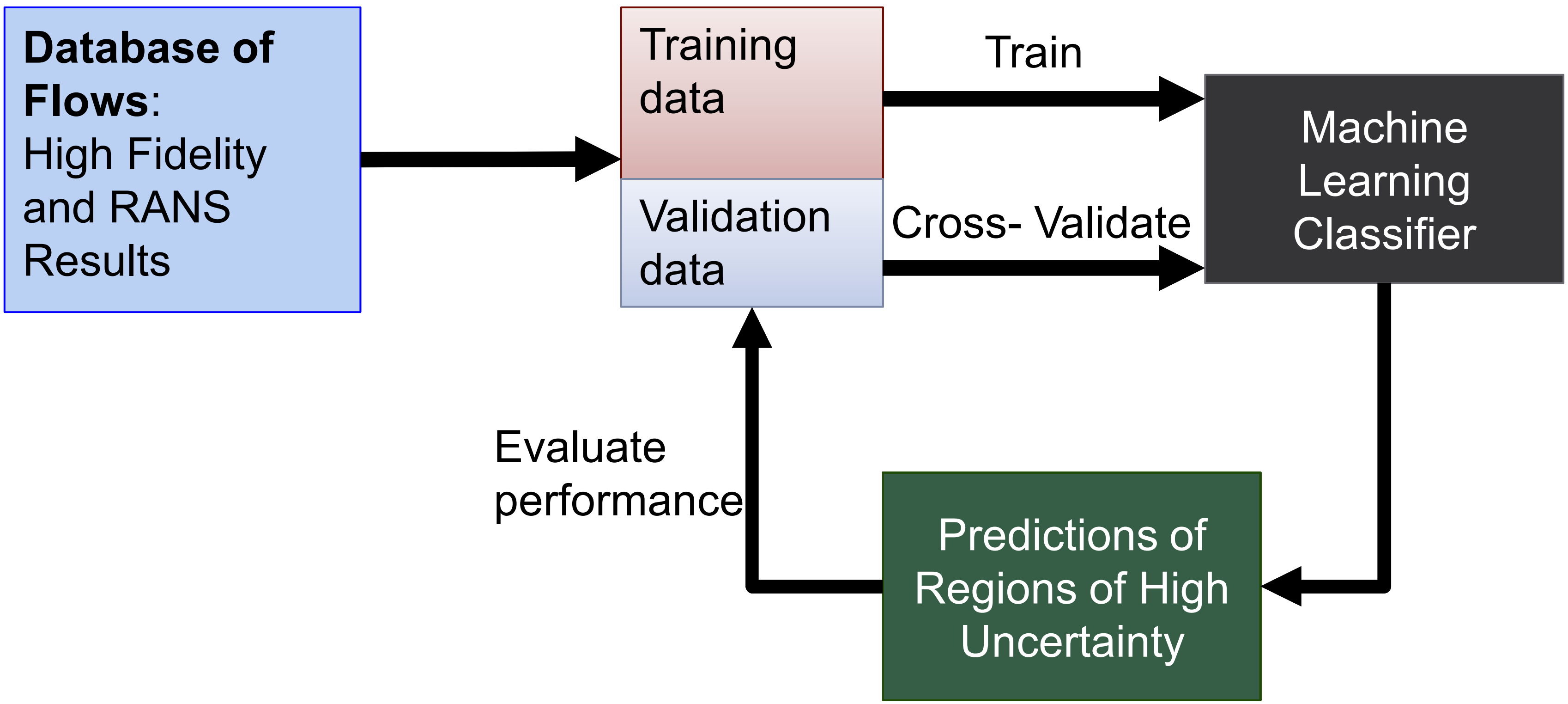
- Binary Decision Trees:
  - Simple, easy to understand and use
  - Tendency to overfit, poor performance with non-linear behavior





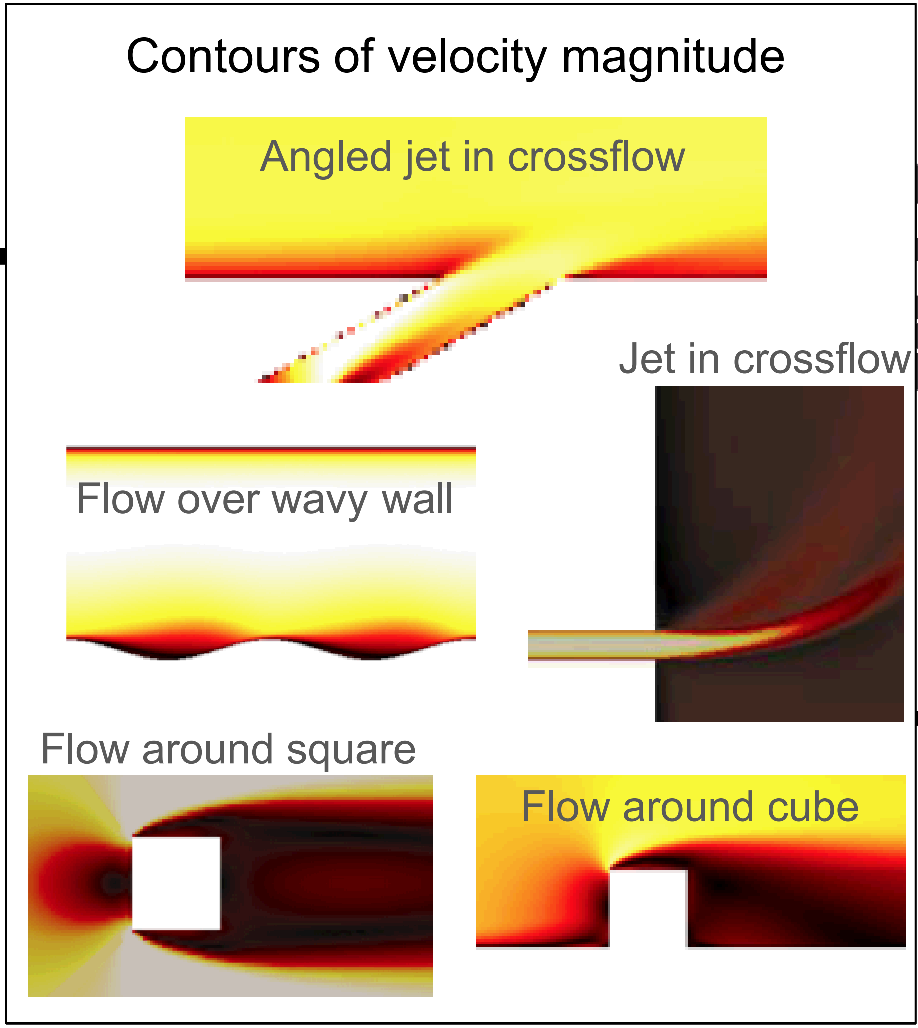
- Ensembles of Decision Trees:
  - Much more robust
  - Random Forests are a type of ensemble of decision trees

Classifier Development



Classifier Development

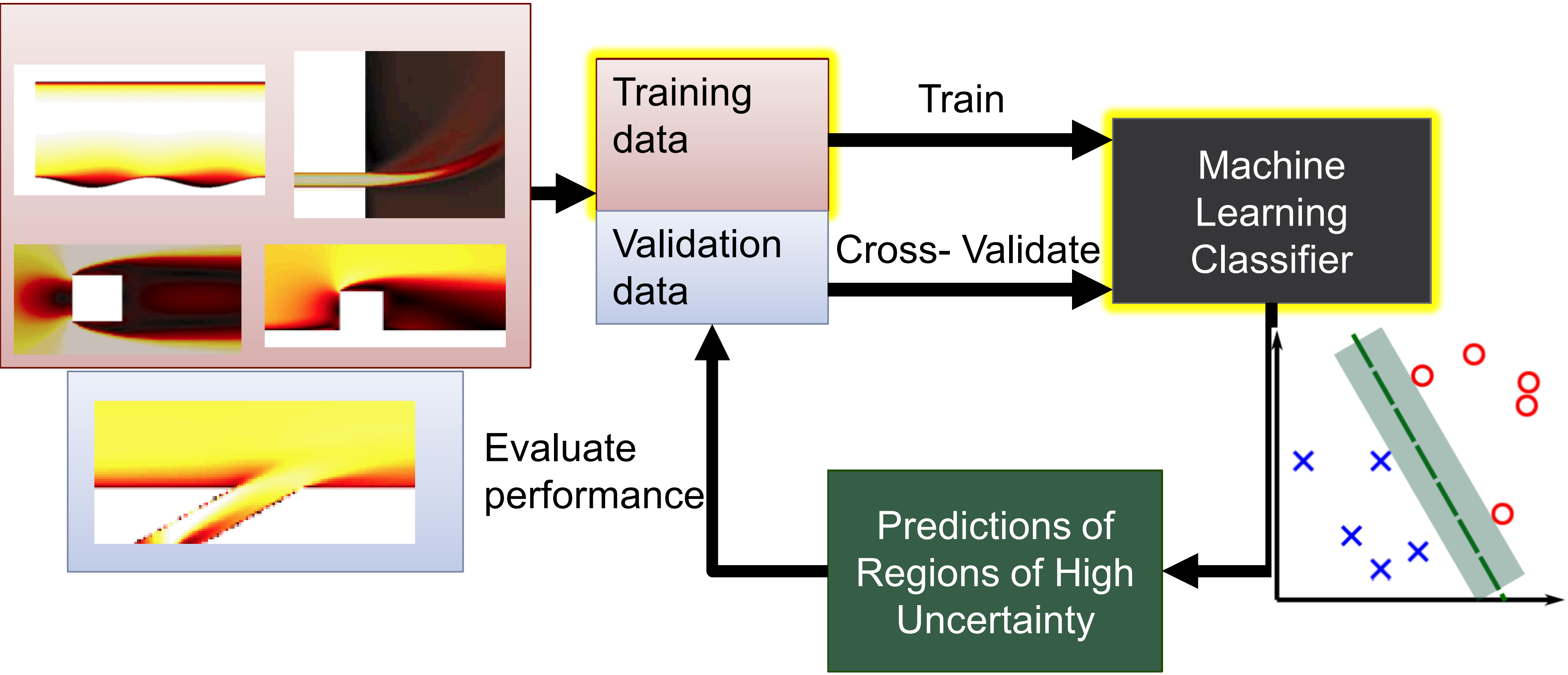
Database of Flows:
High Fidelity and RANS Results



Machine Learning Classifier

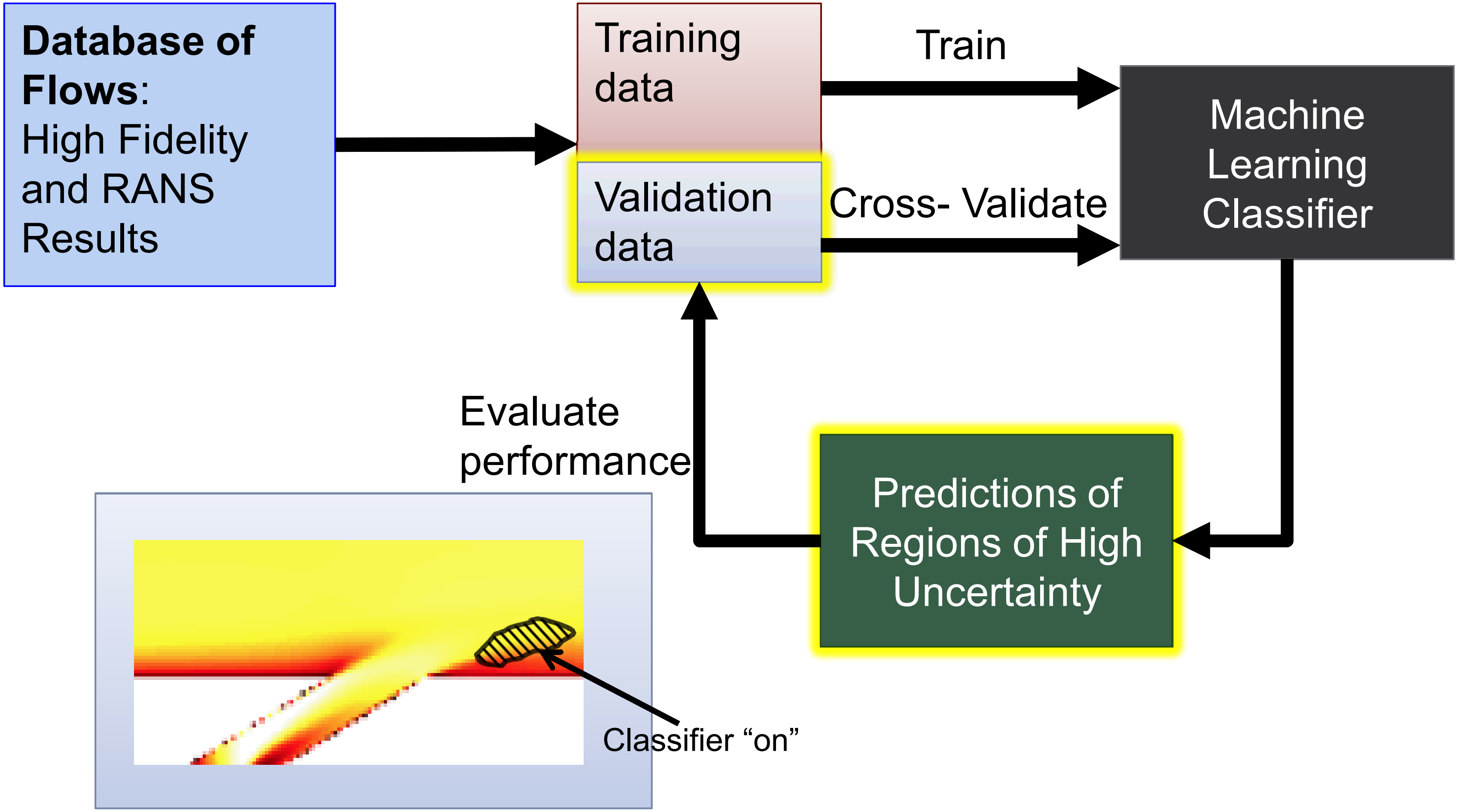
- Have database of canonical “building block” flows

Classifier Development



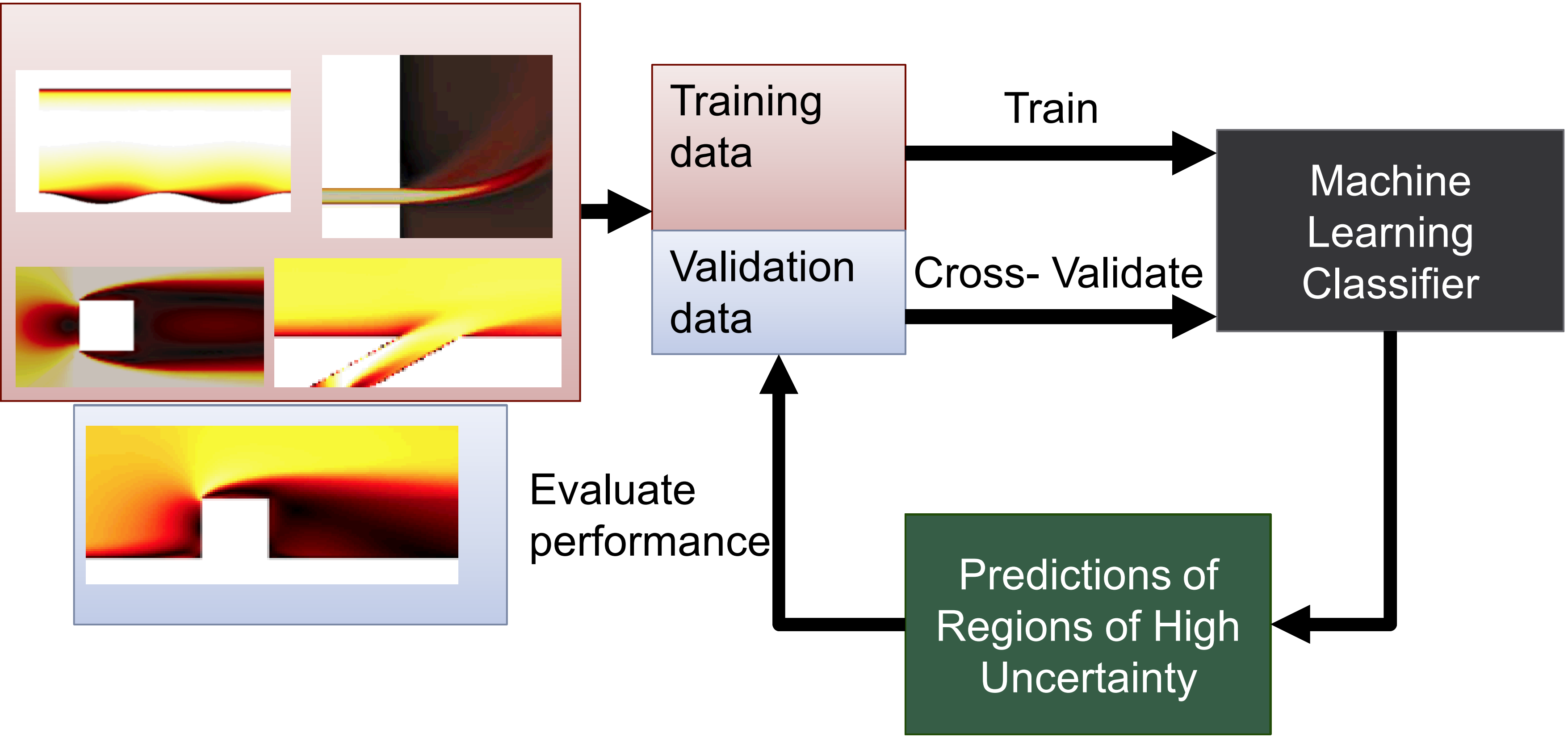
- Split data base into training and validation sets
- Train classifier
  - Input: Local flow variables from RANS
  - Output: Binary flag– “on” if RANS assumption violated, “off” otherwise

Classifier Development



- Use classifier to make predictions on validation set
- Evaluate classifier by comparing to high fidelity results

Classifier Development



- Cross-validate to ensure generalization

Assumptions Tested

$$\overline{u_i'u_j'} = \frac{2}{3}k\delta_{ij} - 2\nu_t S_{ij}$$

1. Non-negativity of eddy viscosity
   - Can extract eddy viscosity from LES/DNS
     $$\nu_t = \frac{-\overline{u_i'u_j'}S_{ij} + \frac{2}{3}k\delta_{ij}S_{ij}}{2S_{kl}S_{kl}}$$
   - Classifier should be "on" when LES/DNS eddy viscosity goes negative
2. Isotropy of Reynolds stresses
   - Classifier should be "on" when second invariant of anisotropy tensor exceeds a set threshold
3. Linearity of Boussinesq hypothesis
   - Extract linear and cubic eddy viscosity from LES/DNS data
   - If these values differ significantly, then uncertainty associated with linearity assumption is high

Inputs:

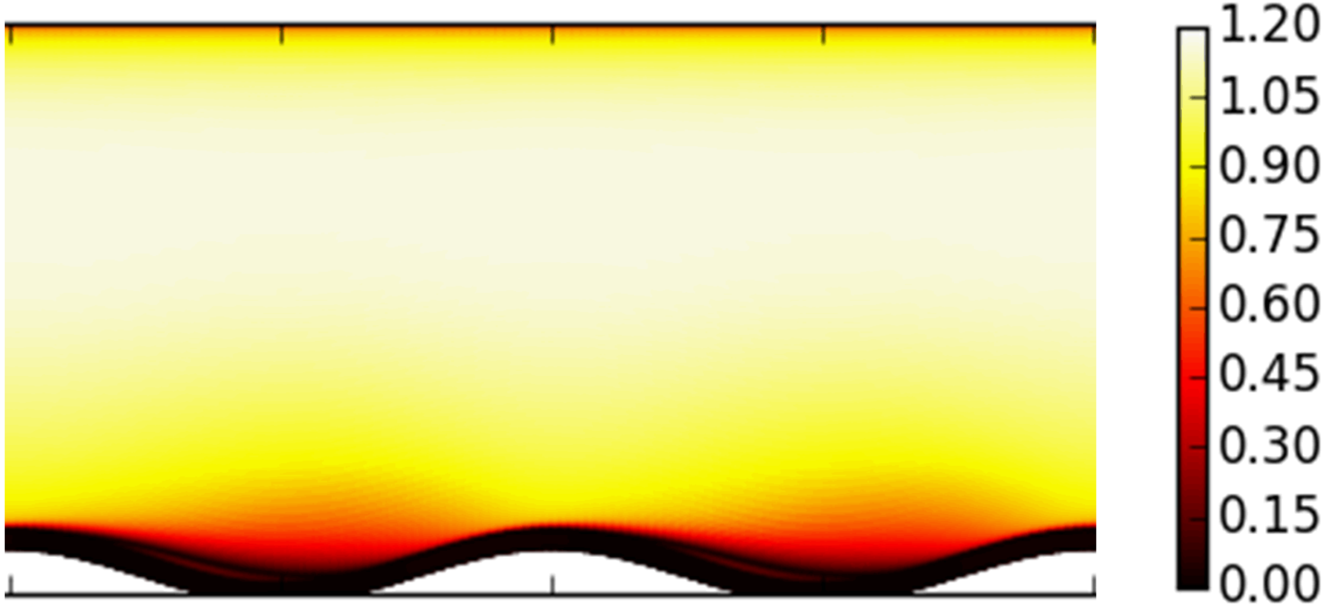
- Non-dimensional, rotationally invariant local flow variables from RANS

Applications of Classifiers

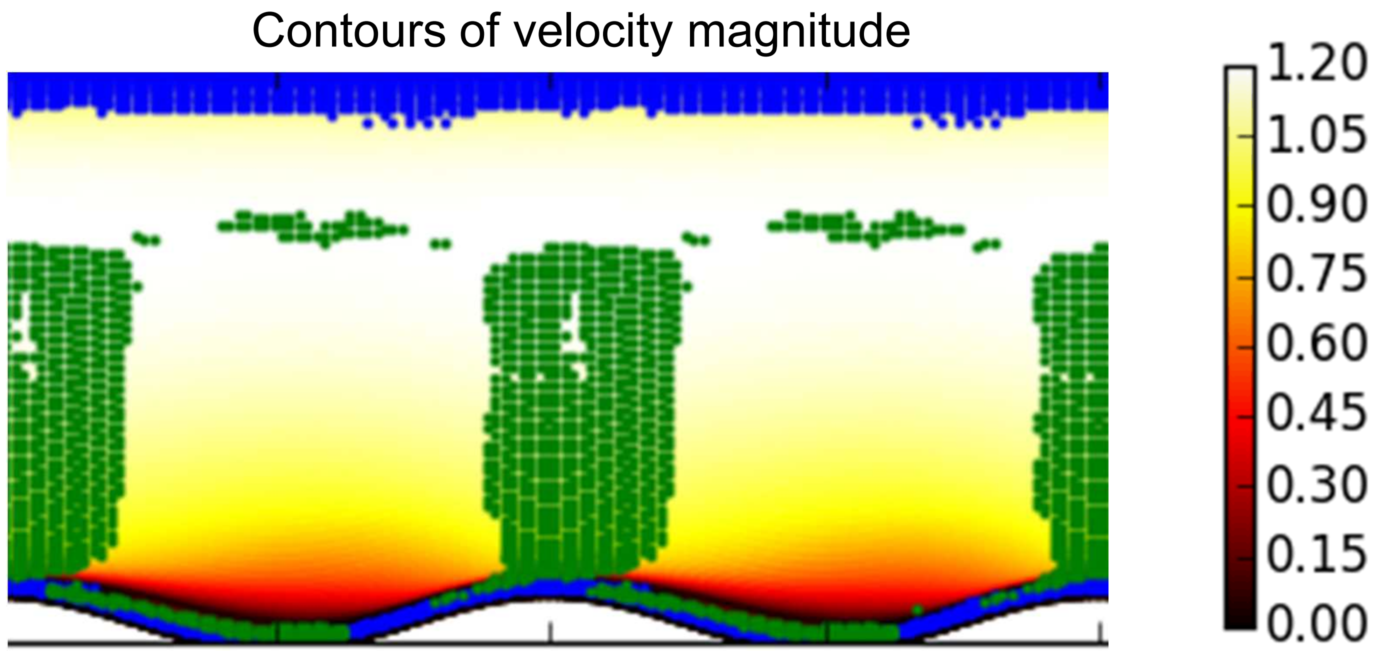
- Can quickly post-process RANS simulation to determine whether it's reliable in region of interest
  - Don't have to wait around for validation data set
  - Can determine what corrections to implement
- Can enable adaptive corrections during run time
- Experimental design
  - Design experiments to provide the strongest validation
- LES-RANS hybrids
  - Use classifiers to inform switching function

The Status Quo

Contours of velocity magnitude

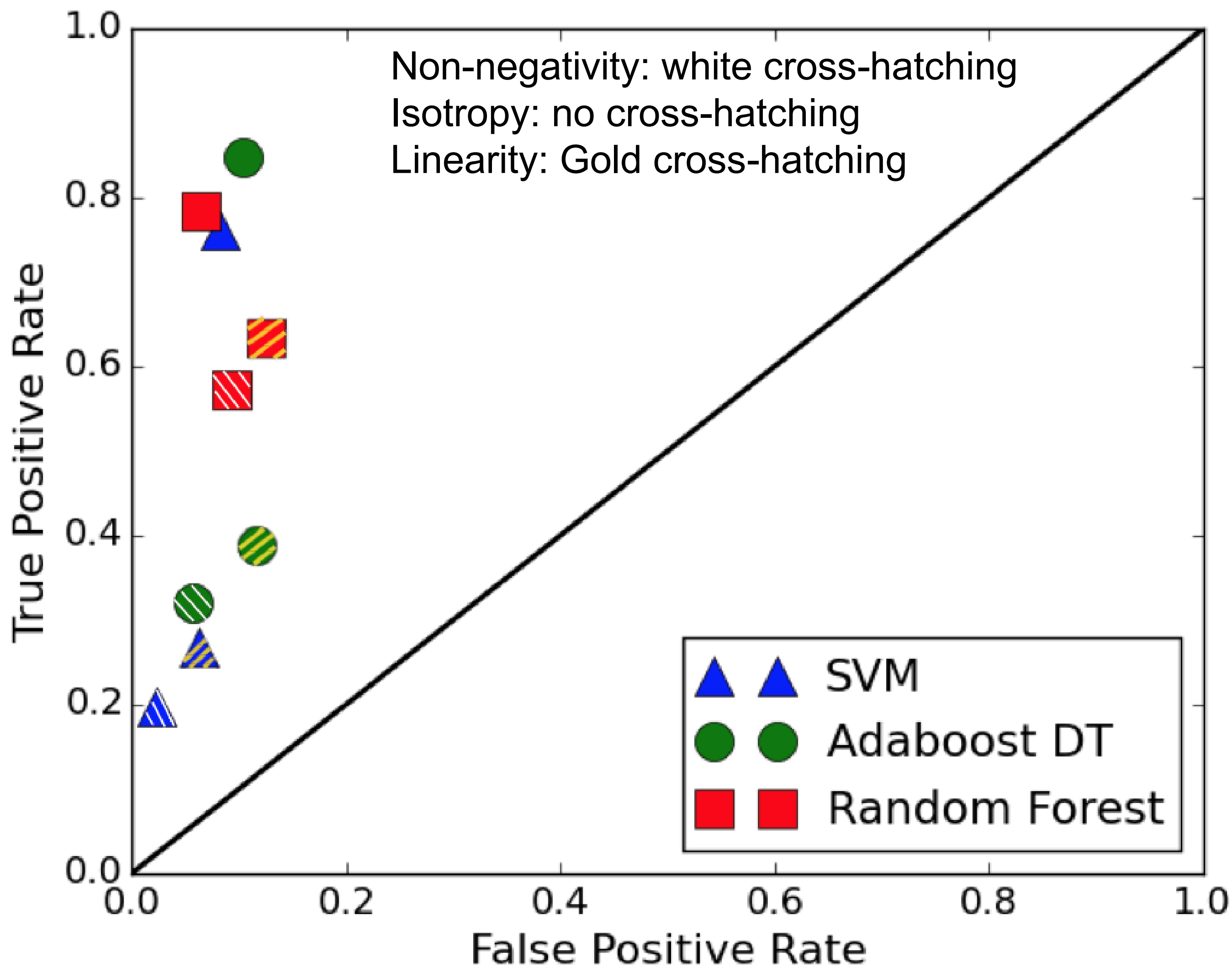


A Better Option

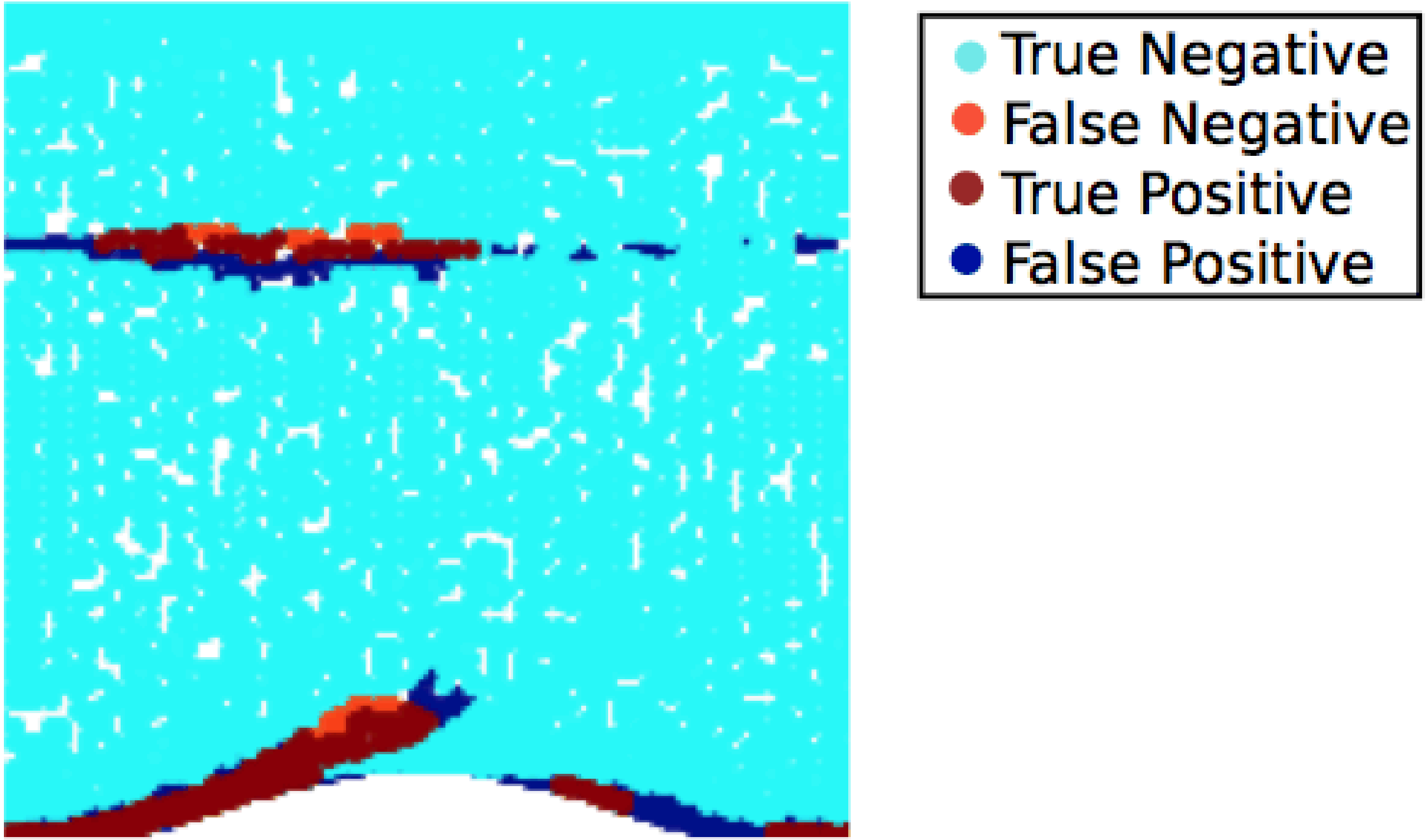


Blue: Regions where classifier predicts isotropy assumption violated
Green: Regions where classifier predicts linearity assumption violated

Classifier Performance



Classifier Performance



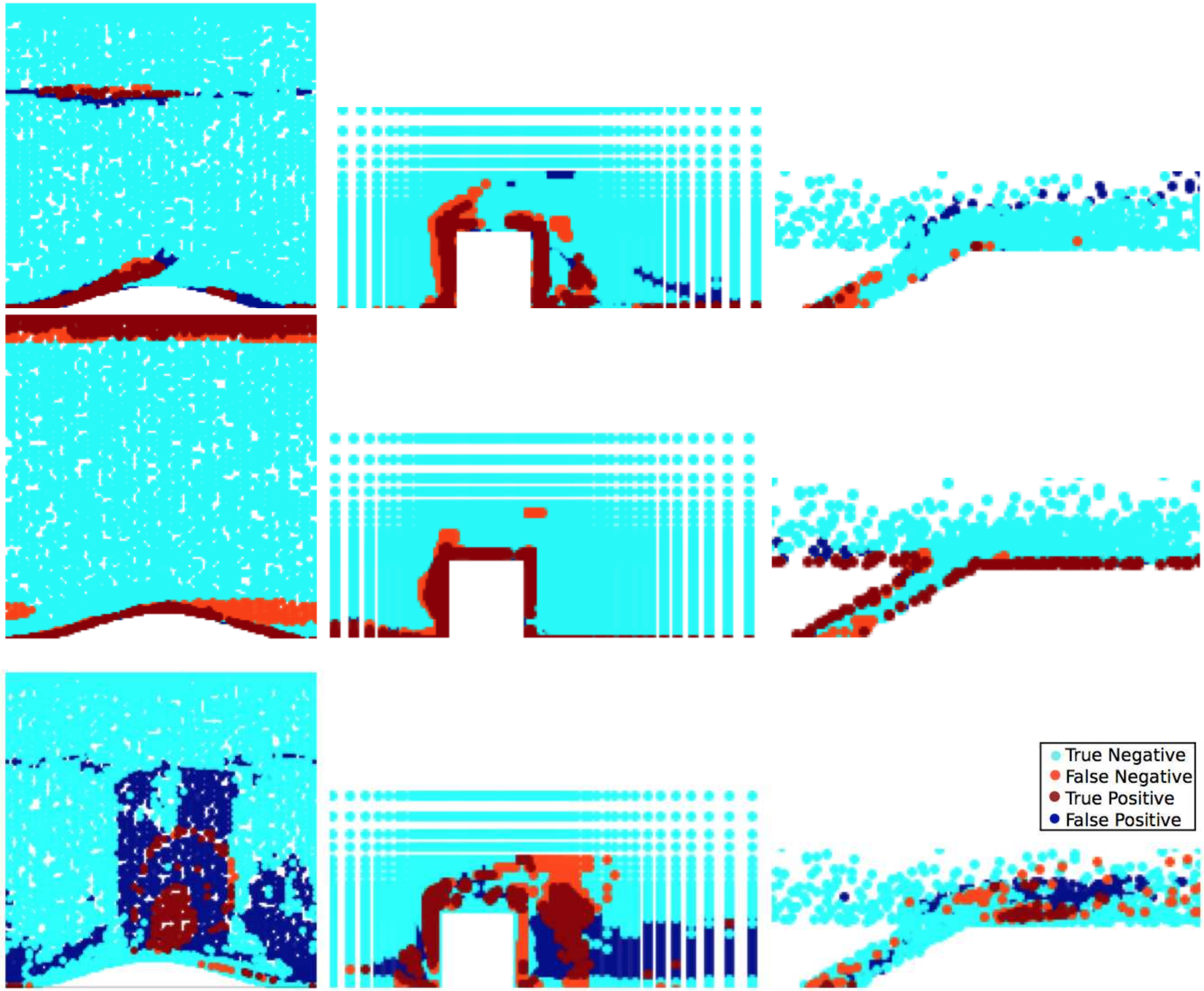
(a) Case 1, Marker 1:
Negative ν_t

Classifier Performance

Non-negativity assumption

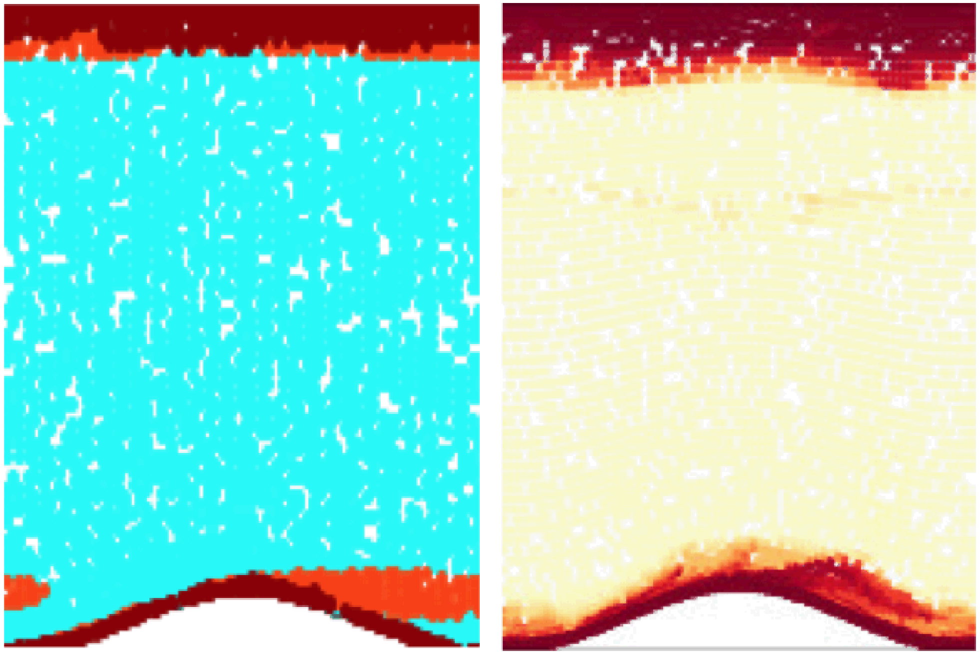
Isotropy assumption

Linearity assumption

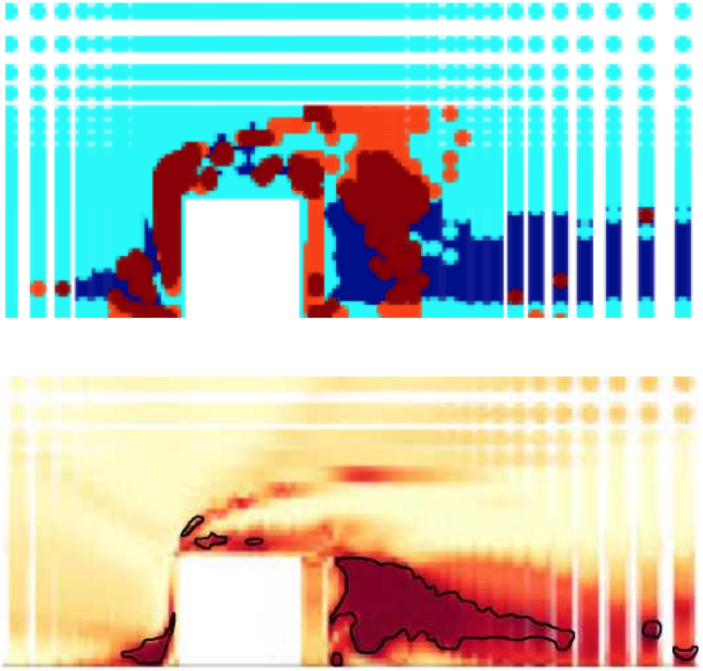


Classifier Confidence

Uncertain classifications

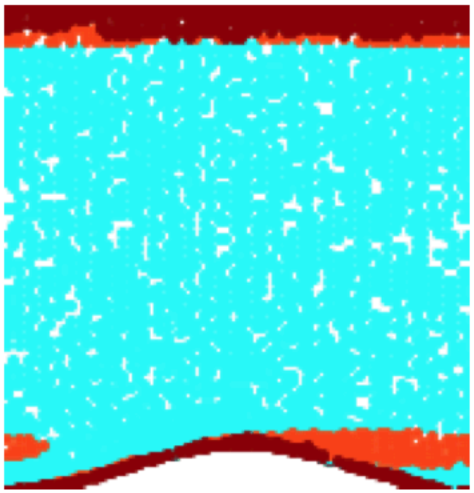


Extrapolation Detection



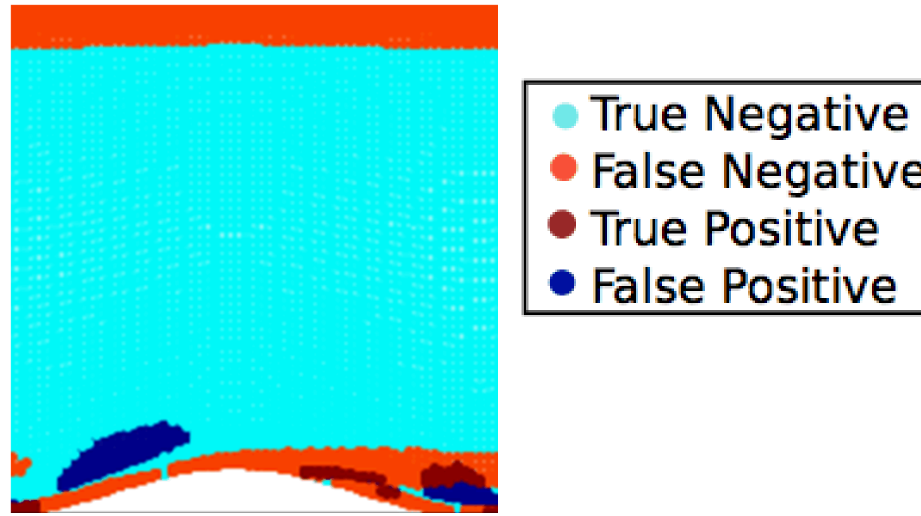
Comparison against State of the Art

Machine Learned Classifier



Cross-validation
Error rate: 11%

Physics-based Classifier of Gorle et al.



Cross-validation
Error rate: 33%

- Cross-validated classifier error rate: 11%
- 3 X more accurate than current state of the art physics-driven classifier of Gorle et al.
  - Gorle et al.'s classifier is used as an input to the ML classifier

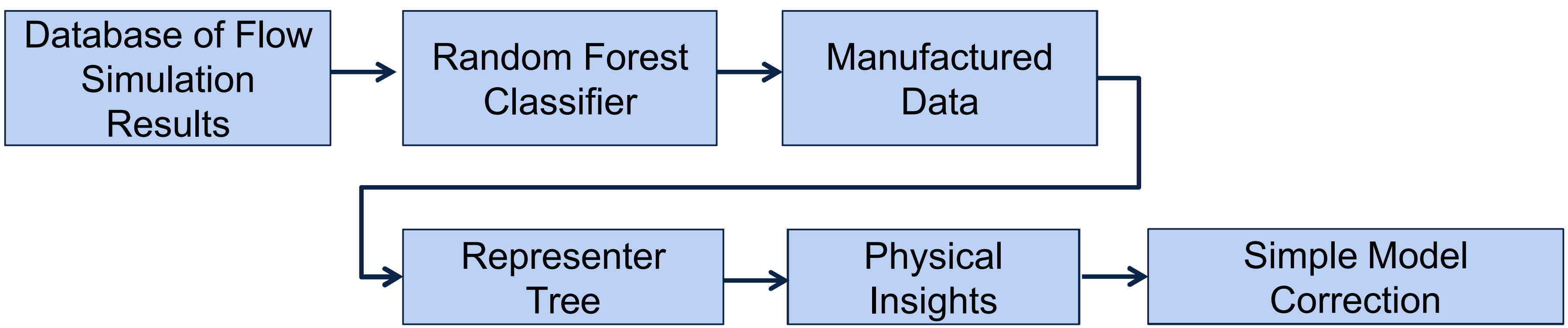
Impacts

- Classifiers for RANS model uncertainty can transform the way RANS results are post-processed and understood
  - Clarify when RANS simulations are predictive
  - Enable adaptive modeling corrections

- Develop techniques for using machine learning algorithms on physical systems
  - Leverage domain knowledge and physical constraints to develop smarter models
  - Use data-driven models to learn about the physical system

Rule Extraction

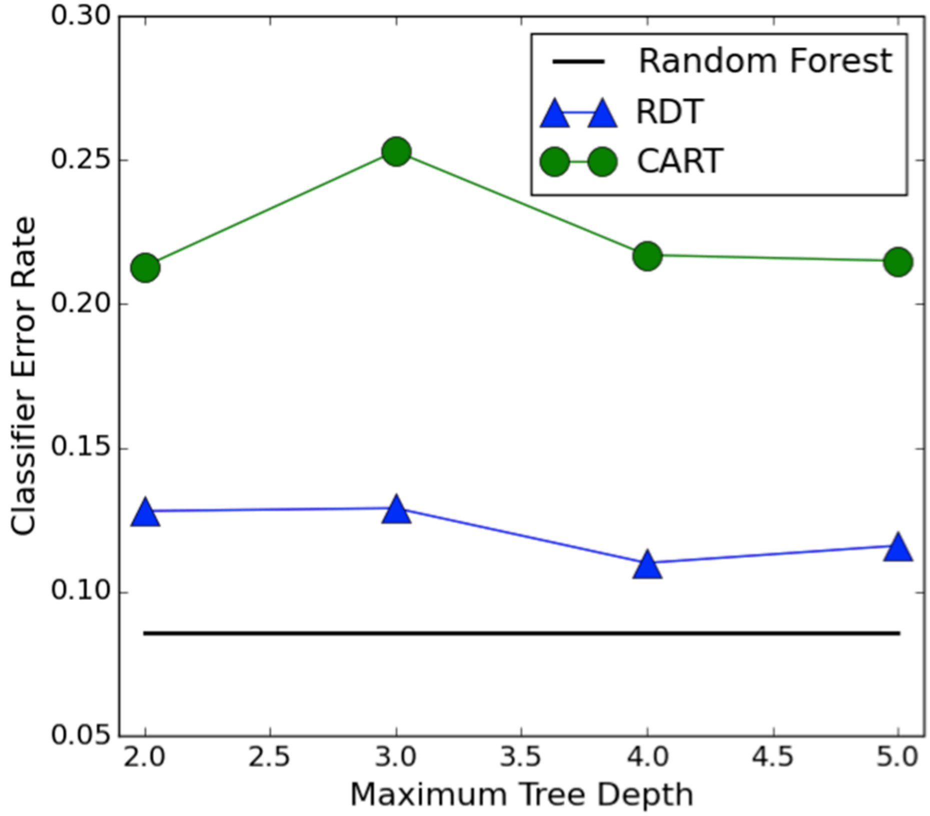
- Random Forests are much more robust and high-performance than single decision trees, but what have we lost?
  - Clarity—how can we understand these machine learned models?
- Representer Trees



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

Representer Decision Trees

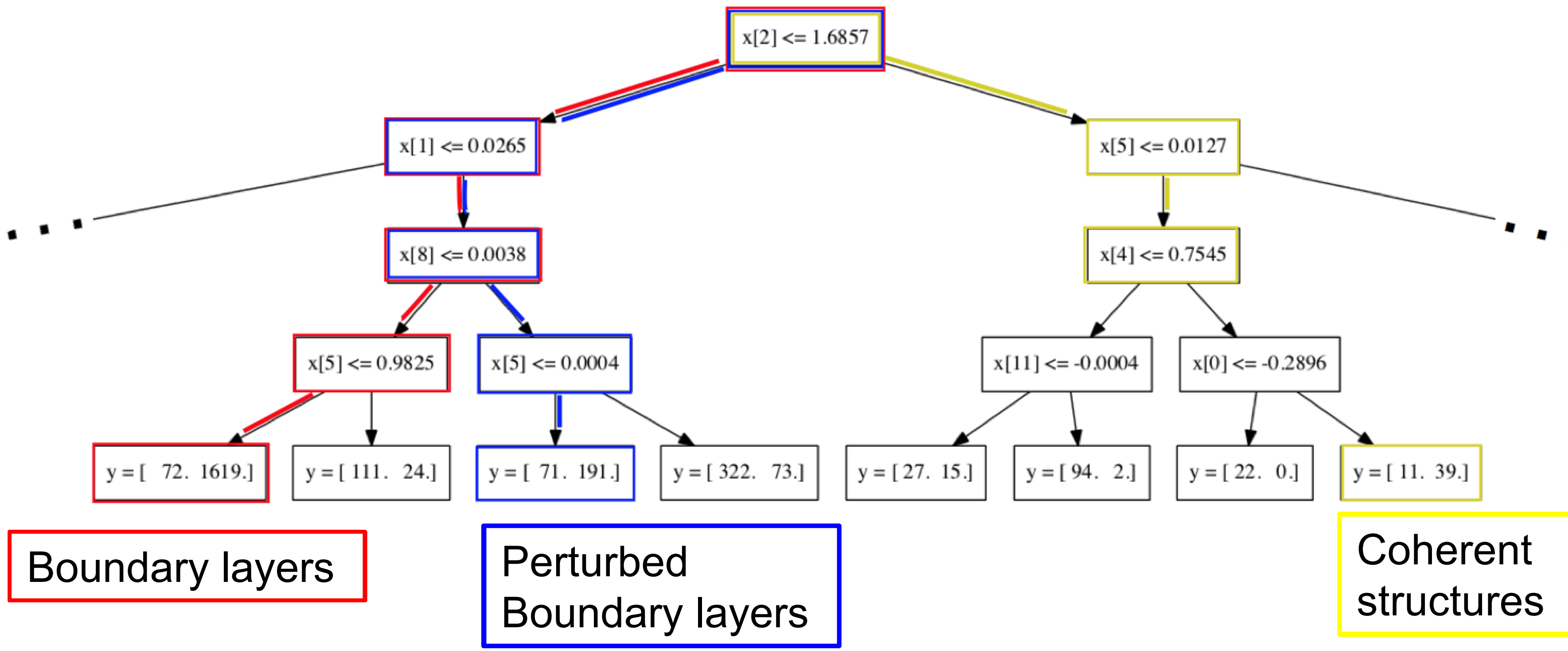
- Surprising result: the representer tree has better performance and is more stable than a tree trained on the original tra



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

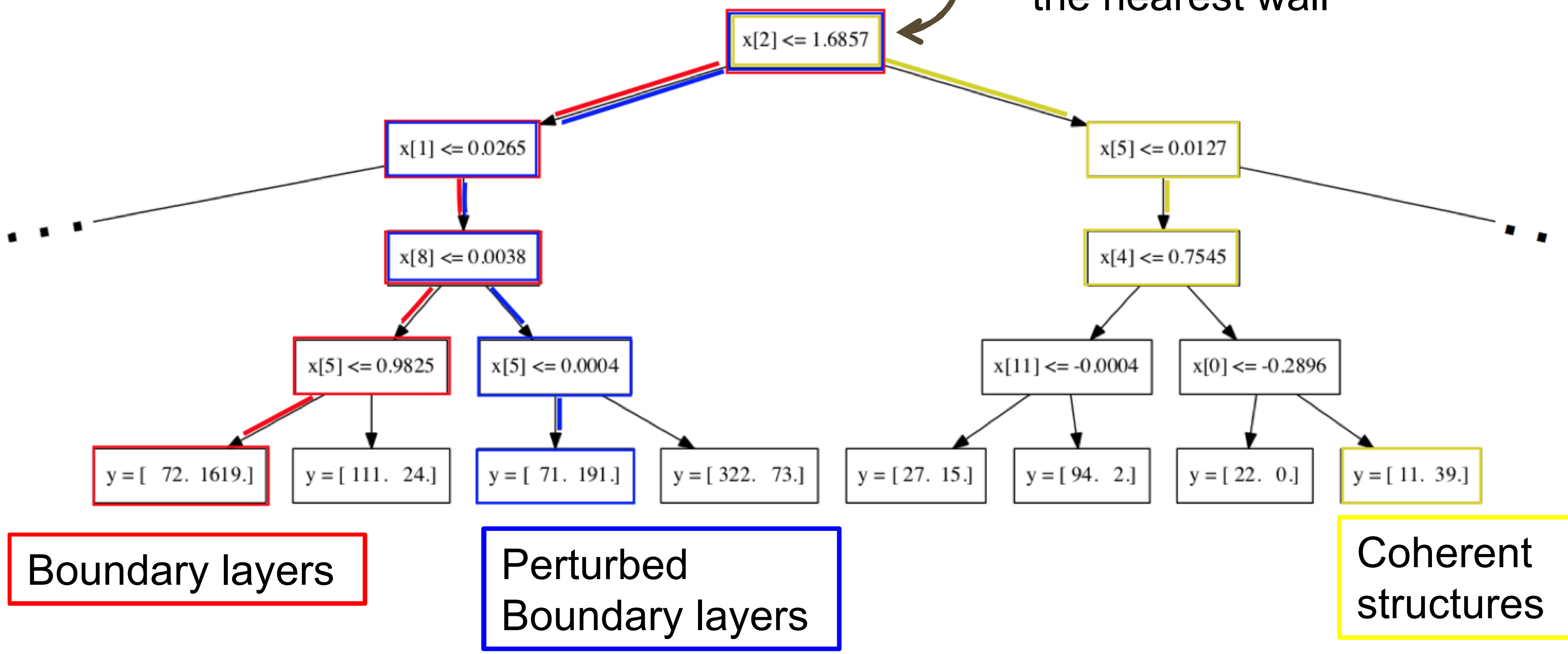
Analyzing the Representer Tree

- Look for consistent branches

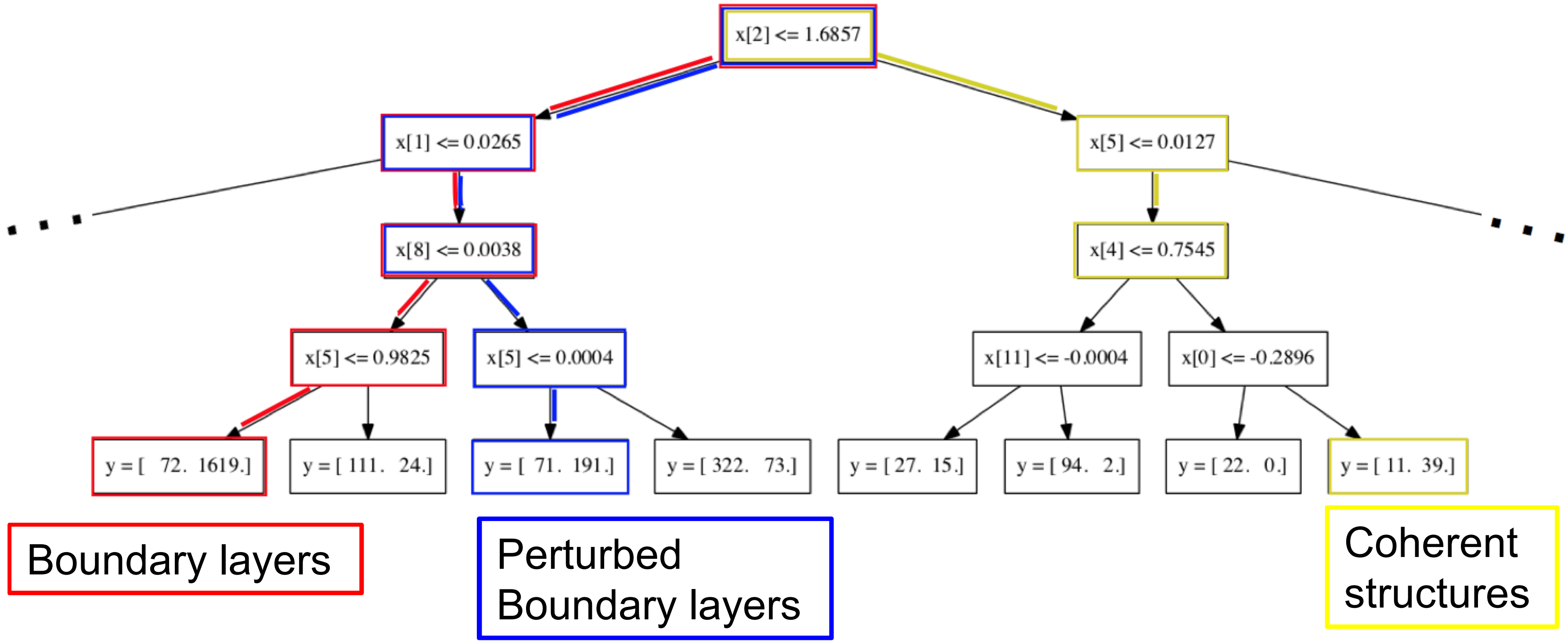


Analyzing the Representer Tree

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



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

Conclusions

- Machine learning was used to detect when RANS assumptions break down
- These data-driven methods achieved significantly improved classification accuracy by leveraging the high-dimensional data
- Rule extraction techniques were then used to regain physical intuition from the machine learning classifiers

Acknowledgments

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C. Gorle, J. Larsson, M. Emory, G. Iaccarino, “The deviation from parallel shear flow as an indicator of linear eddy viscosity model inaccuracy,” Physics of Fluids, (2014).