Developing Data-Augmented Turbulence Models using Field Inversion and Machine Learning

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Motivation

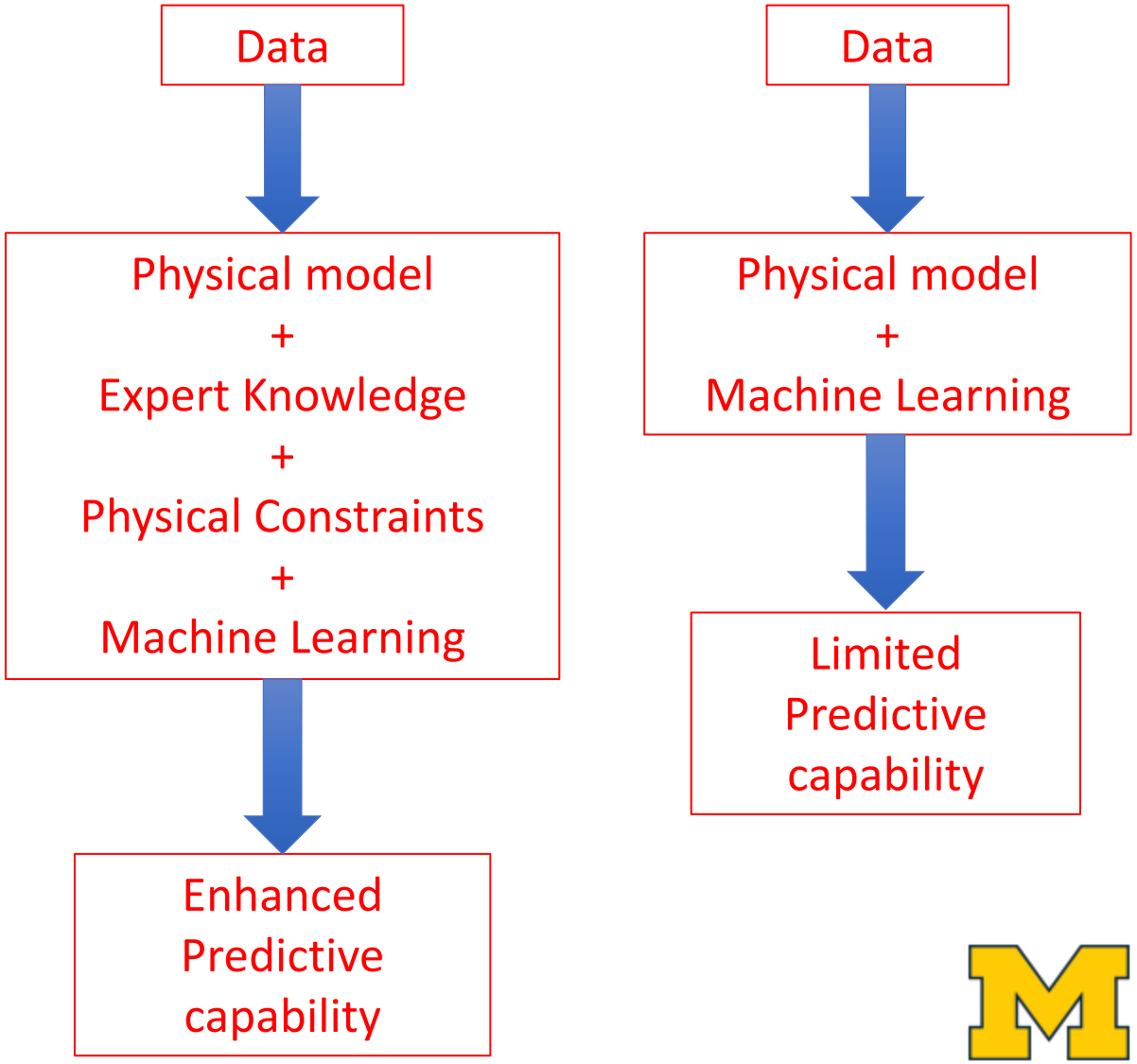
- ***RANS is fast and inexpensive*** – Ideal choice for design and optimization

- Turbulence models for RANS are ***insufficiently accurate***
  - Due to inadequacy in the model-form
  - Due to calibration over only a handful of flows

- Despite their shortcomings, ***RANS models do capture some basic physics very accurately***
  - Data-driven augmentation is a way forward to improve accuracy

Goals

- Leverage Machine Learning to augment turbulence models
- Conserve physical laws and known properties
- Improve predictive capabilities – towards generalizable models – Augmentation to be expressed in terms of lowest possible number of flow quantities (“*features*”)
- Develop interpretable augmentations



Challenges

- Modeled quantities can have a drastically different behavior from corresponding physical quantities
  - **Inferring usable information about the behavior of *modeled* terms from *physical* data** is of key importance
- **Predictive capability** depends on the ability to express the augmentation correctly in terms of specific features
- **Predictive accuracy** requires mindful application of an augmentation and knowledge of its limitations
  - Correcting the intended discrepancy without deteriorating performance in other regions/flows where the augmentation is applied is crucial

Truth:

$$\frac{\partial u}{\partial t} + \mathcal{R}(u) = 0$$

Coarse-graining: $\bar{u} = \mathbb{P}(u)$

$$\frac{\partial \bar{u}}{\partial t} + \mathcal{R}(\bar{u}) = \mathcal{R}(\bar{u}) - \overline{\mathcal{R}(u)}$$

Model discrepancy and augmentation:

$$\frac{\partial \bar{u}}{\partial t} + \mathcal{R}(\bar{u}) = \epsilon(u) + \left(M_1(\bar{u}) + M_2(\bar{u})\right) \approx M_1(\bar{u}) + \beta(\bar{u}) M_2(\bar{u})$$

Is it possible to formulate such a $\beta(\bar{u})$? If yes, how?

Outline

- Augmentation
  - Philosophy
  - Implementation

- Field Inversion

- Field Inversion and Machine Learning
  - Traditional FIML

- Towards Generalizable FIML model augmentations
  - A brief introduction to Spalart-Allmaras turbulence model
  - Physics-Constrained and Physics-Informed Augmentation options
  - Results for Channel Flow

- Prediction Improvements from FIML (Flow over airfoils)

- Newer variants of FIML
  - Tightly-Coupled FIML
  - Loosely-Coupled FIML

Augmentation – Philosophy

Where to augment?

- What is the intended correction?
- How will the augmentation affect cases where correction is not required?

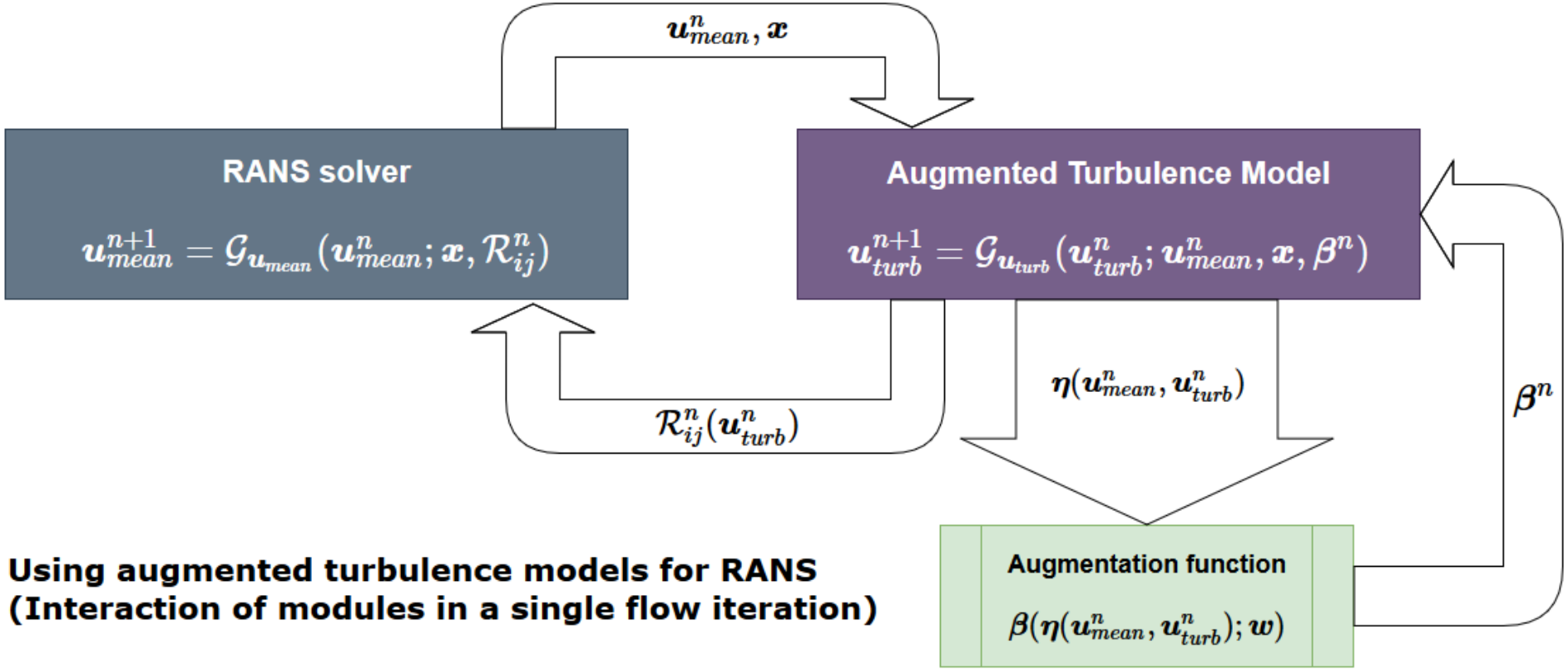
What are the relevant features?

- Based on Expert Knowledge
- Should not be specific to a problem
- Does the available data span the feature space sufficiently?

What is the functional form?

- Non-linear with unknown structure:
  - Neural Networks
  - Gaussian Processes
  - Decision Trees, etc.
- Custom-built based on some knowledge of the structure
- Hybrid – Non-linear with constraints

Augmentation – Implementation



Using augmented turbulence models for RANS (Interaction of modules in a single flow iteration)

How can the parameters $\boldsymbol{w}$ be determined?

MACHINE LEARNING!!

Augmentation – Implementation

What ***not*** to do (in many problems)

Supervised Learning

$$\boldsymbol{w} = \arg\min_{\boldsymbol{w}_m} \|\boldsymbol{\beta}(\boldsymbol{\eta}(\boldsymbol{u}_{\text{data}}); \boldsymbol{w}_m) - \boldsymbol{\beta}_{\text{data}}\|_2^2$$

Model Augmentation

$$\mathcal{R}(\boldsymbol{u}, \boldsymbol{\beta}(\boldsymbol{\eta}(\boldsymbol{u}); \boldsymbol{w})) = 0$$

- Inconsistent because learning does not go through the model
  - Learning and injection environment can be very different
  - Only works when $\boldsymbol{u} = \boldsymbol{u}_{data}$
- Requires full fields of $\boldsymbol{u}_{data}$, $\boldsymbol{\beta}_{data}$

Augmentation – Implementation

- Assume the available higher-fidelity data, $\boldsymbol{d}$, consists of a few measured flow quantities and let the RANS predictions for the same quantities be $\boldsymbol{h}(\boldsymbol{u})$

- Assume that the **optimal** values of the augmentation function are given as $\boldsymbol{\beta}_k$, such that after solving the augmented model

$$\boldsymbol{R}(\boldsymbol{u}_k, \boldsymbol{\beta}_k) = 0$$

the prediction $\boldsymbol{h}(\boldsymbol{u}_k)$ matches the higher-fidelity data $\boldsymbol{d}$ as closely as possible.

Supervised Learning

$$\boldsymbol{w} = \arg\min_{\boldsymbol{w}_m} \|\boldsymbol{\beta}(\boldsymbol{\eta}(\boldsymbol{u}_k); \boldsymbol{w}_m) - \boldsymbol{\beta}_k\|_2^2$$

Model Augmentation

$$\mathcal{R}(\boldsymbol{u}, \boldsymbol{\beta}(\boldsymbol{\eta}(\boldsymbol{u}); \boldsymbol{w})) = 0$$

How to determine $\boldsymbol{\beta}_k$?

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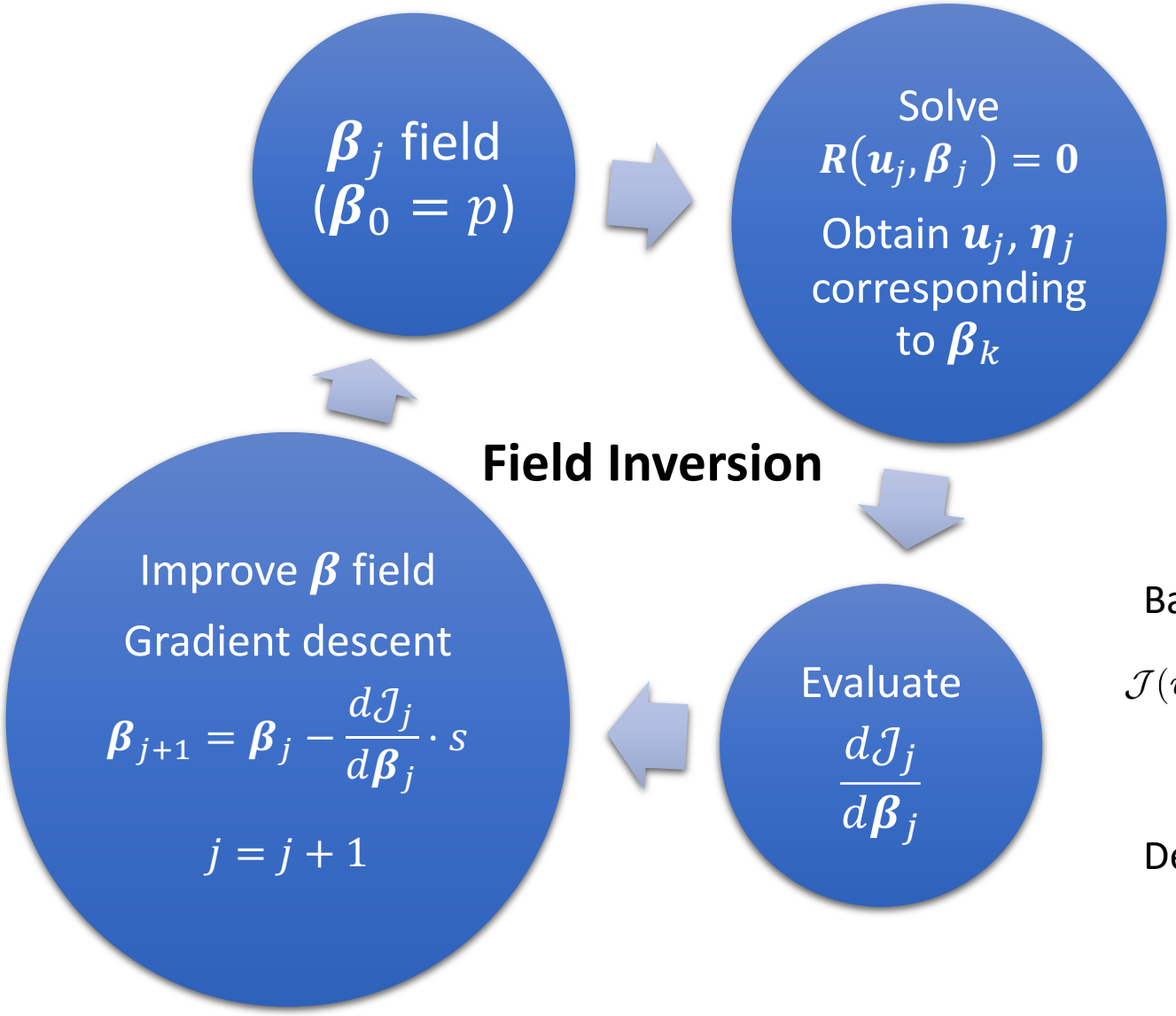
Field Inversion



Field Inversion as an optimization problem

$$\boldsymbol{\beta}_k = \arg\min_{\boldsymbol{\beta}_j} \mathcal{J}(\boldsymbol{u}_j, \boldsymbol{\beta}_j)$$

Subject to

$$\mathcal{R}(\boldsymbol{u}_j, \boldsymbol{\beta}_j) = 0$$

Bayesian Objective Function

$$\mathcal{J}(\boldsymbol{u}_j, \boldsymbol{\beta}_j) = \frac{1}{2}\left((\boldsymbol{d} - \boldsymbol{h}(\boldsymbol{u}_j))^T C_m^{-1} (\boldsymbol{d} - \boldsymbol{h}(\boldsymbol{u}_j))\right) + \left((\boldsymbol{\beta}_j - \boldsymbol{p})^T C_p^{-1} (\boldsymbol{\beta}_j - \boldsymbol{p})\right)$$

Deterministic Objective Function

$$\mathcal{J}(\boldsymbol{u}_j, \boldsymbol{\beta}_j) = \frac{1}{2}\|\boldsymbol{d} - \boldsymbol{h}(\boldsymbol{u}_j)\|_2^2 + \lambda\|\boldsymbol{\beta}_j - \boldsymbol{p}\|_2^2$$

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Field Inversion and Machine Learning

Field Inversion

$$\mathcal{J}(\boldsymbol{u}_j, \boldsymbol{\beta}_j) = \frac{1}{2}\|\boldsymbol{d} - \boldsymbol{h}(\boldsymbol{u}_j)\|_2^2 + \lambda\|\boldsymbol{\beta}_j - \boldsymbol{p}\|_2^2$$

$$\boldsymbol{\beta}_k = \arg\min_{\boldsymbol{\beta}_j} \mathcal{J}(\boldsymbol{u}_j, \boldsymbol{\beta}_j) \qquad s.t. \qquad \mathcal{R}(\boldsymbol{u}_j, \boldsymbol{\beta}_j) = 0$$

$\boldsymbol{\beta}_k$ is spatio-temporally discretized

Supervised Learning

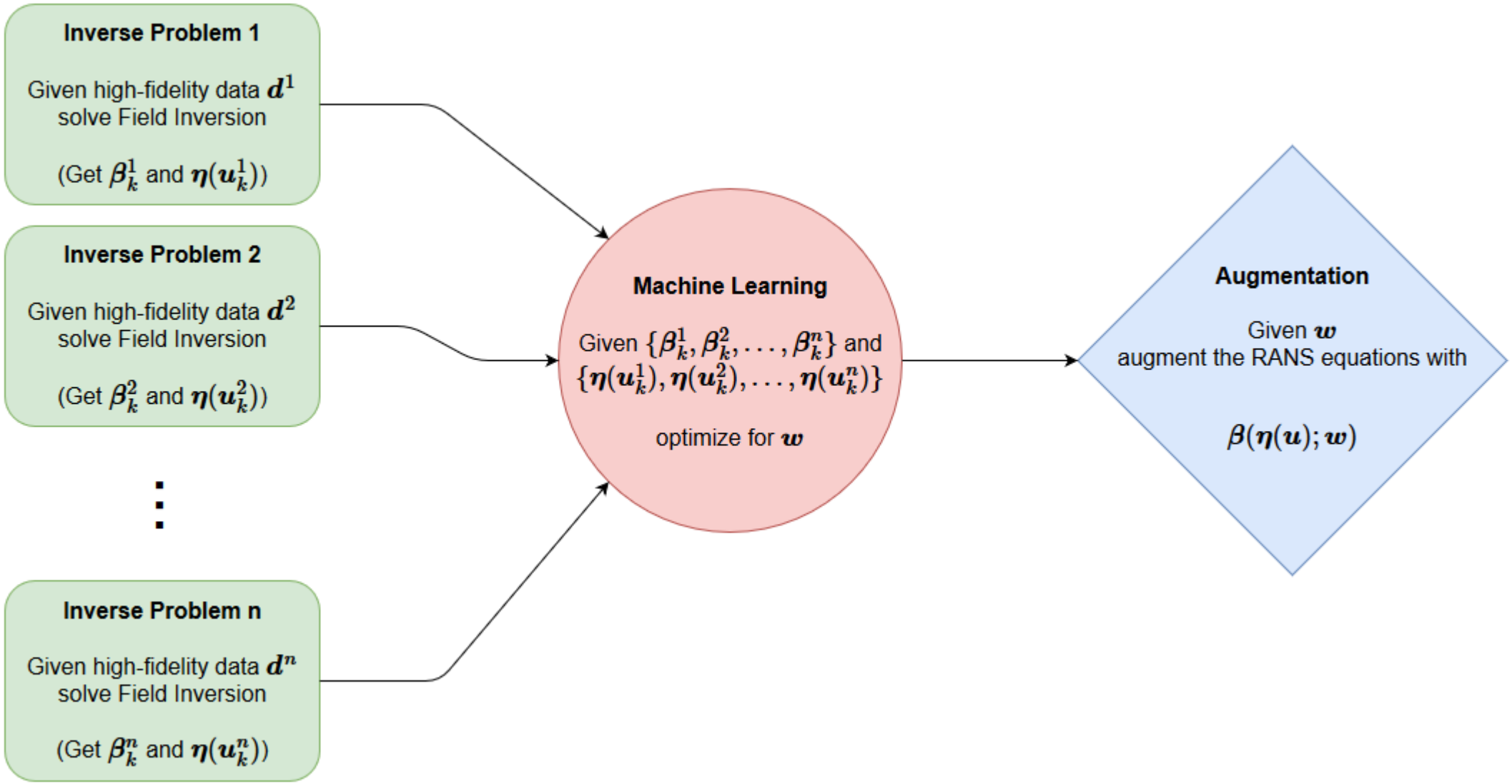
$$\boldsymbol{w} = \arg\min_{\boldsymbol{w}_m} \|\boldsymbol{\beta}(\boldsymbol{\eta}(\boldsymbol{u}_k); \boldsymbol{w}_m) - \boldsymbol{\beta}_k\|_2^2$$

Model Augmentation

$$\mathcal{R}(\boldsymbol{u}, \boldsymbol{\beta}(\boldsymbol{\eta}(\boldsymbol{u}); \boldsymbol{w})) = 0$$

- Consistency between learning and injection environments
- Does not require full fields of $\boldsymbol{u}_{data}$ and $\boldsymbol{\beta}_{\text{data}}$

Field Inversion and Machine Learning



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Spalart-Allmaras Turbulence Model

Basic Version

$$\frac{D\nu_t}{Dt} = c_{b1}\nu_t\Omega + \frac{1}{\sigma}\left(\nabla\cdot((\nu_t+\nu)\nabla\nu_t) + c_{b2}(\nabla\nu_t)^2\right)$$

- c_{b1} scales the Production term
- Lower $\sigma \Rightarrow$ Higher Diffusion
- c_{b2} controls the speed of turbulent front (must be greater than -1.0)

Calibration

- Choosing a σ, optimize c_{b1} and c_{b2} such that the maximum shear stress for a fully developed mixing layer and far wake is matched

Spalart-Allmaras Turbulence Model

Wall-bounded version for High Reynolds Numbers

$$\frac{D\nu_t}{Dt} = c_{b1}\nu_t\Omega + \frac{1}{\sigma}\left(\nabla\cdot((\nu_t+\nu)\nabla\nu_t) + c_{b2}(\nabla\nu_t)^2\right) - c_{w1}f_w\frac{\nu_t^2}{d^2}$$

- c_{w1} defined to obtain a perfect log layer

$$c_{w1} = \frac{c_{b1}}{\kappa^2} + \frac{1+c_{b2}}{\sigma}$$

- f_w designed to limit destruction in the outer layer – depends on c_{w2}, c_{w3}, $r = \nu_t/S\kappa^2 d^2$

$$f_w = g\left(\frac{1+c_{w3}^6}{g^6+c_{w3}^6}\right)^{1/6} \qquad g = r + c_{w2}(r^6 - r)$$

Calibration

- c_{w2} chosen to match friction coefficient of a ZPG boundary layer at $Re = 10^4$

Spalart-Allmaras Turbulence Model

Wall-bounded version for Finite Reynolds Numbers

$$\frac{D\widetilde{\nu}}{Dt} = c_{b1}\widetilde{\nu}\widetilde{\Omega} + \frac{1}{\sigma}\left(\nabla\cdot((\widetilde{\nu}+\nu)\nabla\widetilde{\nu}) + c_{b2}(\nabla\widetilde{\nu})^2\right) - c_{w1}f_w\frac{\widetilde{\nu}^2}{d^2}$$

- $\tilde{\nu}$ introduced as an operational variable – intended to be same as ν_t in and beyond the log layer
- $\widetilde{\Omega}$ correspondingly introduced to maintain the constant stress in the inner layer

$$\chi = \frac{\widetilde{\nu}}{\nu} \qquad f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3} \qquad \nu_t = \widetilde{\nu} f_{v1} \qquad f_{v2} = 1 - \frac{\chi}{1 + f_{v1}\chi} \qquad \widetilde{\Omega} = \Omega + \frac{\widetilde{\nu}}{\kappa^2 d^2} f_{v2}$$

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Physics-Constrained Augmentation – SA model

Objective: Change the diffusive characteristics of the model

Change intended in: σ

- Changing any of the three quantities in $\{\sigma, c_{b1}, c_{b2}\}$ would mean changing the other two, given the constraints for far wake and fully developed mixing layer
- The relationship between these quantities has been plotted in Spalart et al. (1992) and can be used to express c_{b1} and c_{b2} as $c_{b1}(\sigma)$ and $c_{b2}(\sigma)$, respectively.
- Alternatively, the objective function can be constrained based on the maximum turbulent stress values observed for fully-developed mixing layer and far wake obtained from the model as
- c_{w1} can then be evaluated based on the log layer constraint
- f_w would need to be checked to ensure correct values of friction coefficients in the ZPG boundary layer

Physics-Informed Augmentations – SA model

Objective: Change the behavior of the model in outer layer

Change intended in: f_w

$$f_w = g\left(\frac{1+c_{w3}^6}{g^6+c_{w3}^6}\right)^{1/6} \qquad g = r + c_{w2}(r^6 - r) \qquad r = \frac{\tilde{\nu}}{\tilde{\Omega}\kappa^2 d^2}$$

- $r = 1$ in the log layer
- <u>Option 1</u>: Augment c_{w2} such that $g = r + c_{w2}^{new}(r^6 - r)$ where $c_{w2}^{new} = \beta c_{w2}$ such that the augmentation is nullified in the log layer and thus only applied in the outer layer. This can augment the model form for g.
- <u>Option 2</u>: Augment f_w such that $f_w^{new} = \beta(f_w - 1) + 1$ such that the augmentation is again nullified in the log layer and the original SA model is preserved for $\beta = 1$. This can augment the model form for f_w.
- Since f_w is a function of r which depends on $\tilde{\nu}$ and $\tilde{\Omega}$, we can make the augmentation β a function of $\nu/(\tilde{\Omega}\kappa^2 d^2 + \nu)$ and $\nu/(\tilde{\nu} + \nu)$ to ensure that the features are bounded and non-dimensional

Physics-Informed Augmentations – SA model

Objective: Change the behavior of the model in buffer layer

Change intended in: f_{v1}

$$\nu_t = f_{v1}\tilde{\nu} \qquad f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3} \qquad \chi = \frac{\tilde{\nu}}{\nu}$$

- <u>Option 1</u>: Augment χ such that $\chi^{new} = \beta\chi$. Here the dampening model-form is left untouched.
- <u>Option 2</u>: Augment f_{v1} such that $f_{v1}^{new} = \beta f_{v1}$. Here the model-form for dampening is changed too.
- Since χ and hence f_{v1} are functions of $\tilde{\nu}$ the choice for a bounded non-dimensional feature could be between $\nu/(\tilde{\nu} + \nu)$ and $\nu/(\nu_t + \nu)$

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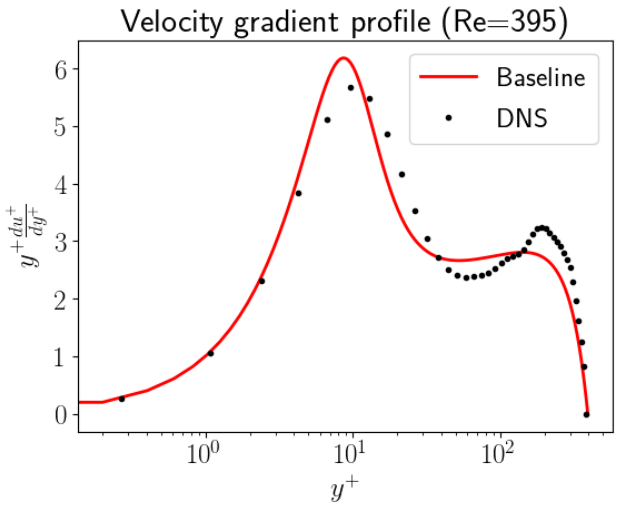
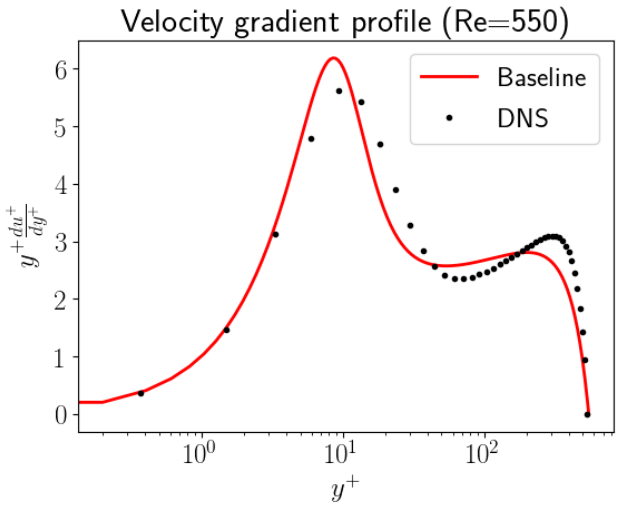
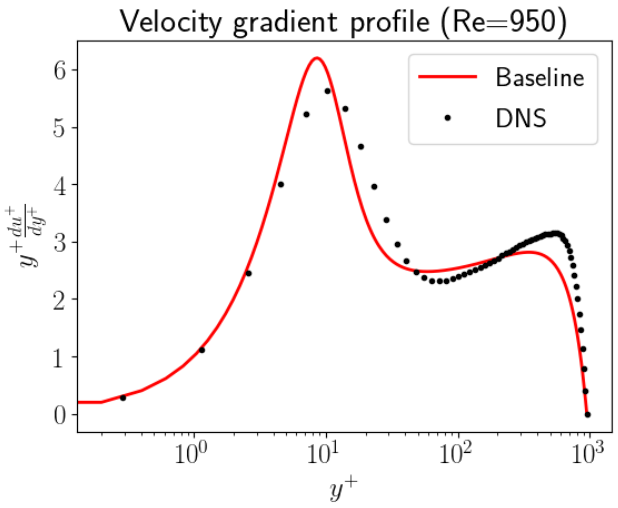
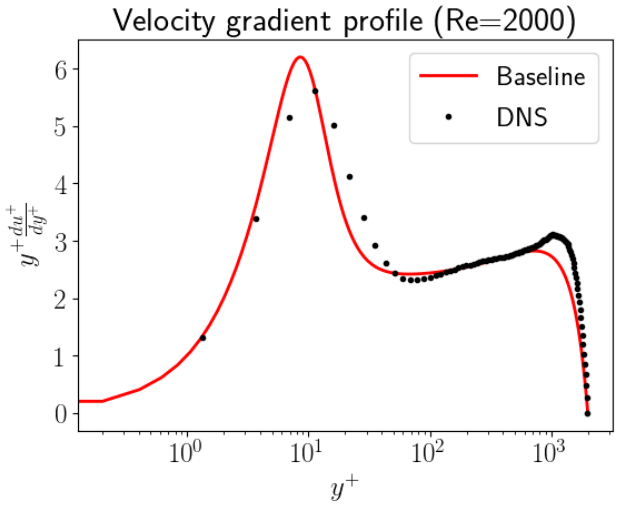
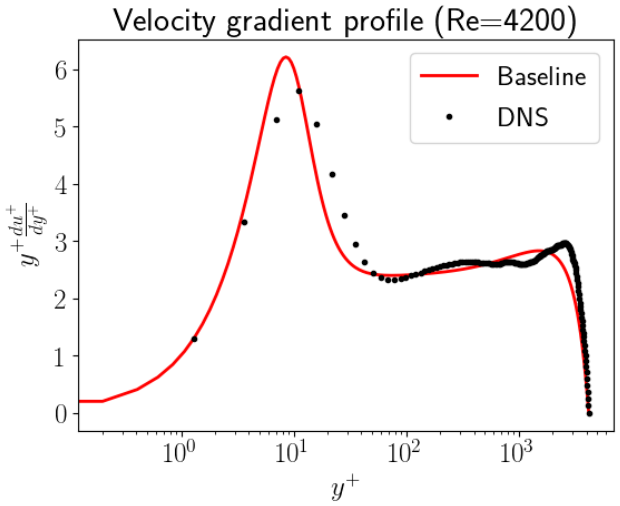
Results for Channel Flow

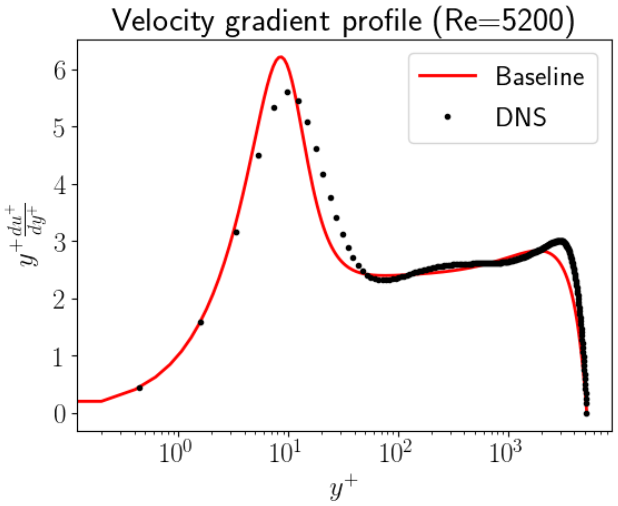












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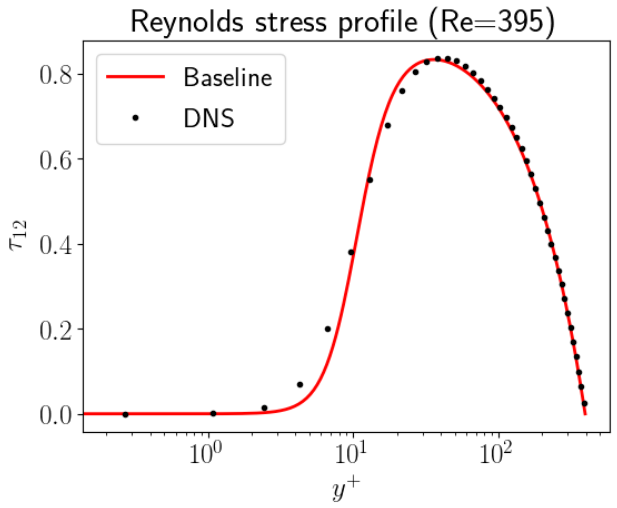

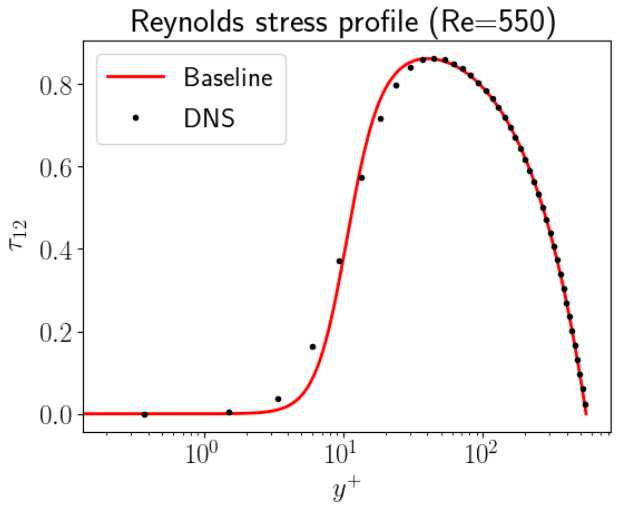

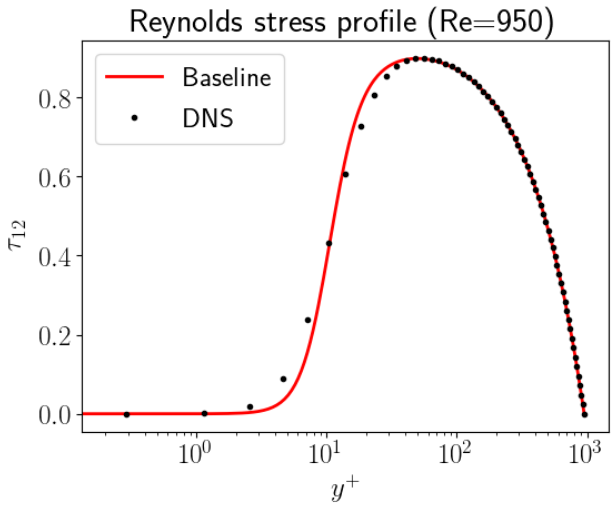

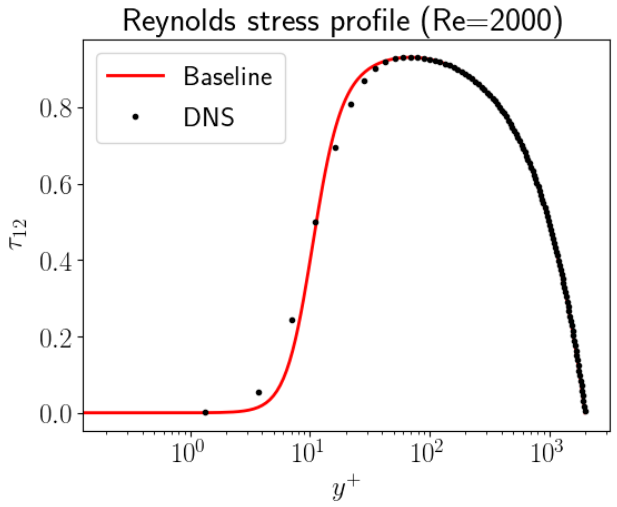

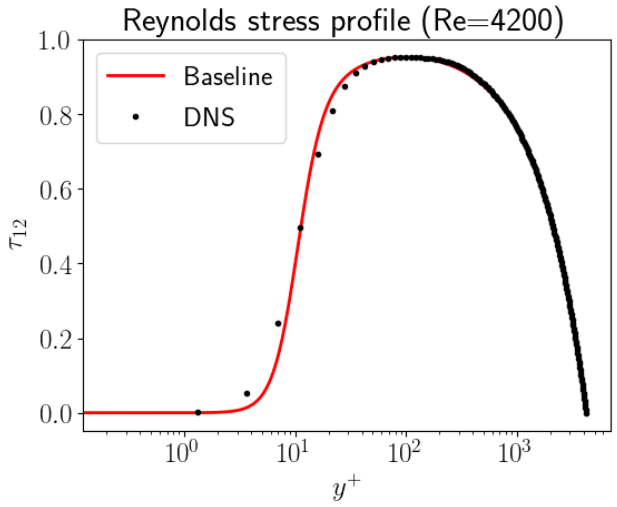

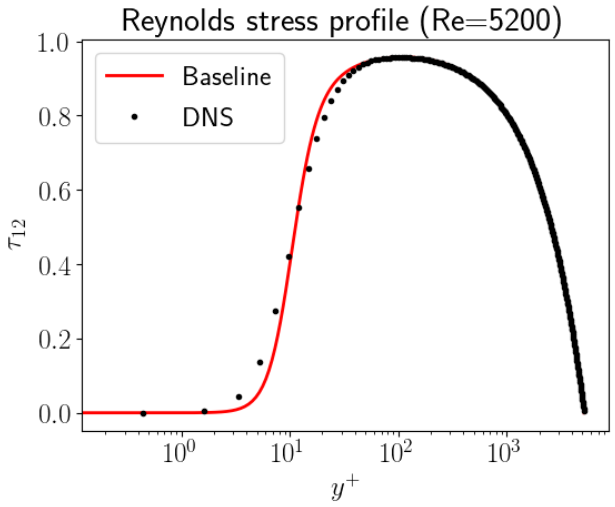

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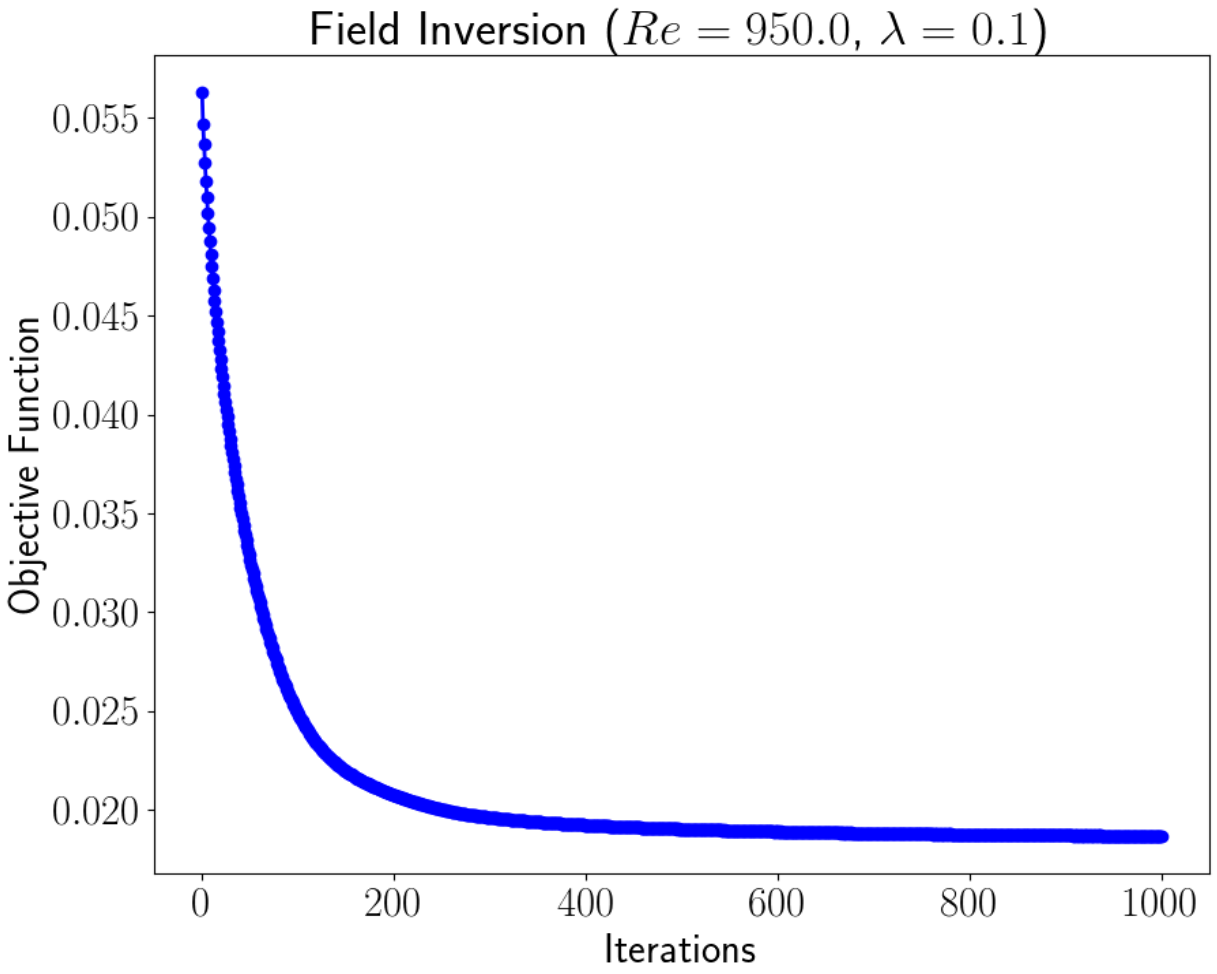
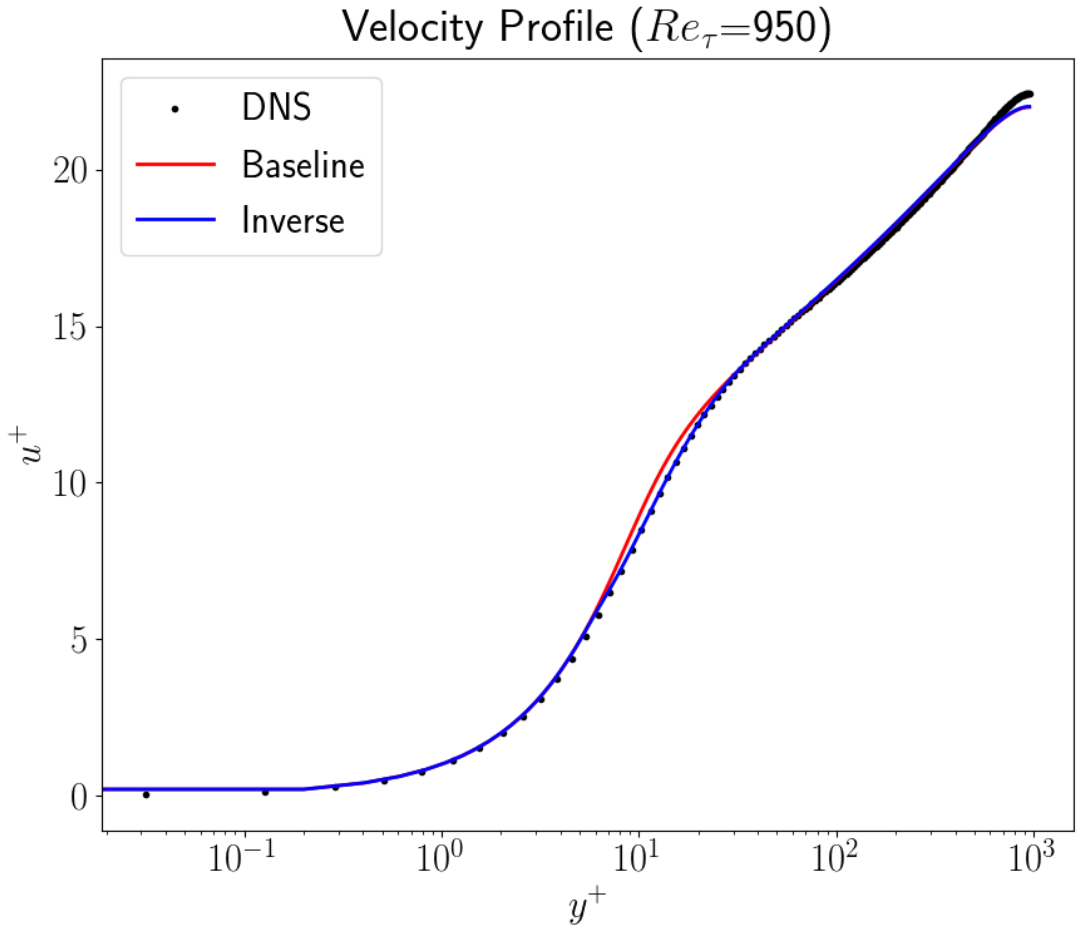
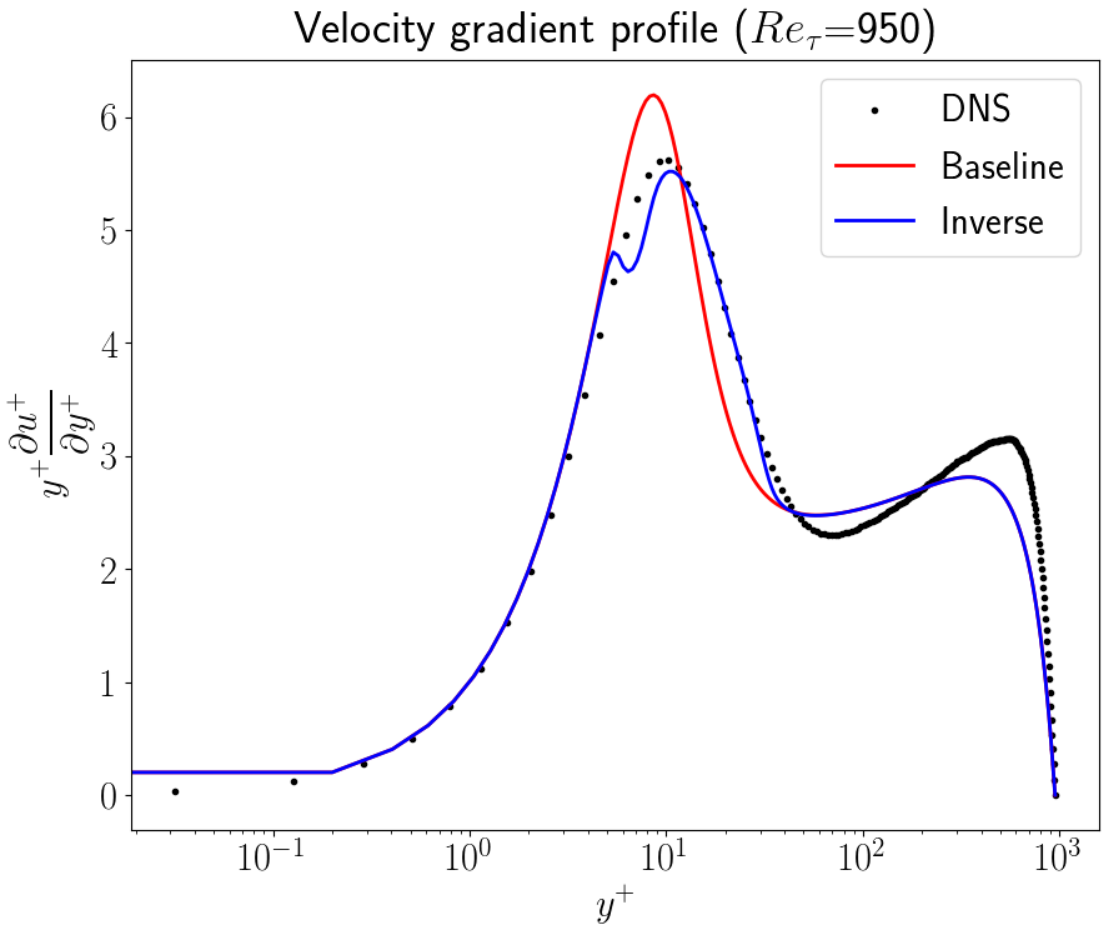
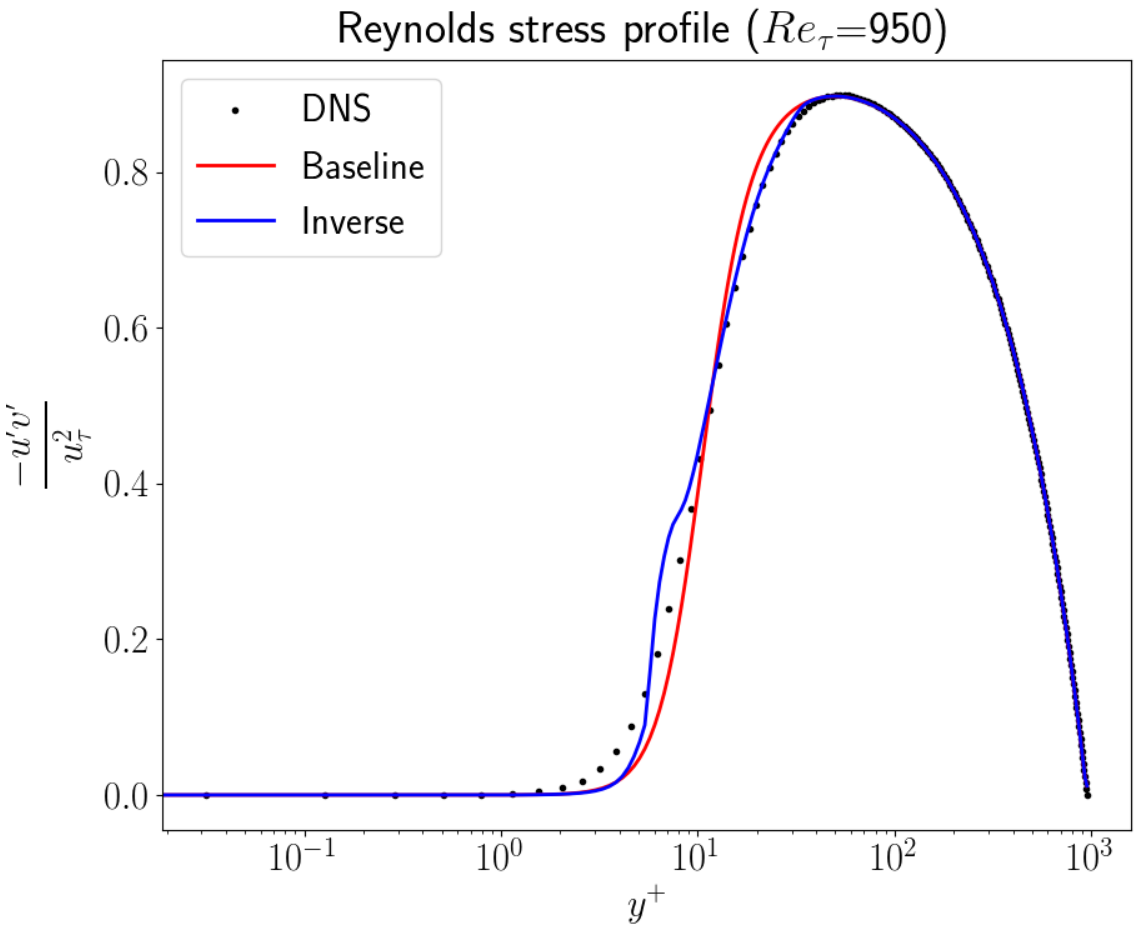




$$\mathcal{J} = \|\boldsymbol{u}^+ - \boldsymbol{u}^+_{DNS}\|_2^2 + \lambda\|\boldsymbol{\beta} - 1\|_2^2$$

Results for Channel Flow





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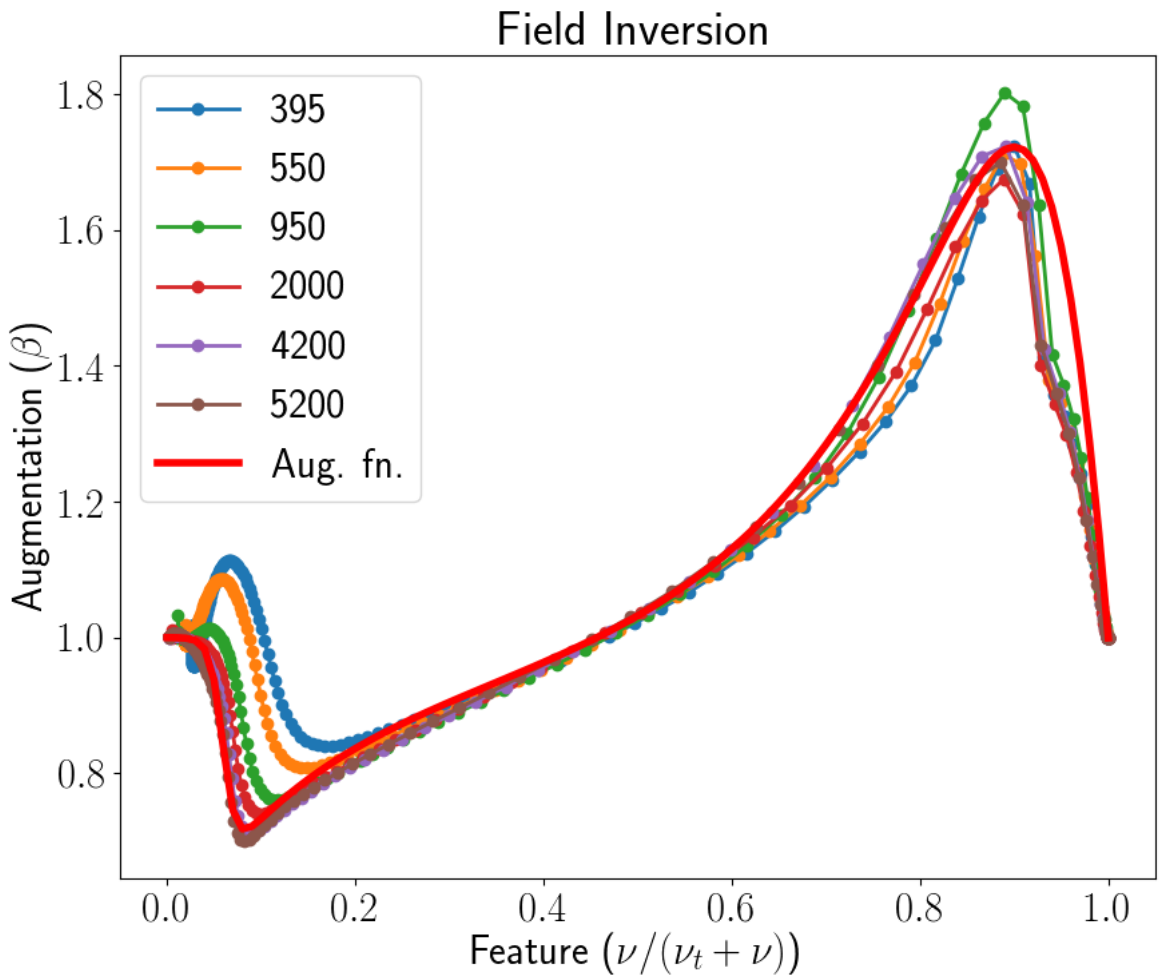


Learnable augmentation for higher Reynolds numbers !!

Augmentation function (Feature: $\boldsymbol{\eta = \nu/(\nu_t + \nu)}$)

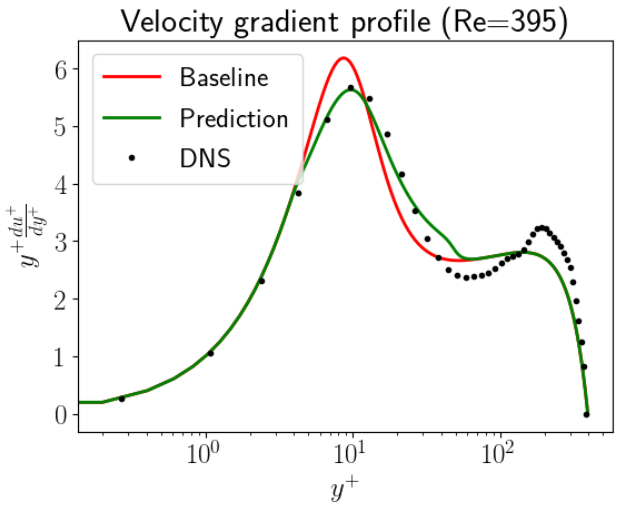
$$\beta(\eta) = 1 + \frac{1}{1+\exp(9-150\eta)}\left(a(\eta)b(\eta) - c(\eta)\right)$$

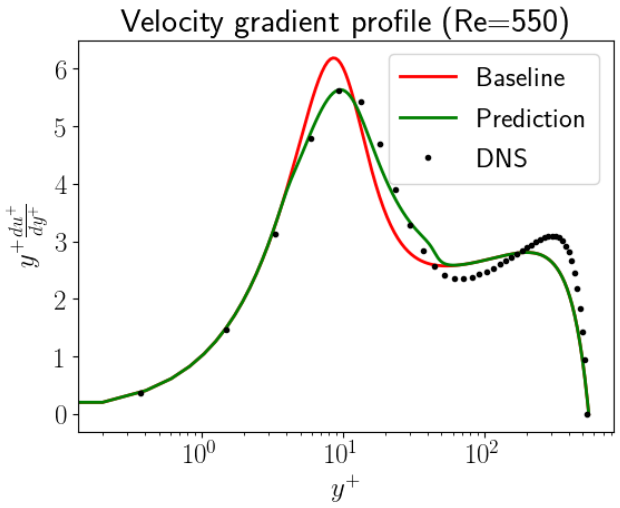
$$a(\eta) = 0.95\tanh(10-10\eta)$$

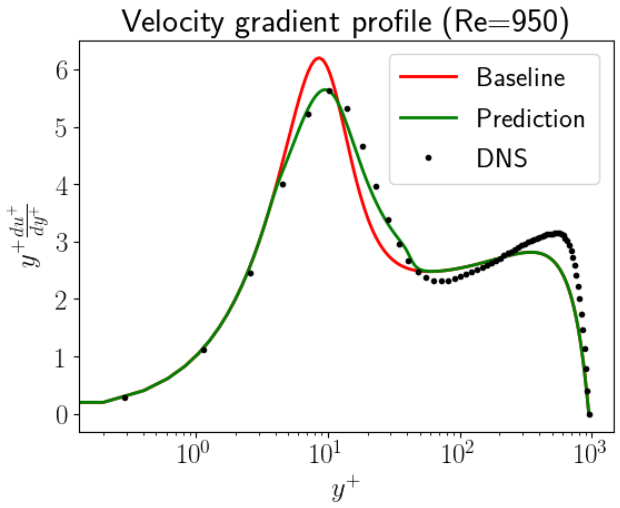
$$b(\eta) = 1.1\exp(5\eta - 0.9) - 0.1$$

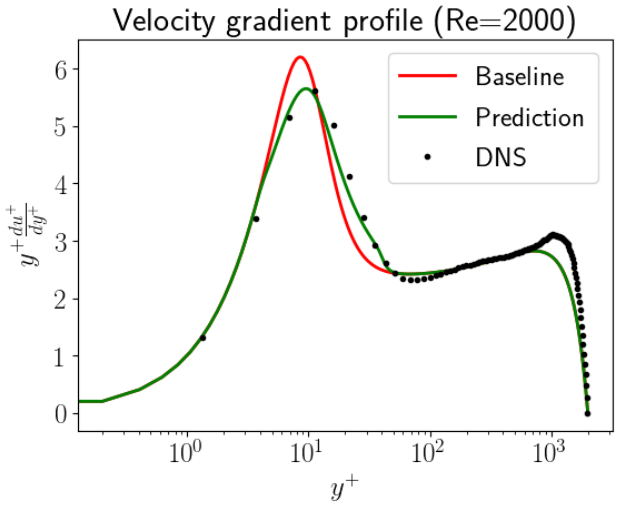
$$c(\eta) = 0.1\exp(1.3 - 6.5\eta)$$

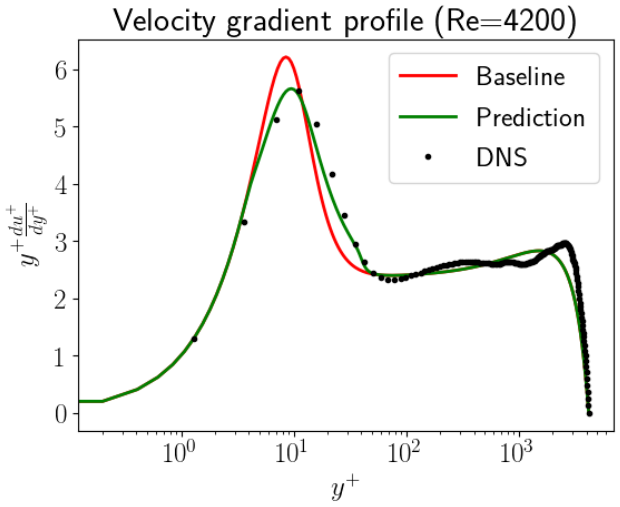
Results for Channel Flow

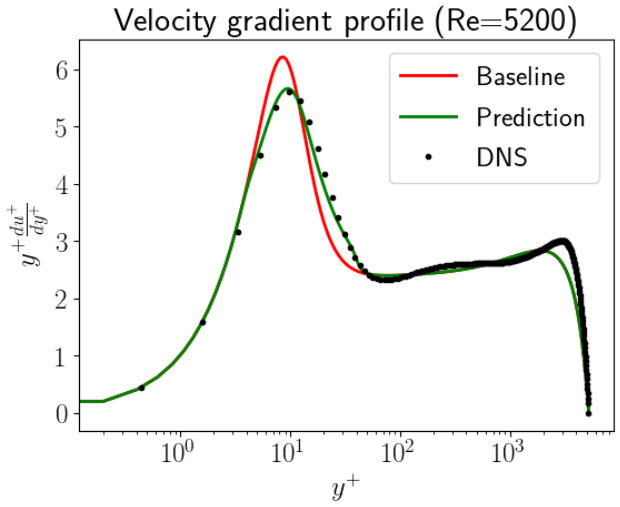




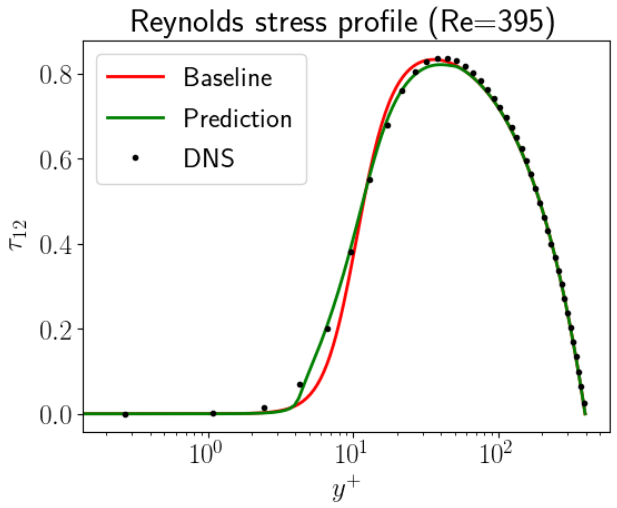


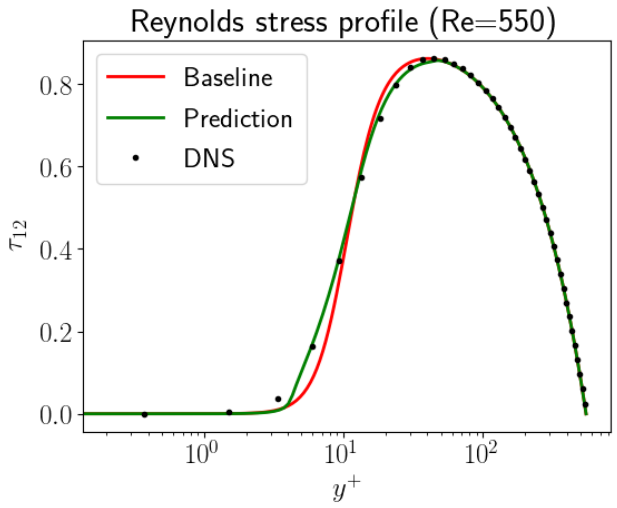


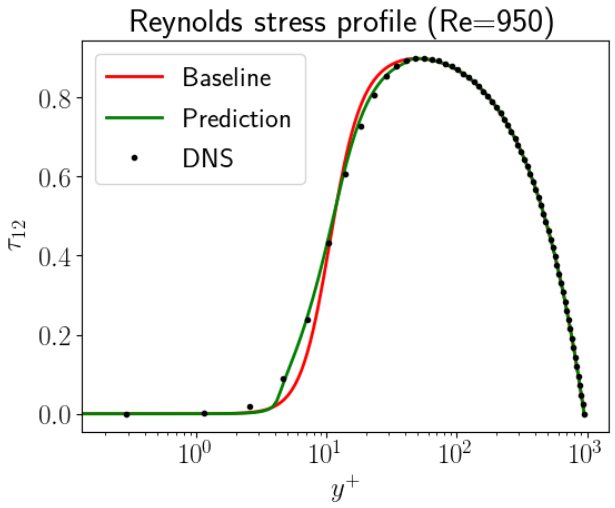


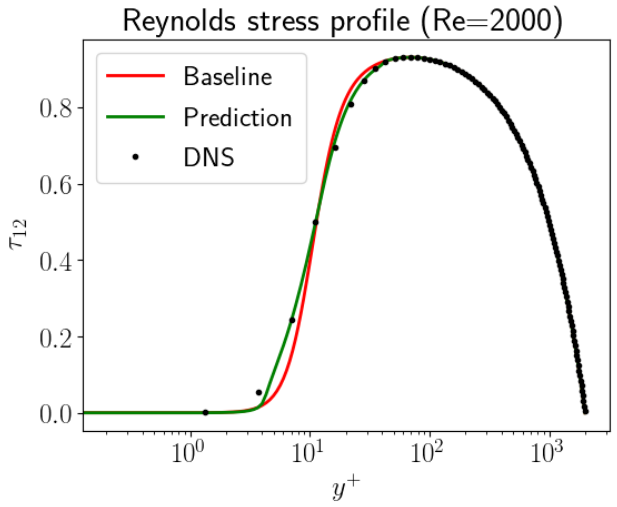


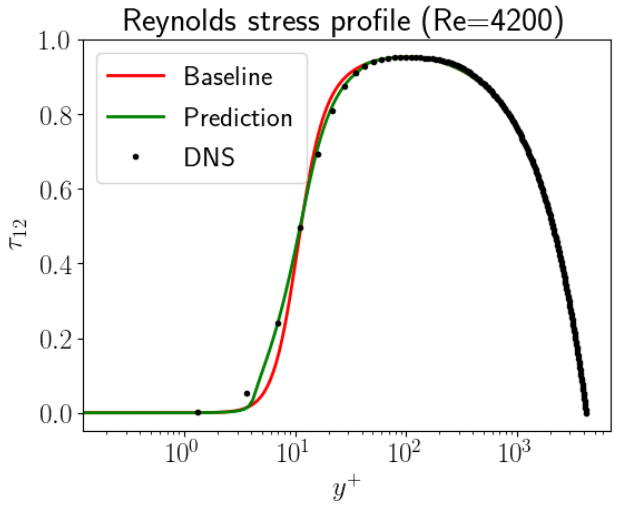
Results for Channel Flow

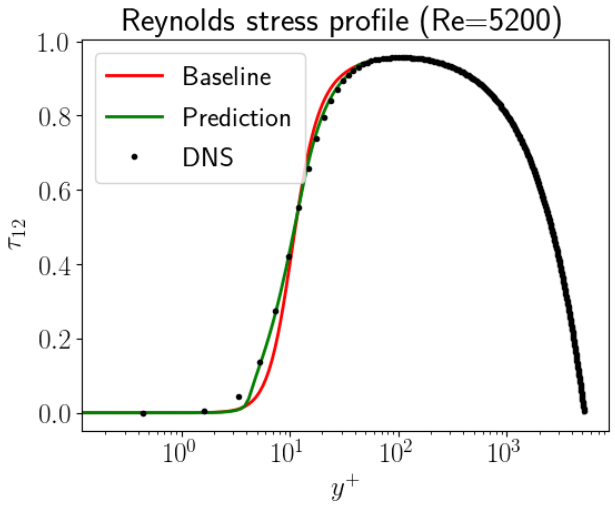












Outline

- Augmentation
  - Philosophy
  - Implementation
- Field Inversion
- Field Inversion and Machine Learning
  - Traditional FIML
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  - A brief introduction to Spalart-Allmaras turbulence model
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Prediction Improvements - Airfoils

Spalart-Allmaras turbulence model: $$\frac{D\widetilde{\nu}}{Dt} = \beta(\eta) c_{b1}\widetilde{\nu}\widetilde{\Omega} + \frac{1}{\sigma}\left(\nabla\cdot((\widetilde{\nu}+\nu)\nabla\widetilde{\nu}) + c_{b2}(\nabla\widetilde{\nu})^2\right) - c_{w1} f_w \frac{\widetilde{\nu}^2}{d^2}$$

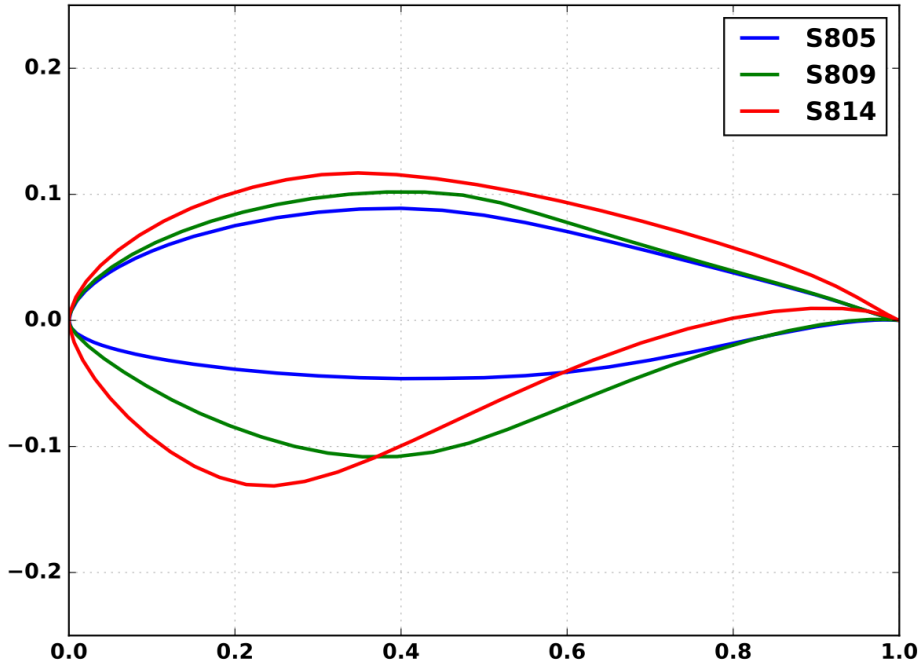
Boussinesq Approximation: $$-\rho\overline{u_i' u_j'} = 2\mu_t \overline{S}_{ij} \qquad \mu_t = \rho\hat{\nu} f_{v1}$$

Momentum Equation (RANS): $$\rho\frac{\partial \bar{u}_i}{\partial t} + \rho\frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = \rho\bar{f}_i + \frac{\partial}{\partial x_j}\left[-\bar{p} + 2\mu\bar{S}_{ij} - \rho\overline{u_i' u_j'}\right]$$

Features(η) : $\left\{\widetilde{\Omega}, \chi, S/\Omega, \tau/\tau_{\text{wall}}, P/D, f_d\right\}$

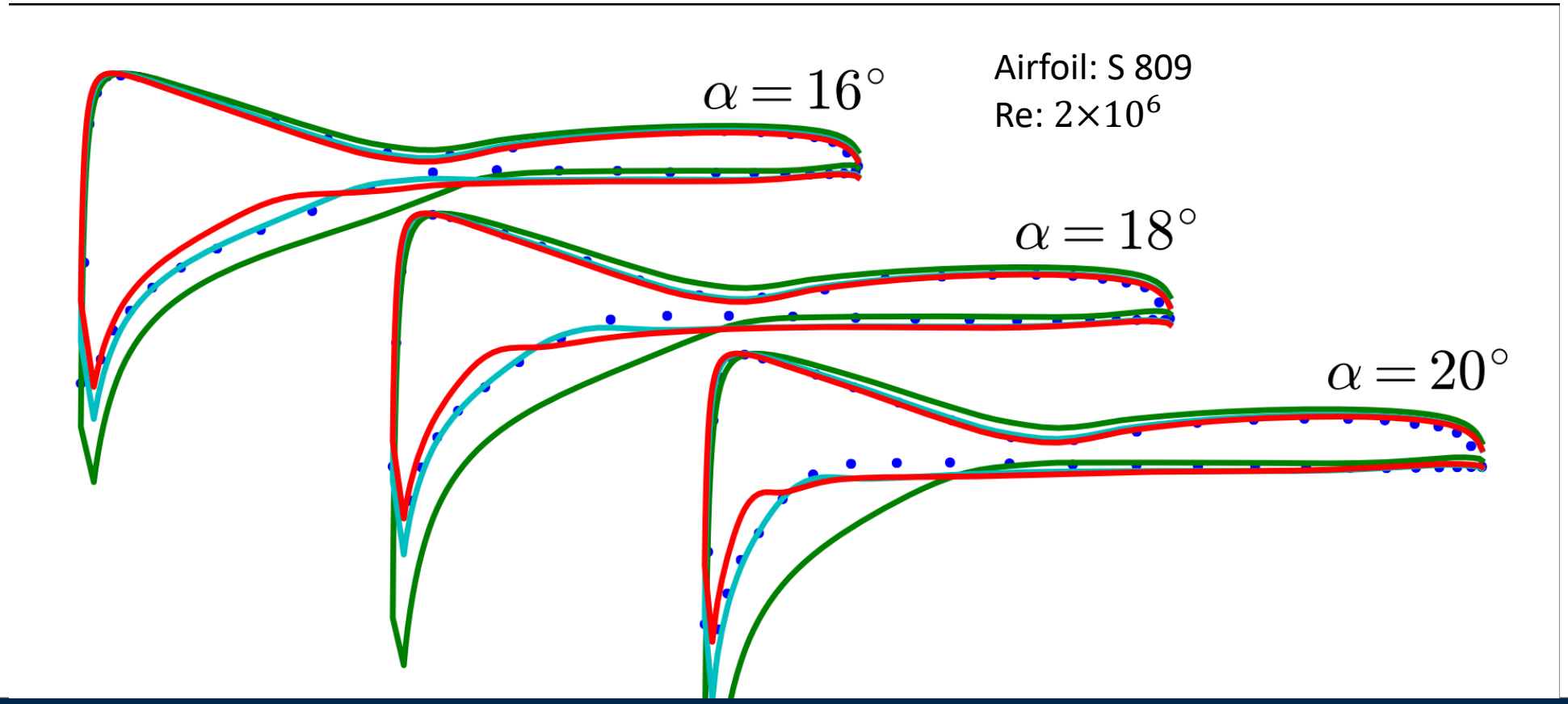
Datasets used for training:

- $S814,\ Re = 1\times10^6$
- $S814,\ Re = 2\times10^6$

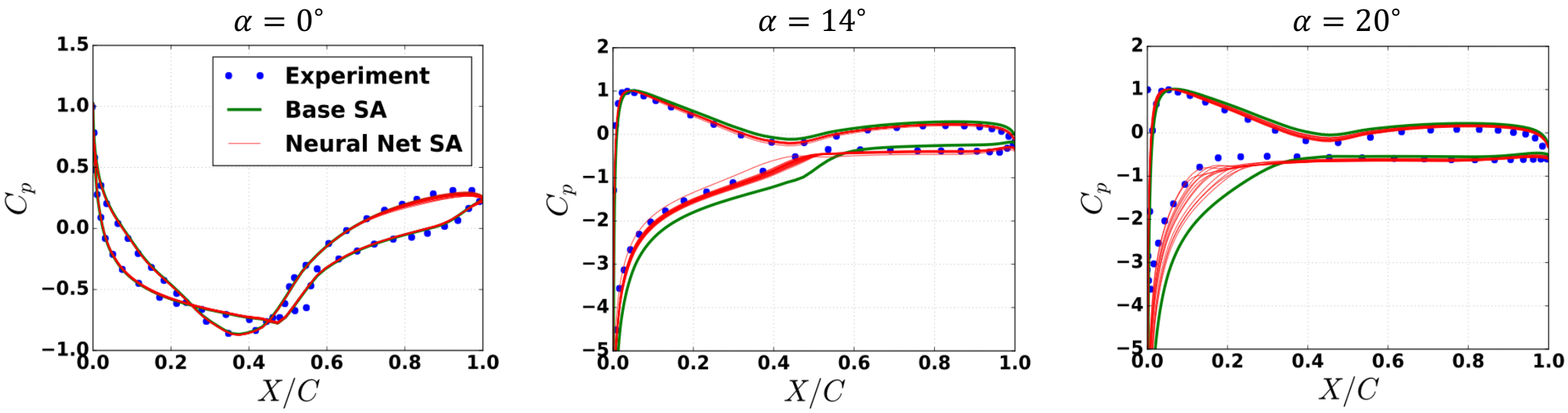


Prediction Improvements - Airfoils

Inference used only C_L data, NN-augmented model provides considerable predictive improvements of C_p



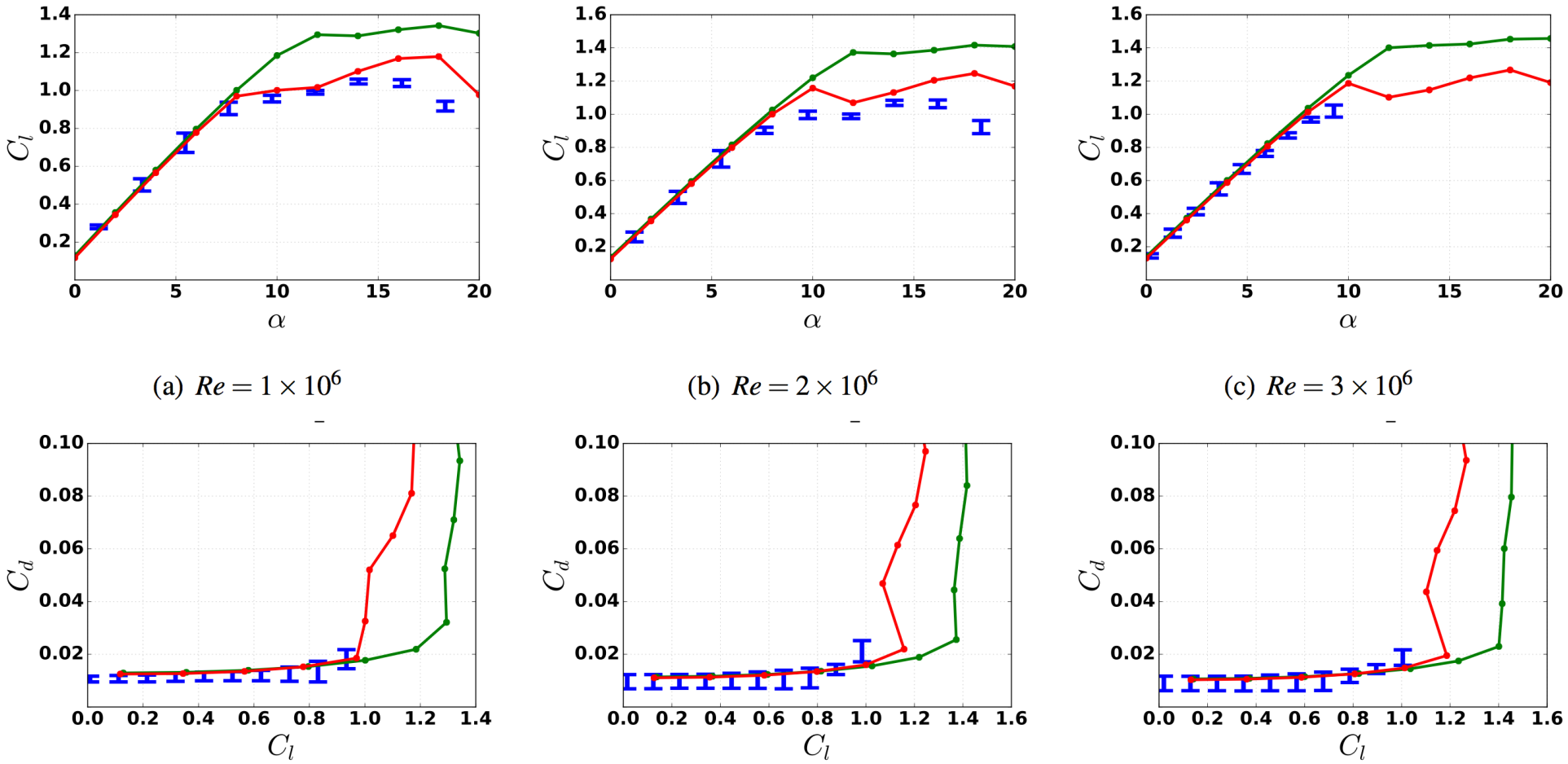
Prediction Improvements - Airfoils



Variability in training from different sets

Singh, A., Medida, S. & Duraisamy, K., Machine-Learning-augmented Predictive Modeling of Turbulent Separated Flows over Airfoils, AIAA Journal, 2017

Prediction Improvements - Airfoils

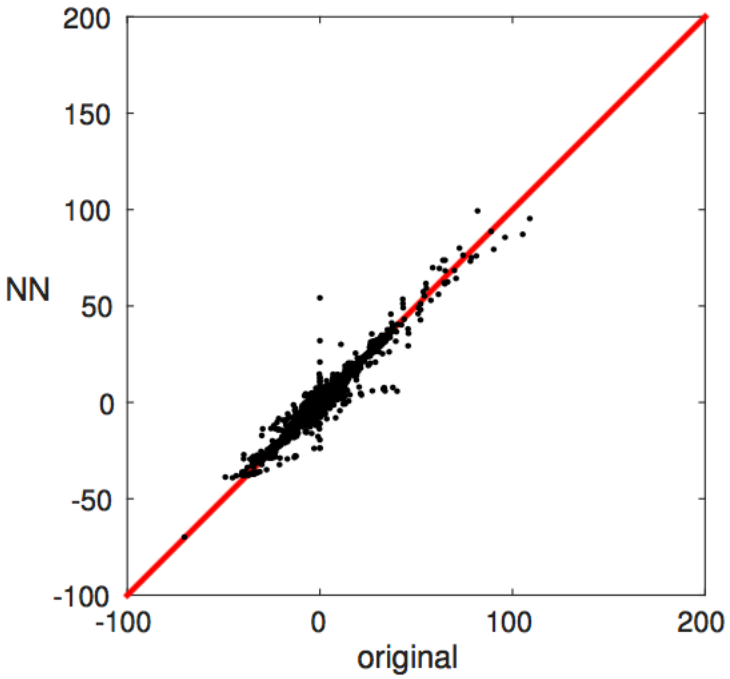


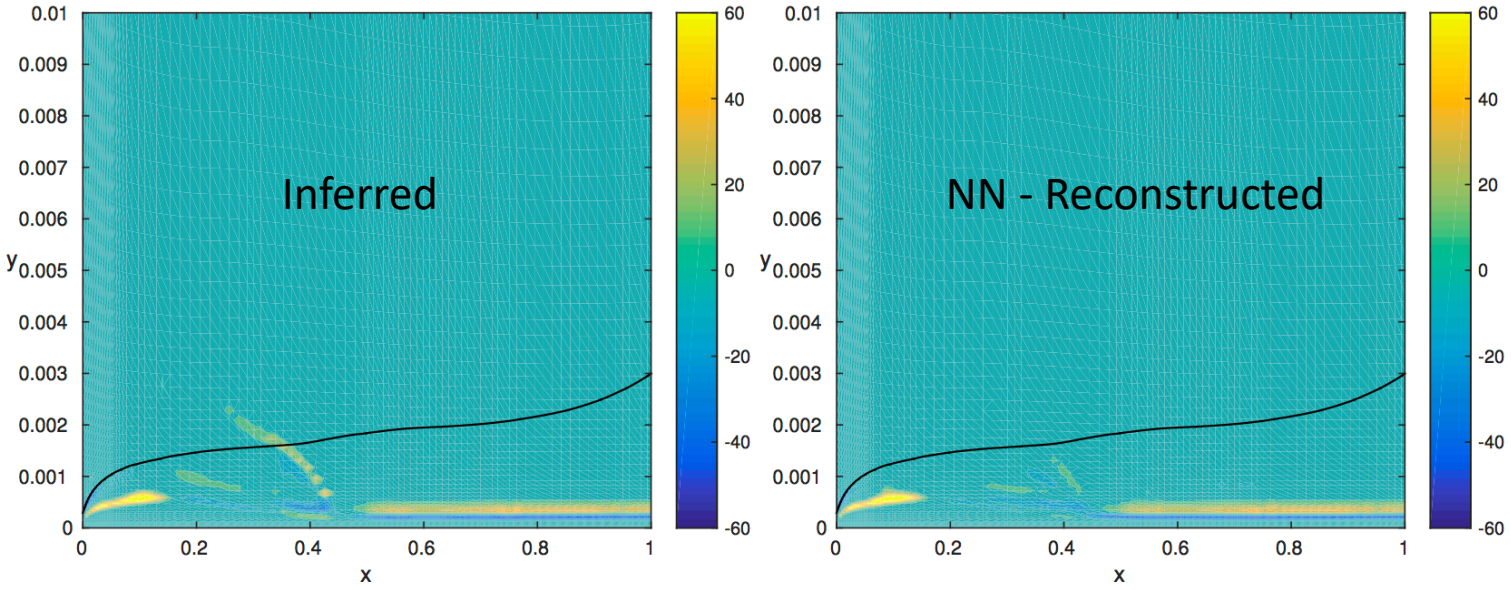
(a) $Re = 1 \times 10^6$ (b) $Re = 2 \times 10^6$ (c) $Re = 3 \times 10^6$

Portability: Implementation in AcuSolve

Field Inversion and Machine Learning

In more complex problems, however, …





What is inferred is not necessarily learnable

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Coupled Field Inversion and Machine Learning (FIML-CT)

Tightly Coupled Inference and Learning

$$\mathcal{J}(\boldsymbol{u}_j, \boldsymbol{w}_j) = \frac{1}{2}\|\boldsymbol{d} - \boldsymbol{h}(\boldsymbol{u}_j)\|_2^2 + \lambda\|\boldsymbol{\beta}(\boldsymbol{\eta}(\boldsymbol{u}_j); \boldsymbol{w}_j) - \boldsymbol{p}\|_2^2$$

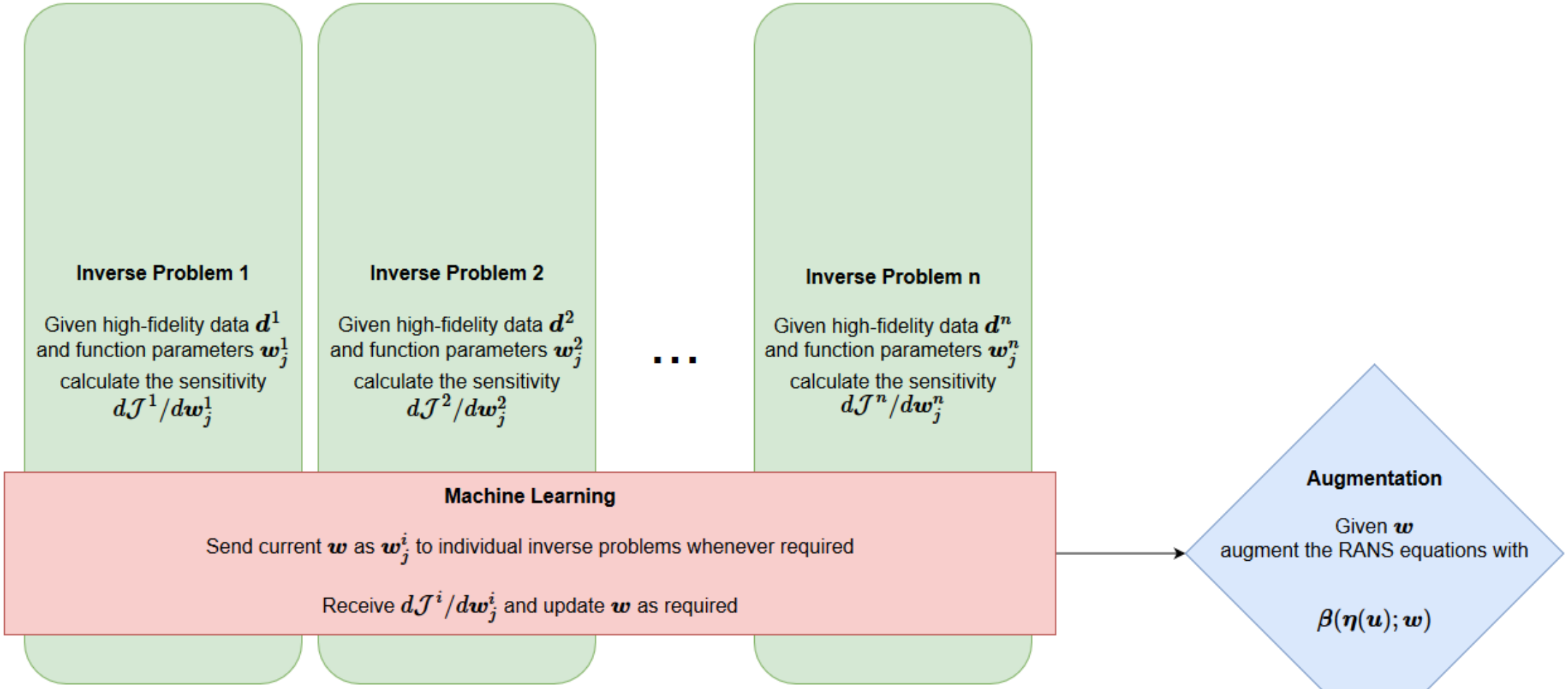
$$\boldsymbol{w} = \arg\min_{\boldsymbol{w}_j} \mathcal{J}(\boldsymbol{u}_j, \boldsymbol{w}_j) \qquad s.t. \qquad \mathcal{R}(\boldsymbol{u}_j, \boldsymbol{\beta}(\boldsymbol{\eta}(\boldsymbol{u}_j); \boldsymbol{w}_j)) = 0$$

Model Augmentation

$$\mathcal{R}(\boldsymbol{u}, \boldsymbol{\beta}(\boldsymbol{\eta}(\boldsymbol{u}); \boldsymbol{w})) = 0$$

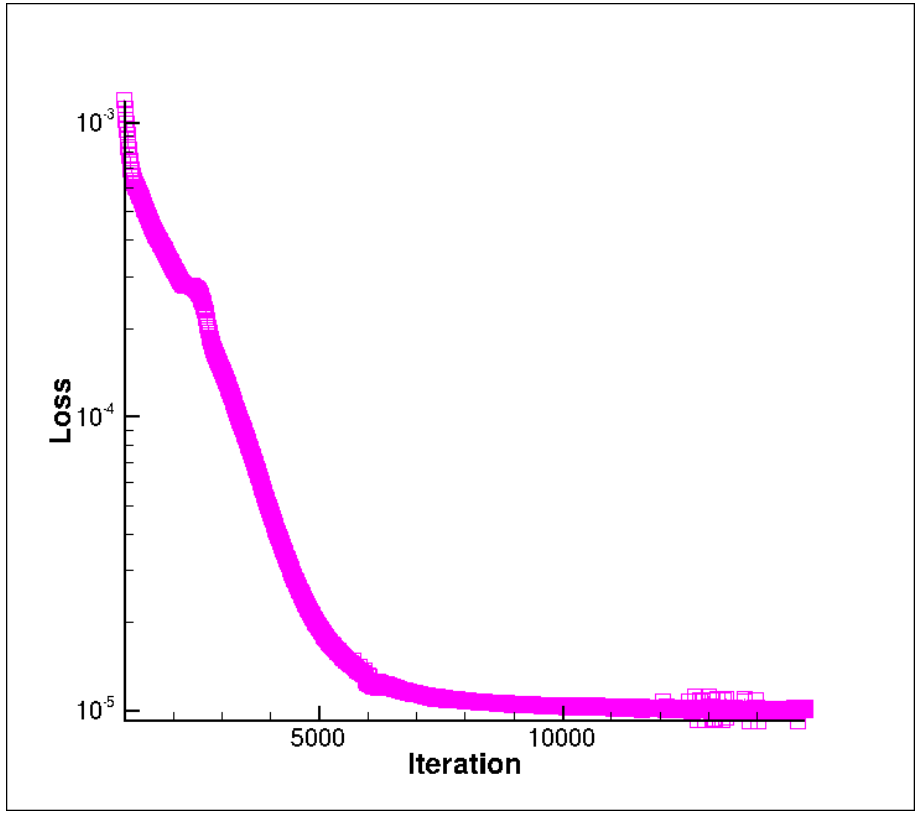
- True consistency between learning and injection environments
- Less prone to overfitting

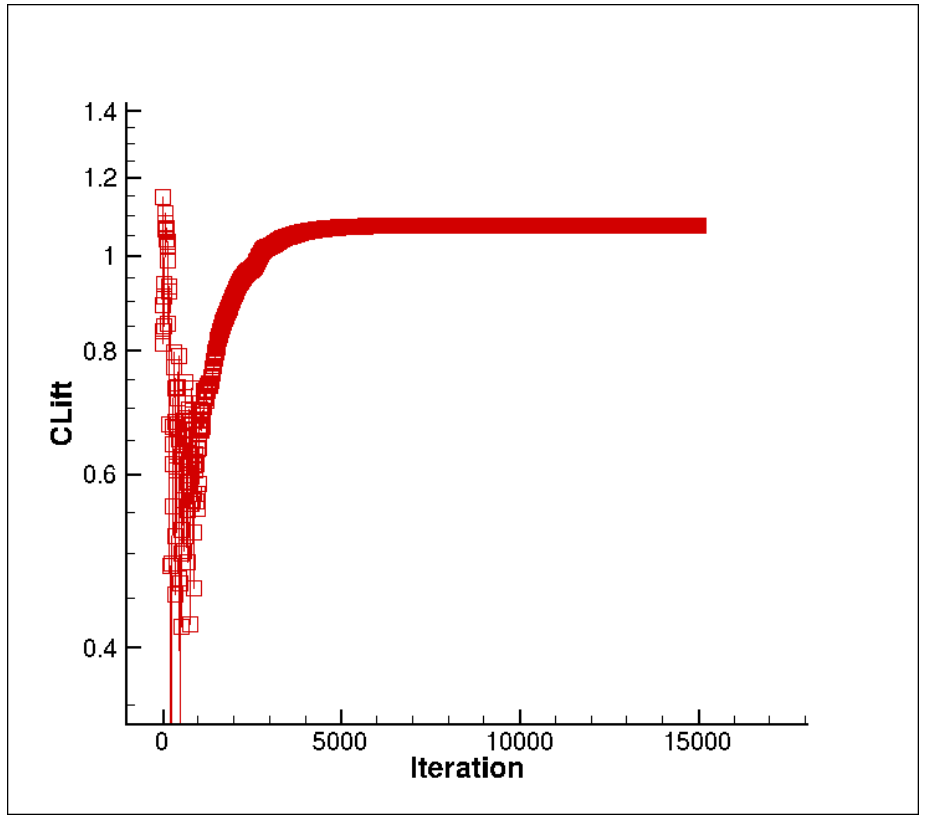
Coupled Field Inversion and Machine Learning (FIML-CT)



Coupled Field Inversion and Machine Learning (FIML-CT)

Learnable inverse, but convergence is slow





Field Inversion is exposed to full non-linearity of NN training

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Coupled Field Inversion and Machine Learning (FIML-CL)

Loosely coupled Inference and Learning

$$\mathcal{J}(\boldsymbol{u}_j, \boldsymbol{w}_j; \boldsymbol{\beta}_j) = \frac{1}{2}\|\boldsymbol{d} - \boldsymbol{h}(\boldsymbol{u}_j)\|_2^2 + \lambda\|\boldsymbol{\beta}(\boldsymbol{\eta}(\boldsymbol{u}_j); \boldsymbol{w}_j) - \boldsymbol{p}\|_2^2$$

$$\boldsymbol{\beta}_k = \arg\min_{\boldsymbol{\beta}_j} \mathcal{J}(\boldsymbol{u}_j, \boldsymbol{w}_j; \boldsymbol{\beta}_j) \quad s.t. \quad \mathcal{R}(\boldsymbol{u}_j, \boldsymbol{\beta}(\boldsymbol{\eta}(\boldsymbol{u}_j); \boldsymbol{w}_j)) = 0, \quad \underbrace{\boldsymbol{w}_j = \arg\min_{\boldsymbol{w}_{j,m}} \|\boldsymbol{\beta}(\boldsymbol{\eta}(\boldsymbol{u}_j); \boldsymbol{w}_{j,m}) - \boldsymbol{\beta}_j\|_2^2}$$

Incremental update from inference

$$\boldsymbol{\beta}_{j+1} = \boldsymbol{\beta}(\boldsymbol{\eta}(\boldsymbol{u}_j); \boldsymbol{w}_j) + \boldsymbol{s} \cdot \left[\frac{d\mathcal{J}}{d\boldsymbol{\beta}'}\right]_{\boldsymbol{\beta}' = \boldsymbol{\beta}(\boldsymbol{\eta}(\boldsymbol{u}_j); \boldsymbol{w}_j)}$$

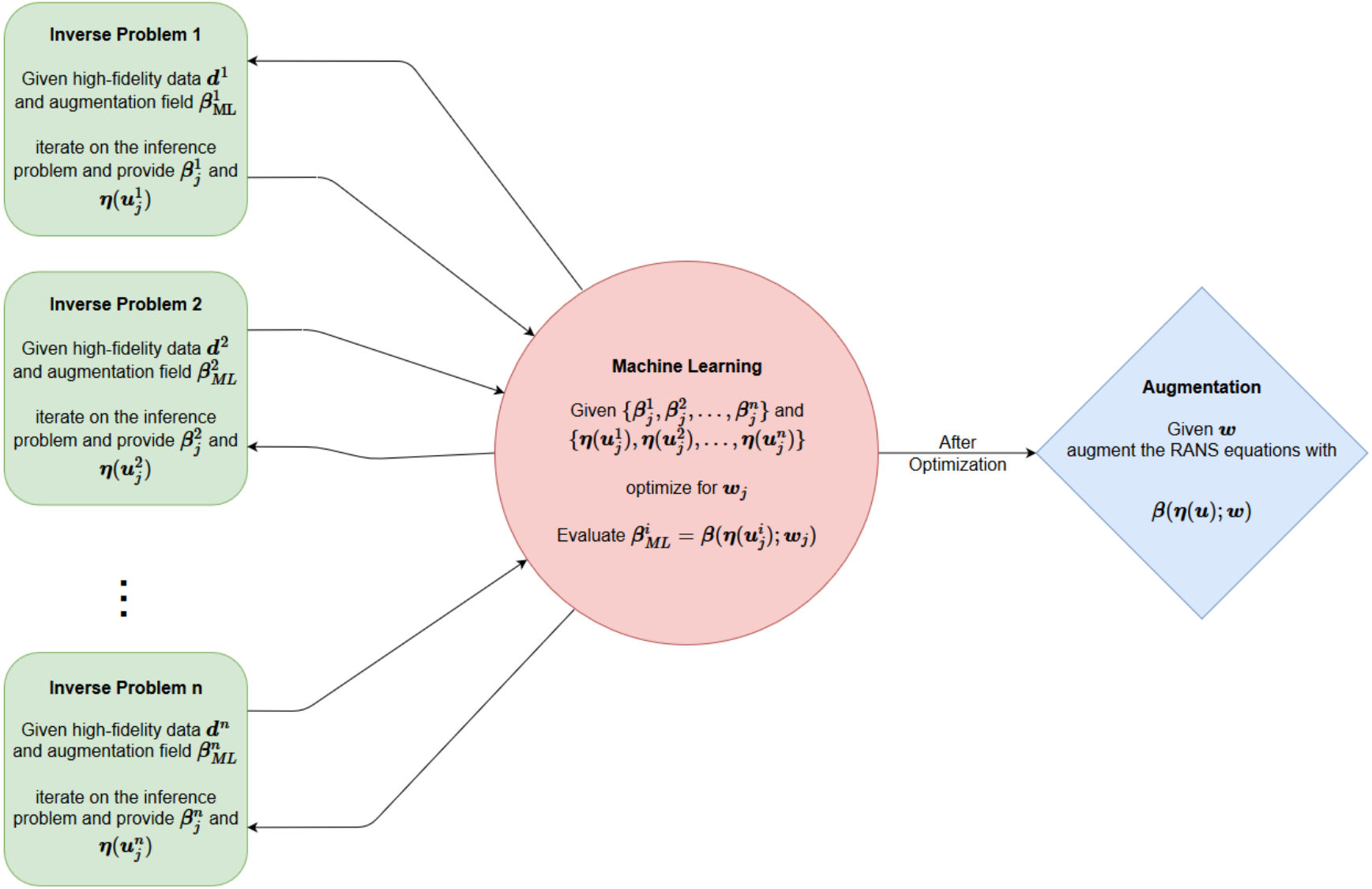
Extract learnable information from inferred field

- Consistency between learning and injection environments
- Does not require full fields of $\boldsymbol{u}_{data}$ and $\boldsymbol{\beta}_{\text{data}}$
- Inference not exposed to NN convergence issues

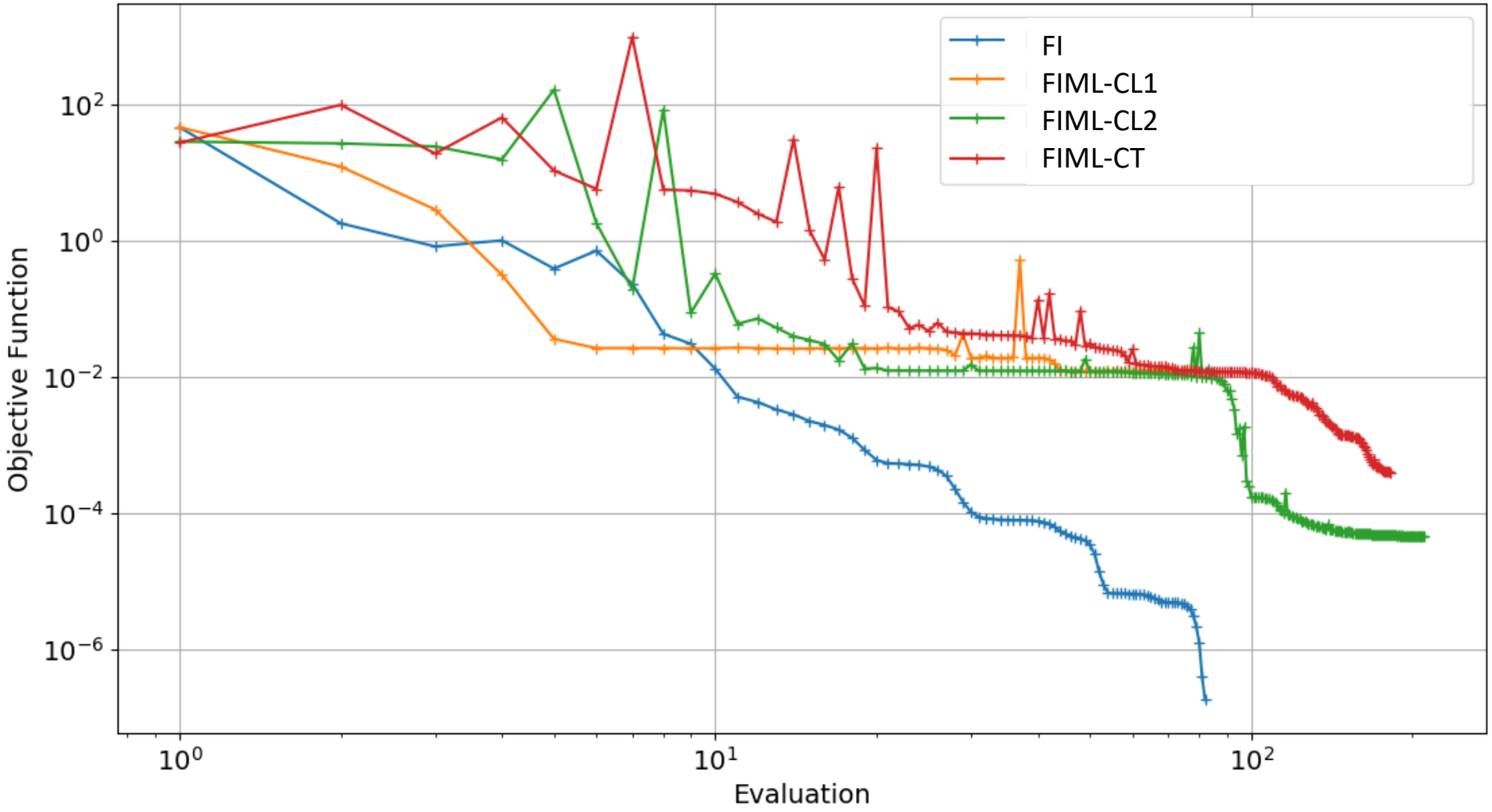
Model Augmentation

$$\mathcal{R}(\boldsymbol{u}, \boldsymbol{\beta}(\boldsymbol{\eta}(\boldsymbol{u}); \boldsymbol{w}_k)) = 0$$

Coupled Field Inversion and Machine Learning (FIML-CL)



Convergence Benefits



In collaboration with J. Holland (University of Maryland)

Summary

- **Predictive capability and accuracy of an augmentation** to a turbulence model **can be improved, if introduced carefully and judiciously** while conserving physical laws and known properties of turbulent flows

- **Field Inversion and Machine Learning** – a useful approach to extract information from the available higher-fidelity data to augment models
  - **Improves predictions** for cases where baseline model doesn't perform well
  - **Consistent** and **Portable**
  - Classical FIML suffers from a **potential deficiency in learnability**

- **Coupled Field Inversion and Machine Learning** – **Ensures maximum learnability** from the data *during* inference
  - **Tightly coupled FIML** – exposed to functional form of augmentation
    - **Convergence issues for highly non-linear augmentations**

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THANK YOU!