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

Vishal Srivastava, Ph.D. Candidate
Advisor: Dr. Karthik Duraisamy

Department of Aerospace Engineering
University of Michigan, Ann Arbor
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

RANS solver

\[ u_{\text{mean}}^{n+1} = g_{\text{mean}}(u_{\text{mean}}^{n}, x, R_{ij}^{n}) \]

Augmented Turbulence Model

\[ u_{\text{turb}}^{n+1} = g_{\text{turb}}(u_{\text{turb}}^{n}, u_{\text{mean}}^{n}, x, \beta^{n}) \]

\[ \eta(u_{\text{mean}}^{n}, u_{\text{turb}}^{n}) \]

Augmentation function

\[ \beta(\eta(u_{\text{mean}}^{n}, u_{\text{turb}}^{n}); w) \]

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

How can the parameters \( w \) be determined?  

MACHINE LEARNING!!
Augmentation – Implementation

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

\[ w = \arg \min_{w_m} \| \beta(\eta(u_{\text{data}}); w_m) - \beta_{\text{data}} \|_2^2 \]

Supervised Learning

\[ R(u, \beta(\eta(u); w)) = 0 \]

Model Augmentation

• Inconsistent because learning does not go through the model
  • Learning and injection environment can be very different
  • Only works when \( u = u_{\text{data}} \)
• Requires full fields of \( u_{\text{data}}, \beta_{\text{data}} \)
• Assume the available higher-fidelity data, $d$, consists of a few measured flow quantities and let the RANS predictions for the same quantities be $h(u)$

• Assume that the optimal values of the augmentation function are given as $\beta_k$, such that after solving the augmented model $R(u_k, \beta_k) = 0$ the prediction $h(u_k)$ matches the higher-fidelity data $d$ as closely as possible.

\[ w = \arg\min_{w_m} \| \beta(\eta(u_k); w_m) - \beta_k \|_2^2 \]

\[ R(u, \beta(\eta(u); w)) = 0 \]

How to determine $\beta_k$?
• 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
Field Inversion as an optimization problem

\[ \beta_k = \arg \min_{\beta_j} \mathcal{J}(u_j, \beta_j) \]

Subject to

\[ R(u_j, \beta_j) = 0 \]

Bayesian Objective Function

\[ \mathcal{J}(u_j, \beta_j) = \frac{1}{2} \left((d - h(u_j))^T C_m^{-1} (d - h(u_j))) + ((\beta_j - p)^T C_p^{-1} (\beta_j - p) \right) \]

Deterministic Objective Function

\[ \mathcal{J}(u_j, \beta_j) = \frac{1}{2} \|d - h(u_j)\|^2 + \lambda \|\beta_j - p\|^2 \]
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
Field Inversion and Machine Learning

- Consistency between learning and injection environments
- Does not require full fields of $u_{data}$ and $\beta_{data}$

**Field Inversion**

$$\mathcal{J}(u_j, \beta_j) = \frac{1}{2} \| d - h(u_j) \|_2^2 + \lambda \| \beta_j - p \|_2^2$$

$$\beta_k = \arg \min_{\beta_j} \mathcal{J}(u_j, \beta_j) \quad \text{s.t.} \quad \mathcal{R}(u_j, \beta_j) = 0$$

**Supervised Learning**

$$w = \arg \min_{w_m} \| \beta(\eta(u_k); w_m) - \beta_k \|_2^2$$

**Model Augmentation**

$$\mathcal{R}(u, \beta(\eta(u); w)) = 0$$
Field Inversion and Machine Learning

**Inverse Problem 1**
Given high-fidelity data $d^1$ solve Field Inversion
(Get $\beta_k^1$ and $\eta(u_k^1)$)

**Inverse Problem 2**
Given high-fidelity data $d^2$ solve Field Inversion
(Get $\beta_k^2$ and $\eta(u_k^2)$)

**Inverse Problem n**
Given high-fidelity data $d^n$ solve Field Inversion
(Get $\beta_k^n$ and $\eta(u_k^n)$)

**Machine Learning**
Given $\{\beta_k^1, \beta_k^2, \ldots, \beta_k^n\}$ and $\{\eta(u_k^1), \eta(u_k^2), \ldots, \eta(u_k^n)\}$
optimize for $\mathbf{w}$

**Augmentation**
Given $\mathbf{w}$ augment the RANS equations with
$\beta(\eta(u); \mathbf{w})$
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
Spalart-Allmaras Turbulence Model

Basic Version

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

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

Calibration

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

Spalart P. R., Allmaras S. R., A one-equation turbulence model for aerodynamic flows, 30th Aerospace Sciences Meeting and Exhibit
Spalart-Allmaras Turbulence Model

Wall-bounded version for High Reynolds Numbers

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

- \(c_{w1}\) 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 \(c_{w2}, c_{w3}, r = \nu_t/S\kappa^2 d^2\)
  \[f_w = g \left( \frac{1 + c_{w3}^6}{g^6 + c_{w3}^6} \right)^{1/6} \quad g = r + c_{w2}(r^6 - r)\]

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

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

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

\[
\chi = \frac{\tilde{\nu}}{\nu} \quad f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3} \quad \nu_t = \tilde{\nu} f_{v1} \quad f_{v2} = 1 - \frac{\chi}{1 + f_{v1}\chi} \quad \tilde{\Omega} = \Omega + \frac{\tilde{\nu}}{\kappa^2 d^3} f_{v2}
\]
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
Physics-Constrained Augmentation – SA model

**Objective:** Change the diffusive characteristics of the model

**Change intended in: \( \sigma \)**

- 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.
**Objective:** Change the behavior of the model in outer layer

**Change intended in:** $f_w$

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

$$g = r + c_{w2}(r^6 - r)$$

$$r = \frac{\tilde{v}}{\Omega k^2 d^2}$$

- $r = 1$ in the log layer

- **Option 1:** 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 $g$.

- **Option 2:** 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 $\tilde{v}$ and $\Omega$, we can make the augmentation $\beta$ a function of $v/(\Omega k^2 d^2 + v)$ and $v/(\tilde{v} + v)$ to ensure that the features are bounded and non-dimensional.
Objective: Change the behavior of the model in buffer layer

Change intended in: $f_{v1}$

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

• **Option 1:** Augment $\chi$ such that $\chi^{new} = \beta \chi$. Here the dampening model-form is left untouched.

• **Option 2:** Augment $f_{v1}$ such that $f_{v1}^{new} = \beta f_{v1}$. Here the model-form for dampening is changed too.

• Since $\chi$ 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 $\nu/(\nu_t + \nu)$
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
Results for Channel Flow

Velocity gradient profile (Re=395)

Velocity gradient profile (Re=550)

Velocity gradient profile (Re=950)

Velocity gradient profile (Re=2000)

Velocity gradient profile (Re=4200)

Velocity gradient profile (Re=5200)
Results for Channel Flow

Reynolds stress profile (Re=395)

Reynolds stress profile (Re=550)

Reynolds stress profile (Re=950)

Reynolds stress profile (Re=2000)

Reynolds stress profile (Re=4200)

Reynolds stress profile (Re=5200)
Results for Channel Flow

Field Inversion ($Re = 950.0$, $\lambda = 0.1$)

Velocity Profile ($Re_\tau=950$)

$J = \|u^+ - u^+_{DNS}\|^2_2 + \lambda \|\beta - 1\|^2_2$
Results for Channel Flow

Velocity gradient profile ($Re_y=950$)

- DNS
- Baseline
- Inverse

Reynolds stress profile ($Re_y=950$)

- DNS
- Baseline
- Inverse
Learnable augmentation for higher Reynolds numbers!!

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

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

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

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

$$c(\eta) = 0.1 \exp(1.3 - 6.5\eta)$$
Results for Channel Flow
Results for Channel Flow

Reynolds stress profile (Re=395)

Reynolds stress profile (Re=550)

Reynolds stress profile (Re=950)

Reynolds stress profile (Re=2000)

Reynolds stress profile (Re=4200)

Reynolds stress profile (Re=5200)
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
Prediction Improvements - Airfoils

Spalart-Allmaras turbulence model:

\[
\frac{D \tilde{\nu}}{Dt} = \beta(\eta) c_{b1} \tilde{\nu} \hat{\Omega} + \frac{1}{\sigma} (\nabla \cdot ((\tilde{\nu} + \nu) \nabla \tilde{\nu}) + c_{b2} (\nabla \tilde{\nu})^2) - c_{w1} f_w \frac{\tilde{\nu}^2}{d^2}
\]

Boussinesq Approximation:

\[
-\rho \bar{u}_i \bar{u}_j = 2 \mu_t \bar{S}_{ij} \quad \mu_t = \rho \tilde{\nu} f_{v1}
\]

Momentum Equation (RANS):

\[
\rho \frac{\partial \bar{u}_i}{\partial t} + \rho \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = \rho \bar{f}_i + \frac{\partial}{\partial x_j} \left[ -p + 2 \mu \bar{S}_{ij} - \rho \bar{u}_i \bar{u}_j \right]
\]

Features(\eta) : \{\hat{\Omega}, \chi, S/\Omega, \tau/\tau_{wall}, P/D, f_d\}

Datasets used for training:

- S814, \( Re = 1 \times 10^6 \)
- S814, \( Re = 2 \times 10^6 \)
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

Prediction Improvements - Airfoils

Portability: Implementation in AcuSolve

In more complex problems, however, ...

What is inferred is not necessarily learnable
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
Coupled Field Inversion and Machine Learning (FIML-CT)

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

\[ \mathcal{J}(u_j, w_j) = \frac{1}{2} \| d - h(u_j) \|^2 + \lambda \| \beta(\eta(u_j); w_j) - p \|^2 \]

\[ w = \arg \min_{w_j} \mathcal{J}(u_j, w_j) \quad s.t. \quad \mathcal{R}(u_j, \beta(\eta(u_j); w_j)) = 0 \]

Model Augmentation

\[ \mathcal{R}(u, \beta(\eta(u); w)) = 0 \]
Coupled Field Inversion and Machine Learning (FIML-CT)

Inverse Problem 1
Given high-fidelity data $d^1_j$ and function parameters $w^1_j$
calculate the sensitivity $dJ^1/dw^1_j$

Inverse Problem 2
Given high-fidelity data $d^2_j$ and function parameters $w^2_j$
calculate the sensitivity $dJ^2/dw^2_j$

Inverse Problem n
Given high-fidelity data $d^n_j$ and function parameters $w^n_j$
calculate the sensitivity $dJ^n/dw^n_j$

Machine Learning
Send current $w$ as $w^j_j$ to individual inverse problems whenever required
Receive $dJ^j/dw^j_j$ and update $w$ as required

Augmentation
Given $w$
augment the RANS equations with $\beta(\eta(u); w)$

In collaboration with J. Holland (University of Maryland)
Learnable inverse, but convergence is slow

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

In collaboration with J. Holland (University of Maryland)
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
Coupled Field Inversion and Machine Learning (FIML-CL)

Loosely coupled Inference and Learning

\[ J(u_j, w_j; \beta_j) = \frac{1}{2} \| d - h(u_j) \|_2^2 + \lambda \| \beta(\eta(u_j); w_j) - p \|_2^2 \]

\[ \beta_k = \arg\min_{\beta_j} J(u_j, w_j; \beta_j) \quad \text{s.t.} \quad R(u_j, \beta(\eta(u_j); w_j)) = 0, \quad w_j = \arg\min_{w_j,m} \| \beta(\eta(u_j); w_{j,m}) - \beta_j \|_2^2 \]

Incremental update from inference

\[ \beta_{j+1} = \beta(\eta(u_j); w_j) + s \cdot \left[ \frac{dJ}{d\beta'} \right]_{\beta' = \beta(\eta(u_j); w_j)} \]

Extract learnable information from inferred field

Model Augmentation

\[ R(u, \beta(\eta(u); w_k)) = 0 \]

- Consistency between learning and injection environments
- Does not require full fields of \( u_{data} \) and \( \beta_{data} \)
- Inference not exposed to NN convergence issues

In collaboration with J. Holland (University of Maryland)
Coupled Field Inversion and Machine Learning (FIML-CL)

In collaboration with J. Holland (University of Maryland)
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
Acknowledgements

Thanks to

• Dr. Philippe Spalart, Dr. Christopher Rumsey, Dr. Gary Coleman, Dr. Ponnampalam Balakumar and Dr. Jonathan Holland for their valuable insights, inputs and suggestions

• The Office of Naval Research for funding this project
THANK YOU!