Uncertainty Quantification For Turbulent Flows with Machine Learning

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Abstract

Turbulent flows are of central importance across applications in science and engineering problems. For design and analysis, scientists and engineers use Computational Fluid Dynamics (CFD) simulations using turbulence models. Turbulent models are limited approximations, introducing epistemic uncertainty in CFD results. For reliable design and analysis, we require quantification of these uncertainties. The Eigenspace Perturbation Method (EPM) is the preeminent physics based approach for turbulence model UQ, but often leads to overly conservative uncertainty bounds. In this study, we use Machine Learning (ML) models to moderate the EPM perturbations and introduce our physics constrained machine learning framework for turbulence model UQ. We test this framework in multiple problems to show that it leads to improved calibration of the uncertainty estimates.

1 Overview

Turbulent fluid flows are of central importance across problems in Science and Engineering. For example, the design of transcatheter aortic valves (TAV) focuses on minimizing turbulence in the blood flow for patient safety[1]. The design of automobiles aims to reduce turbulence in the automobile wake to save energy[2]. Such design studies use Computational Fluid Dynamics (CFD) simulations with turbulence models to account for the effects of turbulence. Turbulence models are simple constitutive equations that relate the effects of turbulence to measurable variables. This simplification is an advantage for computational expense, but also leads to severe limitation in the turbulence physics that these models can replicate. This limitation leads to epistemic uncertainty in CFD predictions, which can have hazardous ramifications on engineering designs. Estimating these uncertainties is essential for reliable design[3–6]. The only physics based approach to estimate turbulence model uncertainty is the Eigenspace Perturbation Method (EPM)[7]. This uses physics based perturbations in the turbulence model predictions to estimate predictive uncertainty. Studies of turbulence model Uncertainty Quantification (UQ) are mainly focused on the EPM based eigenvalue and eigenvector perturbations, such as turbulent flow through scramjets [8], aircraft nozzle jets [9], over steamlined bodies [10], in aeronautical engines[11, 12], supersonic axisymmetric submerged jet [13], canonical cases of turbulent flows over a backward-facing step [7, 14], and benchmark cases of complex turbulent flow [15]. Its theoretical foundations are well established[16] and the EPM's software implementations are widely used[17]. Despite its success, the EPM has limitations. Primarily, the EPM weighs all physically permissible events equally, leading to uncalibrated and conservative prediction intervals. This leads to overly safe and inefficient designs. If we can weigh all physically permissible events by their likelihood, we can improve the calibration of the uncertainty bounds. In this study, we augment the EPM framework with Machine Learning models to infer the strength of the perturbations for better calibration of uncertainty bounds.

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2 Methods & Methodology

In this study, we use the turbulence model of Langtry and Menter [18] to simulate turbulent flow over an SD7003 airfoil at 8° angle of attack (AoA). With the Reynolds number based on the cord length of $Re_c = 60000$, the flow underwent transition to turbulence on the suction side of the airfoil. Hereon, the turbulence model predictions for this airfoil case are referred to as RANS (Reynolds Averaged Navier Stokes) and the true targets as DNS (Direct Numerical Simulation). Such turbulent flows are characterised by random fluctuations in the velocity and pressure fields, where the instantaneous velocity can be decomposed into a mean and fluctuating component, $u = U_{mean} + u_{fluctuation}$. The key quantity of interest for design is the covariance of this fluctuating velocity referred to as the Reynolds Stress Tensor, $\langle u_i u_j \rangle$, that encompasses the effect of turbulence on the flow. The trace of the Reynolds Stress Tensor is referred to as the turbulence kinetic energy, k. In the EPM[7], the perturbed Reynolds stresses are defined as

$$\langle u_i u_j \rangle^* = 2k^* \left(\frac{1}{3}\delta_{ij} + v^*_{in}\hat{b}^*_{nl}v^*_{jl} \right), \tag{1}$$

where k^* is the perturbed turbulence kinetic energy, $\hat{b}^*_{kl}$ is the perturbed eigenvalue matrix for the Reynolds Stress Tensor, v^*_{ij} is perturbed eigenvector matrix, and δ_{ij} is the kronecker delta. In this study the perturbed turbulence kinetic energy can be defined as

$$k^* = k + \Delta_k = M_k, \quad M_k \sim f(x, y), \tag{2}$$

where M_k is a marker function of the x and y coordinate in a computational domain. This marker function predicts the magnitude of the perturbation to be used to modulate EPM perturbations.

In this study, we examined polynomial regression to construct this marker function augmented with eigenvalue perturbations to estimate the uncertainty bound for the predicted skin friction coefficient. We also train a convolutional neural network (CNN) to predict high-fidelity turbulence kinetic energy. Here, we use a one-dimensional convolutional neural network to learn the projection from the functional mapping estimated by the turbulence model $f^{\mathrm{RANS}}(x, y)$ to the true mapping $f^{\mathrm{DNS}}(x, y)$. For a given x, we can rewrite the estimated function as $g_x(k, y)$. Assuming that there exists a morphism F from $g^{\mathrm{RANS}}_x(k, y)$ to $g^{\mathrm{DNS}}_x(k, y)$, every x and $g_x(k, y)$ is smooth. Our CNN is trained to depict F so as to project $g^{\mathrm{RANS}}_x(k, y)$ to $g^{\mathrm{DNS}}_x(k, y)$. This is conducted by training the paired RANS- and DNS-estimated functions at the selected x coordinates. Taking advantage of the smoothness assumption of $g_x(k, y)$, our 1D-CNN is trained to predict DNS estimated function at (x, y_{target}) given a series of RANS estimated function at (x, y_i), where $y_i \in [y - \epsilon, y + \epsilon], \epsilon > 0$ belongs to the neighbor of y_{target}. Our 1D-CNN has four-layers and in total 86 parameters: a single model for all zones at any x to project RANS to DNS. We trained our 1D-CNN with normalized pairs of $\left(g^{\mathrm{RANS}}_x(k, y), g^{\mathrm{DNS}}_x(k, y)\right)$ at only three positions $x = 0.4, 0.56, 0.58$ with mean squared error as the loss function and a 80%–20% split as training–testing dataset. We validated our trained 1D-CNN by comparing the L1 loss of RANS, denoted as $L^1_c(\mathtt{rans}) = |CF^{\mathrm{RANS}}_k - CF^{\mathrm{DNS}}_k|$ with the L1 loss of 1D-CNN projected RANS, denoted as $L^1_c(\mathtt{pred}) = |CF^{\mathrm{CNN}}_k - CF^{\mathrm{DNS}}_k|$.

3 Results

In Figures 2 (a) - (c), the mean of the polynomial regression-based normalized turbulence kinetic energy profile as the representative for each zone shows the discrepancy between RANS and DNS. Note that all profiles are shifted down to the origin of y/c, denoted $y/\left.c\right|_o$. The corresponding marker for each zone is shown in Figs. 2 (d) - (f). Marker functions can be constructed by fitting appropriate models to the discrepancy data for each zone, i.e., a seventh-order polynomial for the ab and ef zone, and a Fourier series for the cd zone. Augmenting the EPM eigenvalue perturbation [1] with the marker function ($1c\_M_k$, $2c\_M_k$ and $3c\_M_k$) using Eqs. 1 and 2, the estimated model-form uncertainty (red envelope) for the predicted skin friction coefficient is constructed and shown in Fig. 3. The $1c$ and $3c$ eigenvalue perturbations are included for reference. It is clear that the uncertainty bound successfully encompasses the ILES/LES data of [19] and [20] for $0.25 < x/c < 0.45$. This region falls into the cd and part of the ef zone, where the separation bubble is forming and the flow is re-attaching on the wall surface. In comparison to the eigenvalue perturbations, the red envelop

[1] The strength of eigenvalue perturbation is denoted Δ_B, which varies from 0 to 1.

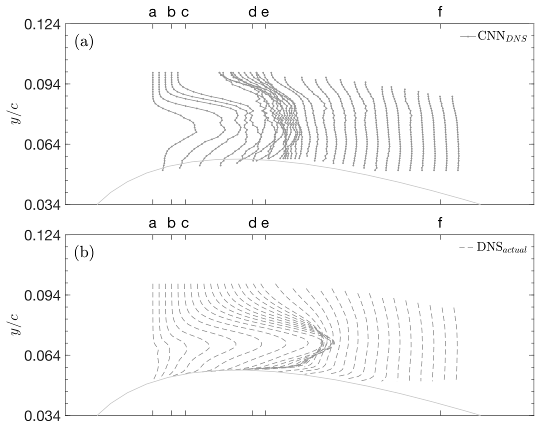

Figure 1: CNN projected DNS (`CNN_DNS`) compared with ground truth (`DNS_actual`). There are 32 positions on the suction side of the airfoil.

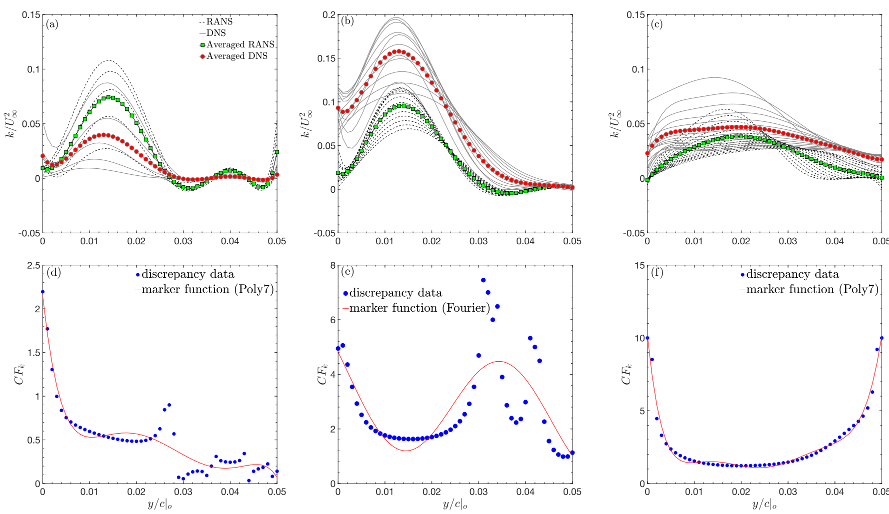

Figure 2: Mean of 7^{th} order polynomials for normalized turbulence kinetic energy (a) - (c), and the corresponding marker function (d) - (f). (a) and (d) zone ab; (b) and (e) zone cd; (c) and (f) zone ef.

exhibits a significant increase in the magnitude of C_f, exhibiting a tendency to retain the shape of the reference data. This marks a significant improvement in the RANS model prediction for C_f. The shape of the red envelope is not as smooth as the eigenvalue perturbations, reflecting the effect of spatial variability in M_k. The 1D-CNN can predict DNS at any zone given RANS, thus acting as the marker function M_k in Eq. 2. From Figs. 1 (a) and (b), the CNN predicted DNS profile for k exhibits agreement with the DNS dataset. In Fig. 4, the series of CNN predicted DNS profiles in the first row are then smoothed with the moving average with a window size of six consecutive estimations. Our CNN predicted DNS profiles resemble the ground truth DNS despite being trained with only a few pairs of RANS and DNS results. From Fig. 4, the discrepancy in general reduces as the flow proceeds further downstream. Consequently, the CNN predicted DNS given the RANS estimated function acts as the marker function M_k in Eq. 2. From the Fig. 4, the second row shows the computed error of the baseline solution and the CNN predicted DNS, and it is clear that the error for CNN predicted DNS is significantly reduced in magnitude compared to that for the baseline solution.

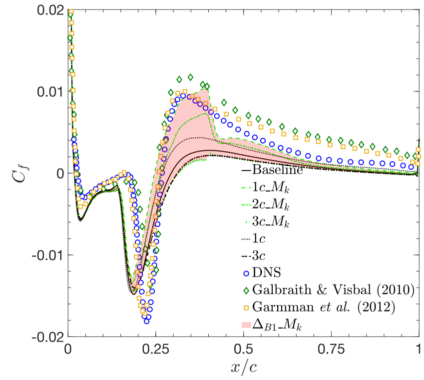

Figure 3: Skin friction coefficient. Displayed are uncertainty bounds for $1c\_M_k$, $2c\_M_k$ and $3c\_M_k$ perturbations (red envelope). Δ_{B1} stands for $\Delta_B = 1$. Profile of the baseline prediction and eigenvalue perturbations ($1c$ and $3c$) are provided for reference.

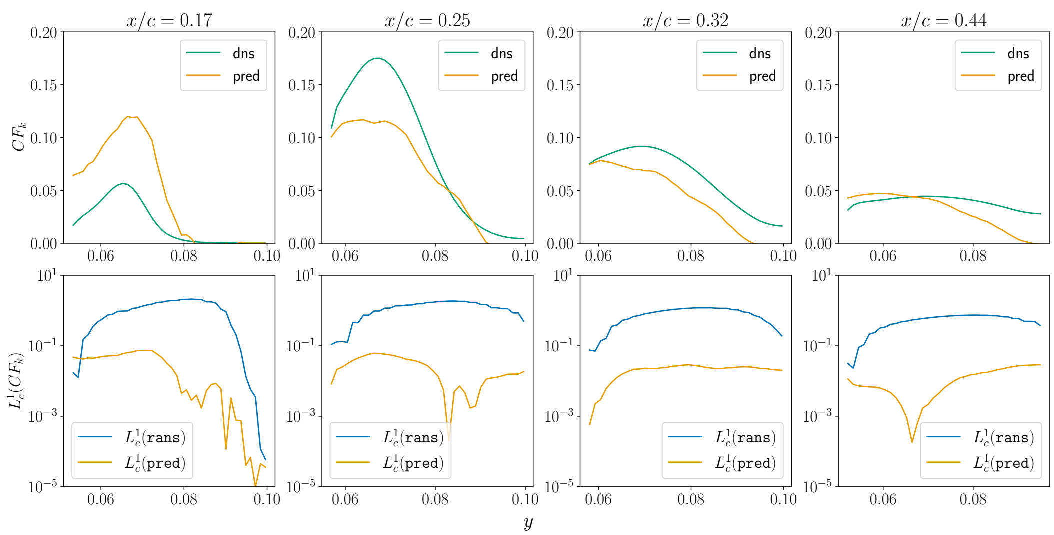

Figure 4: First row: CNN projected DNS (`pred`) compared with ground truth (`dns`). Second row: Validation of 1D-CNN by comparing L1 loss between $L_c^1(\texttt{rans})$ and $L_c^1(\texttt{pred})$.

4 Conclusions

We investigated if ML models, specifically polynomial regression and CNNs, can augment the Eigenspace Perturbation Framework to give better calibration of uncertainty intervals. The learning algorithms need to be coupled to the EPM implemented in OpenFOAM[21] to construct a marker function for the turbulence kinetic energy perturbation. ML models capture the discrepancy in the predicted turbulence kinetic energy between RANS and DNS. Correspondingly, the marker function is augmented with the eigenvalue perturbation to significantly increase the uncertainty bound for C_f. Around the peak of the C_f curve, the uncertainty bound successfully encompassed separation bubble. While researchers have attempted to use ML models to augment the EPM[22–24], we are the first to examine the projection from RANS to DNS using the CNN approach. Our experiment results suggest that the CNN approach can help us project the RANS estimated marker function to DNS data. A projection that can approximate the DNS reasonably well from RANS might exist independent of x. Our methodology can be easily extended to analyze flows over different airfoils. Future work may include evaluating other machine learning models in generating marker functions with different types of airfoils, as well as integrating the CNN approach into the EPM.

5 Impact statement

Transitional flows are frequently encountered in aerospace and medical applications. While turbulence models have severe challenges in such flows, they are the only pragmatic recourse. Thus the estimation of turbulence model uncertainty is valuable for improving the usefulness of turbulence models in engineering applications. A recent physics-based eigenspace perturbation method evaluates the accuracy of turbulence models for practical usage based on physically possible perturbations, which is less reliable in terms of giving exact strength of perturbation. We propose a machine learning augmented eigenspace perturbation method that can effectively increase the precision of the estimates of turbulence model uncertainty and build confidence in engineering simulations. Our method is generalizable to a variety of flow scenarios. Our method can also be employed to shed lights on predicting errors in turbulence model predictions, enabling a correction to turbulence models to improve their accuracy.

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