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Bayesian Deep Learning for RANS Modeling with Uncertainty Quantification Applied to Wall-Mounted Obstacles

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SUMMARY:
In the present work, a deep Bayesian neural network is trained to predict the anisotropic contribution of the Reynolds stress tensor. The neural network is trained with the Stein Variational Gradient Descent algorithm to generate different tensor samples. The resulting uncertainty is propagated through a forward Monte Carlo RANS simulation. The training data are generated via Large-Eddy Simulation of flow past a wall-mounted cube at moderate/high Reynolds number $\mathrm{Re}_H = 10\,000$ and are assumed as ground-truth. The data-driven prediction based on the different samples enables major enhancement compared to a baseline RANS simulation as it closely matches the LES. In addition, probabilistic interval of confidence is also computed for quantities of interest such as the velocity. The uncertainty bounds takes into account model-form error but also epistemic-form error related to the finite size of the training dataset. The variance predicted by the model is in-line with prior physical expectations as the largest uncertainty occurs in the wake of the bluff-body, where the flow is highly turbulent and RANS is known to provide low-accurate predictions.

Keywords: RANS, Deep Learning, Uncertainty Quantification

1. INTRODUCTION

The use of Reynolds-Averaged Navier-Stokes (RANS) simulations is common in engineering to model complex flows due to its good trade-off between accuracy and computational cost. However, a turbulence models is required to close the RANS equations and the latter introduces uncertainty in the results. This uncertainty can limit the application of numerical simulations in decision making. To overcome this issue, several advanced RANS turbulence models have been successfully introduced for wall-mounted obstacles e.g. (Longo et al., 2017; Parente et al., 2011) for the $k-\varepsilon$ model and (Bellegoni et al., 2023) for $k-\omega$ SST.

Recently, the use of data-driven methods to model turbulence as emerged as a powerful tool due to the increase of computational resources. Data-driven RANS modeling uses machine learning techniques to accurately predict the Reynolds stress tensor. This approach can be used to improve the accuracy of RANS simulations, especially in complex flows where traditional RANS models may not perform well. Nevertheless, these approaches have mainly been limited to two-dimensional or low-Reynolds flows. Furthermore, the use of black-box models increases the need of uncertainty quantification. This uncertainty may be related directly to the turbulence model form itself, but also to the training data/method of the black-box framework. The objective of the present work is to develop a data-driven framework to reduce the model-form error in RANS simulation of flow past wall-mounted obstacles while providing uncertainty range for the corrected quantities of interest.

2. PROBLEM FORMULATION AND METHODOLOGY

The Reynolds stress tensor $\overline{\mathbf{u}'\mathbf{u}'}$ can be expressed as the sum of an isotropic contribution, depending on the turbulent kinetic energy (k), and an anisotropic tensor ($\mathbf{b}$):

$$\overline{\mathbf{u}'\mathbf{u}'} = \frac{2}{3}k\mathbf{I} + k\mathbf{b}. \tag{1}$$

The anisotropic tensor can be re-written as a linear combination of the five strain-rate and rotation invariants ($\Lambda_{1:5}$):

$$\mathbf{b}(\mathbf{s},\omega) = \sum_{n=1}^{n=10} C^{(n)}(\Lambda_{1:5})\mathbf{T}^{(n)} \quad \text{and} \quad \begin{cases} \Lambda_{1:5} &= \left[Tr(\mathbf{s}^2),\ Tr(\omega^2),\ Tr(\mathbf{s}^3),\ Tr(\omega^2\mathbf{s}),\ Tr(\omega^2\mathbf{s}^2)\right] \\ \mathbf{T}^{(n)} &= \left[\mathbf{s},\ \mathbf{s}\omega - \omega\mathbf{s},\ \mathbf{s}^2 - \frac{1}{3}\mathbf{I}Tr(\mathbf{s}^2),\ \omega^2 - \frac{1}{3}\mathbf{I}Tr(\omega^2),\ \cdots\right] \end{cases}, \tag{2}$$

with $\mathbf{s}$ the strain-rate tensor, ω the rotational tensor, $\mathbf{T}^{(n)}$ the symmetric tensors and $C^{(n)}$ are the coefficients of the linear model. For more information regarding their rigorous definitions, the reader is refereed to the original paper (Pope, 1975).

2.1. Data-Driven Methodology

In this work, we use the same invariant network architecture with a deep Bayesian neural network ($\mathcal{B}$) as a function approximator to predict the anisotropic tensor as introduced in (Geneva and Zabaras, 2019):

$$\mathbf{b} = \mathcal{B}\left([\mathbf{s},\omega],\mathbf{w}\right). \tag{3}$$

The model parameters are treated as random variables such that the weights $\mathbf{w}$ have a probability density function assumed to be fully-factorizable zero mean Gaussian with a learnable precision β that is Gamma distributed.

The network is trained with the Stein Variational Gradient Decent (SVGD) algorithm (Liu and Wang, 2016) that minimizes the Kullback-Leibler discrepancy between the true posterior $p(\mathbf{w},\beta|\mathcal{D})$ and the variational one $q(\mathbf{w}|\mathcal{D})$ in each batch of N i.i.d training data $\mathcal{D} = \mathbf{b}_{i=1}^{N}$:

$$\min_q \mathrm{KL}(q||p) \quad \text{where} \quad \mathrm{KL}(q||p) \equiv \mathbb{E}_q(\log q(\mathbf{w},\beta)) - \mathbb{E}_q(\log \tilde{p}(\mathbf{w},\beta|\mathcal{D})) + \mathcal{K} \tag{4}$$

with $\tilde{p}(\mathbf{w},\beta|\mathcal{D}))$ being the unormalized posterior and $\mathcal{K}$ the log normalization constant.

The SVGD algortihm approximates a variational distribution by training a set of S independent neural networks and therefore enables the sampling of the posterior $p(\mathbf{w}_i,\beta_i|\mathcal{D})$, with $i \in [0,S]$. If $\mathcal{R}(\mathbf{b},\mathbf{u}(\mathbf{b}))$ represents the RANS operator, the uncertainty quantification based on a Monte-Carlo RANS simulation can be obtained following:

$$\mathbb{E}_{p(\mathbf{w},\beta|\mathcal{D})} \approx \frac{1}{S}\sum_{i=0}^{S}\mathcal{R}(\mathbf{b}_i,\mathbf{u}_i) \quad \text{and} \quad \sigma_{p(\mathbf{w},\beta|\mathcal{D})} \approx \sqrt{\frac{1}{S-1}\sum_{i=0}^{S}\left[\mathcal{R}(\mathbf{b}_i,\mathbf{u}_i) - \mathbb{E}_{p(\mathbf{w},\beta|\mathcal{D})}\right]^2}. \tag{5}$$

2.2. Neural Network Architecture

The neural network architecture is composed of firstly 3 hidden layers of 200 neurons each and two tapered layers of 40 and 20 neurons at the end to prevent too small weights. The inputs of the network are the five invariants and the outputs are the ten coefficients of the symmetric tensors (see Eq. 2). A Leaky ReLU activation function is used between each layer. The ADAM optimizer is used to train the networks with a learning rate of 5×10^{-6}. The training data is composed of 10 000 sample points that are randomly re-sampled every 10 epochs, for a total of 100 training epochs. As the computational mesh is well-refined close to the wall-mounted obstacle, no specific probability density function is used to sample the training points. Finally, a mini-batch size of 20 is used and the SVGD algorithm is trained for 20 samples. The architecture is inspired by the work of (Geneva and Zabaras, 2019).

3. RESULTS AND DISCUSSION

The predictive capabilities of the data-driven model are investigated for the flow past a wall-mounted cube at $\mathrm{Re}_H = 10\,000$, where H is the height of the cube. The computational domain size is $14H \times 7H \times 3H$ where H is the cube height. The latter is discretized with $180 \times 130 \times 90$ cells for both RANS and LES.

Fig.1 shows a comparison between mean stream-wise velocity components obtained with a baseline RANS (blue), a LES (purple), the different samples generated via the SVGD algorithm (light gray) with their associated means (orange) and two standard deviation uncertainty ranges (shaded orange). A noticeable improvement is made with the Bayesian Neural Network RANS (BNN-RANS) for both the bulk region and the recirculation zone. Particularly, the predictions of the BNN-RANS in the wake for $x/H < 6$ are superimposed with the LES while the baseline RANS fails to catch the highly turbulent physics. Regarding the far-wake locations, $x/H > 6$, there are small discrepancies between the BNN-RANS and the LES while providing a higher accuracy than the baseline RANS. Those discrepancies occur for $z/H < 1$ where the flow is expected to be highly turbulent.

As far as the uncertainty is concerned, the standard deviation in the velocity samples is only noticeable in the recirculation zone, which is promising. Particularly, the range of uncertainty grows with x/H, where the discrepancies between the baseline RANS and the LES are the largest. Nevertheless, it is worth mentioning that usual uncertainty intervals are represented by the variance rather than two-times the standard deviation. The present choice is made on purpose for the sake of visibility. If the uncertainty range had been represented with a two variance width, it would not have been perceptible. This observation confirms that the methodology is robust even for moderate/high Reynolds.

4. CONCLUSIONS AND FUTURE WORK

This study introduces a Bayesian Deep Learning framework that enables data-driven turbulence model with uncertainty quantification for wall-mounted obstacles. The preliminary results indicate that the suggested approach may be suitable for high Reynolds flows with adverse pressure gradient. Particularly, significant improvements have been made regarding the mean stream-wise velocity component compared to a LES. Besides reducing the model-form error of the baseline

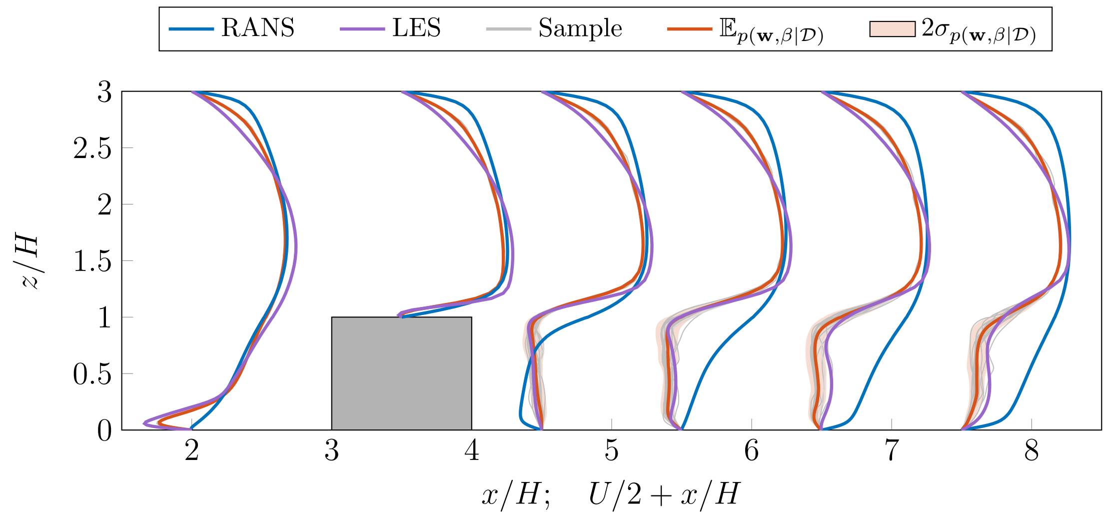

Figure 1. Normalized mean stream-wise velocity component at six different normalized *x*-locations on the plane of symmetry for different turbulence models: baseline RANS, LES, BNN-Samples, BNN-RANS and its uncertainty bounds. The reader is refereed to Eq. (5) for the notation signification.

RANS model, the network enables the quantification of epistemic uncertainty regarding the training data and training method as well. The predicted range of uncertainty is in-line with physical expectations, as the largest variance in the velocity occur in the wake, where the flow is highly turbulent.

In ongoing work, we are performing this analysis for additional Reynolds numbers and different geometries. The final aim would be to obtain a data-driven model that generalizes well for different urban-like configurations.

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