UQFoam: A Computational Library for MultiPhysics Uncertainty Quantification

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Design methodologies that explicitly account for uncertainties are becoming commonplace in engineering. A key source of uncertainty in turbulence simulations arises due to the model form uncertainty of Reynolds Averaged Navier Stokes models. Accounting for the turbulence model form uncertainty has been described by NASA as the “greatest challenge” in simulation based design in aerospace applications. In spite of its importance, OpenFoam does not have an extant module for such turbulence model uncertainty estimation.

In this article, we outline UQFoam, a computation library for OpenFoam that enables the user to estimate the uncertainty in complex turbulence flows, extending from simple shear turbulent flows, buoyancy driven turbulent flows and variable-density turbulence. To this end, the library includes UQ enabled versions of popular turbulence models like k-epsilon, k-omega, along with advanced closures such as the BHR (Besnard-Harlow-Rauenzahn) variable density turbulence model.. We outline the methodology utilized to obtain these interval estimates on the Quantities of Interest. The performance of this library is presented for a range of test cases.

Section I. Introduction

The flow of fluids represents the driving physics in a multitude of occurrences all round us. These range from flows over aircraft and inside turbomachinery, atmospheric flows for weather prediction and through the heart for cardiac auscultation, from biological cases such as the flow of plasma inside a cell to galactic instances such as the Giant Red Spot over Jupiter. In this context, most flows of engineering interest are turbulent. As stated in Moin and Kim (1997) [1] “turbulence is the rule, not the exception in fluid dynamics".

Turbulent flows exhibit chaotic behavior in space and time; lead to increased mixing and high rates of momentum, heat and mass transfer; and a spectrum of interacting scales of motion. Turbulence represents a central problem in diverse and manifold disciplines such as engineering, biomedical sciences, astrophysics, mathematics, geophysics, etc. A thorough understanding of the properties of turbulence is expected to lead to important advances in all these fields. For instance, the turbulent flow of blood in the human heart causes sclerosis leading to cardiovascular complications such as strokes and heart attacks. A resolution of the problem of turbulence would enable the Biomedical community to understand, treat and cure such disorders associated with malfunctioning heart valves. In Meteorology, improved prediction of turbulence occurring in the atmosphere and oceans would lead to superior forecasts of the weather and of climate change. In this vein, Richard Feynman had described turbulence as "the most important unsolved problem of classical physics".

Understanding and predicting the evolution of turbulent flows has remained an important avenue of research for well over a century. In spite of these efforts, there are no closed form theories explaining turbulence, or explicit analytical solutions predicting their evolution. In industrial applications, turbulent flows and their effects are accounted for using Computational Fluid Dynamics simulations, using turbulence models.

Turbulence models are constitutive relations attempting to relate unknown quantities of interest (including higher-order statistical moments that may be expensive to compute exactly) to local, low order flow statistics using simplifying assumptions. In this context, the goal of Reynolds-averaged Navier–Stokes closures is to determine the Reynolds stress tensor as a function of mean flow quantities that are directly computable. RANS models use the concept of an isotropic eddy viscosity along with the modeling of turbulence processes via the gradient diffusion hypothesis. Because of their simplicity and cost-effectiveness, simple RANS models such as linear two-equation $k-\epsilon$ or $k-\omega$ closures are widely used in industrial applications. However, in spite of their wide spread use, RANS-based models suffer from an inherent structural inability to replicate fundamental turbulence processes. Because of the simplifications invoked in model formulation, RANS models can only represent certain features of turbulence with limited fidelity. For instance, in turbulent flows with significant effects of mean rotation, such as swirl or strong streamline curvature, the fidelity of linear eddy-viscosity-based closures is often unsatisfactory [2-3]. Similarly, the performance of two-equation models is found to be erroneous for cases with noninertial frames of reference. In turbulent flows with flow separation and reattachment, eddy-viscosity-based models have had limited success [4]. For instance, in turbulent flows in ducts, isotropic eddy-viscosity-based models are not able to reproduce the secondary flows that develop near the corners of the domain [5].

To aid in the establishment of RANS simulations as reliable tools for the engineering design process, there is need for quantification of margins and uncertainties in such models. In the most rudimentary manifestation, explicit quantification of the uncertainty in model predictions is needed in the form of uncertainty interval estimates for the quantities of interest. While OpenFoam has validated and verified implementations for most turbulence models, there are no extant libraries available in OpenFoam for Uncertainty Quantification for these models.

This is exacerbated by the changes in the engineering design methodology over the past decade. With the advent of improved computational resources, engineering design has shifted from a testing-based process to a simulation-driven procedure, where uncertainties in design and operating conditions are explicitly accounted for. Methodologies like Robust Design, Reliability based design, etc have become commonplace, leading to the advent of the Design Under Uncertainty approach.

In light of these developments, there is urgent for a turbulence model uncertainty quantification library for OpenFoam. In this article, we outline UQFoam, an OpenFoam library that enables the user to estimate the turbulence model uncertainty in complex flows, from simple shear turbulent flows, buoyancy driven turbulent flows and variable-density turbulence. To this end, the library includes UQ enabled versions of popular turbulence models like k-epsilon, k-omega, along with advanced closures such as the BHR model. We outline the methodology utilized to obtain these interval estimates on the Quantities of Interest. The performance of this library is presented for a range of test cases.

With respect to the arrangement of the article, after a broad overview motivating the need for this research in Section I, we detail the mathematical nuances of the UQ procedure and its implementation in Section II. In Section III, we apply this turbulence model uncertainty quantification library to a range of complex turbulent flows and discuss its performance. We conclude with a summary of important results in Section IV.

Section II. Methodology of eigenspace perturbation

The Reynolds stress tensor R_{ij} for incompressible flow and compressible or variable density flow are defined as

$$R_{ij} = \langle u_i^{'} u_j^{'} \rangle \text{ and } R_{ij} = \langle u_i^{"} u_j^{"} \rangle$$

respectively, which are obtained by Reynolds decomposition $u_i = \overline{u}_i + u_i^{'}$ and Favre decomposition $u_i = u_i + u_i^{"}$ respectively. The turbulence models based on eddy-viscosity hypothesis approximate the Reynolds stress by the product of the mean rate-of-strain and the eddy-viscosity, taking variable density flow as example:

$$R_{ij} = \frac{2}{3}\overline{\rho} k \delta_{ij} - \overline{\rho} \nu_t 2 S_{ij}$$

where $S_{ij} = \frac{1}{2}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)$ for incompressible flow and $S_{ij} = \frac{1}{2}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right)$ for compressible or variable density flow; k is the turbulence kinetic energy. As we know, the right two parts in above equation are calculated separately in OpenFOAM turbulence models. Using the eigenvalue decomposition, the Reynolds stress tensor can be decomposed as

$$R_{ij} = 2\overline{\rho}k\left(\frac{1}{3}\delta_{ij} + \upsilon_{in}\Lambda_{nl}\upsilon_{jl}\right)$$

Where υ represents the eigenvector matrix, and Λ is the diagonal matrix of eigenvalues of the Reynolds stress tensor. The tensors υ and Λ are ordered such that $\lambda 1 \geq \lambda 2 \geq \lambda 3$. The amplitude, the shape, and the orientation of the Reynolds stress are explicitly represented by k, λ_i and υ_{ij}, respectively. By perturbing the eigenvalues and eigenvectors into the modeled Reynolds stress, then

$$R_{ij}^{*} = 2\overline{\rho}k\left(\frac{1}{3}\delta_{ij} + \upsilon_{in}^{*}\Lambda_{nl}^{*}\upsilon_{jl}^{*}\right)$$

where* denotes the perturbated variables. The perturbations to the eigenvalues Λ correspond to varying the componentiality of the flow. There are three extreme states of Reynolds stress componentiality, we consider perturbation directions along the three vertices of the triangle: x1C; x2C, and x3C, representing the limiting states of turbulence anisotropy. The perturbations to the eigenvectors v correspond to varying the alignment of the Reynolds stress ellipsoid. In this work, we focus on the production term in turbulence kinetic energy equation. For the purposes of bounding all permissible dynamics, we seek the extremal values. Hence, the eigenspace perturbation has five distinct extremal states of the Reynolds stress tensor [6-9]. These correspond to three extremal states of the componentiality 1C; 2C; 3C and two extremal alignments of the Reynolds stress eigenvectors. More details can be found in the eigenspace perturbation framework [6-9]. Therefore, five RANS simulations need be conducted to bound the structural uncertainties of flow dynamics based on the eigenspace perturbations. It should be noted that the eigenspace perturbation framework can be applied to any RANS-based model. In this work, we estimated the structural uncertainties of k-epsilon and k-omega models, we also extend it to variable density turbulence flow modeled by BHR model.

From the above illustration of eigenspace perturbation, we can see that it can be implemented very easily in OpenFOAM turbulence models since the model calculate $\frac{2}{3}\overline{\rho}k\delta_{ij}$ and $\overline{\rho}\nu_t 2S_{ij}$ separately. Therefore, we first calculate the anisotropy tensor $\nu_t S_{ij}/k$, then decomposing it with eigenvalue and eigenvectors $\upsilon_{in}\Lambda_{nl}\upsilon_{jl}$, the perturbed anisotropy tensor is obtained by injecting the perturbation into eigenvalues and eigenvectors $\upsilon_{in}^{*}\Lambda_{nl}^{*}\upsilon_{jl}^{*}$, finally, the perturbed Reynolds stress tensor is implemented in turbulence models in OpenFoam. It should be noted that nothing was modified in OpenFOAM except the calculations of $\overline{\rho}\nu_t 2S_{ij}$, hence there is no limitation for the eigenspace perturbation.

Section III. Results

In this section, we considered three cases to test the UQFoam to quantify the structural uncertainties. We stat with the simple plane channel flow using k-epsilon model; followed by the subsonic jet flow from the NASA acoustic response nozzle with k-omega model; and the turbulent mixing flow is simulated using BHR model. The numerical results show that the UQFoam offers good performance and more reliable predictions for the various popular turbulence models.

A. Plane channel flow

Firstly, we considered the plane channel flow using k-epsilon model at $Re_\tau = 2003$ since the DNS results are available [10]. Since the flow is very simple and no separation, we just conducted the three extreme eigenvalue perturbation simulations in UQFoam. The mesh has $y+ \approx 0.1$ for the first cell, with 80 cells up to the symmetry line. Figure 1 shows the estimation of uncertainty in eigenvalue perturbations with the three extreme situations for mean velocity, comparing with the DNS data. The solid line shows the results of k-epsilon model, we can see that the k-epsilon model mismatches the DNS data, alternatively, overpredicted, as $y^+ > 30$, the uncertainty estimate of the three extreme eigenvalue simulations still covers the DNS data in the whole domain.

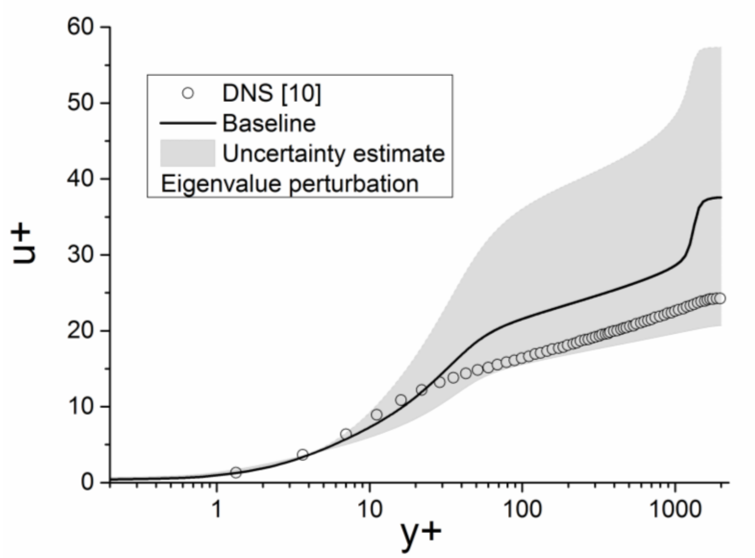


Fig. 1: Uncertainty estimates of the eigenvalue perturbations on mean velocity u^+ for k-epsilon model, comparing with DNS data of [10].

B. NASA Acoustic Response Nozzle

Reliable predictions of turbulent jets exhausting from contoured aircraft nozzles are essential for a variety of aerospace design applications. However, these exhaust jets involve a multitude of complications such as the interaction of the jet efflux and the ambient, complicated nozzle geometries, compressibility effects, under- or overexpanded flows, etc. These pose significant challenges to eddy-viscosity-based models. As an illustration, we may focus on the mixing between the jet and the ambient fluid. In the vicinity of the nozzle exit, RANS models predict a significantly lower rate of jet mixing as compared with high-fidelity data. Farther downstream of the jet potential core, RANS models predict the far-field mixing rate to become substantially higher than is observed in experiments. Similarly, the fidelity of RANS predictions is highly inconsistent, having higher fidelity for cold jets than heated, for axisymmetric than nonaxisymmetric geometries, varying significantly over different quantities of interest, etc.

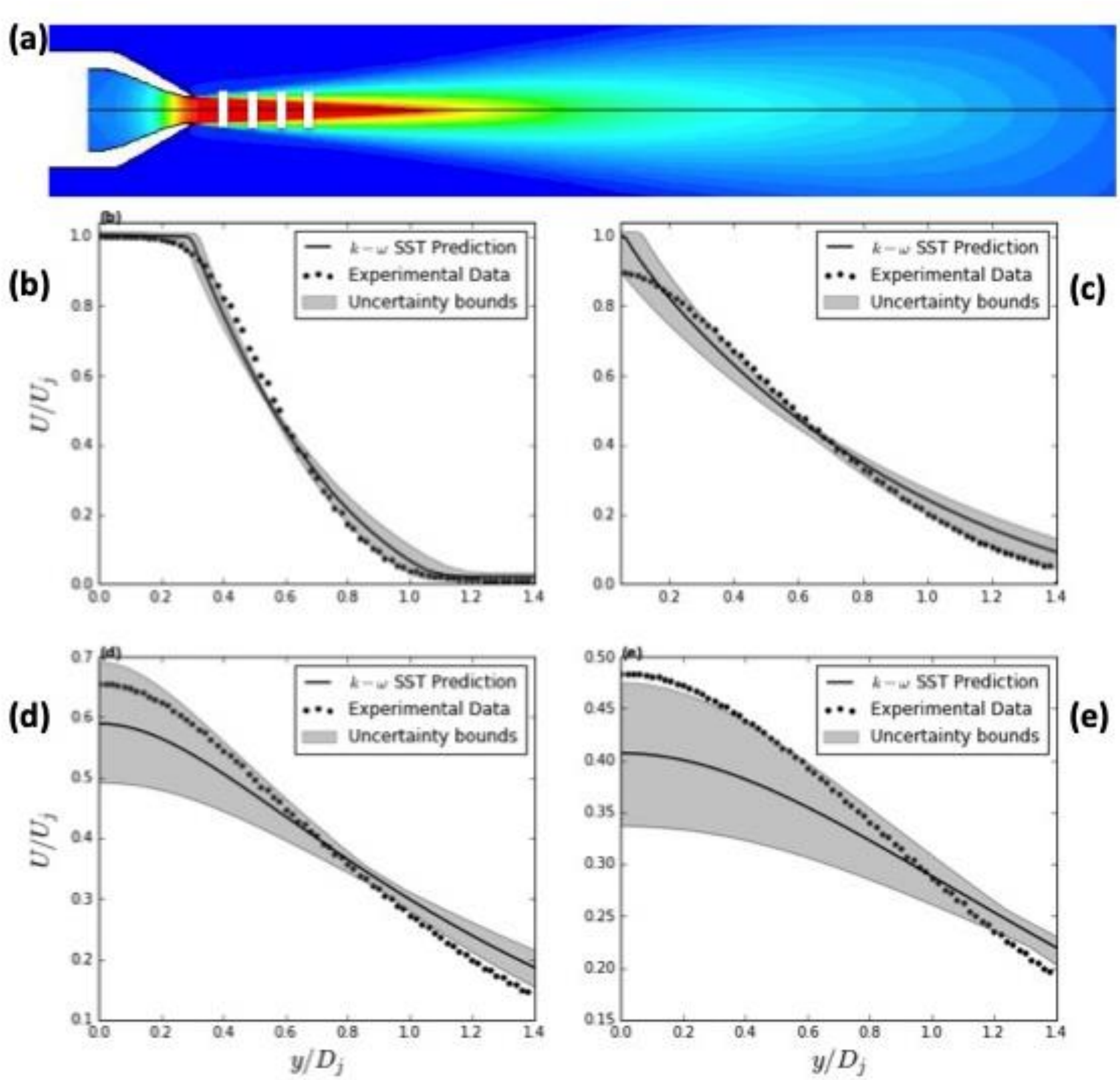


Figure2: Outlining the uncertainty estimates for the NASA ARN Jet. a) Mach number contours, outlining the locations of the mean velocity profiles with white dashes; b),c),d) and e) Outline the mean axial velocity profiles for the NASA ARN heated Jet at Ma=0.37, delineated at x/D=4,8,12, and16 respectively.

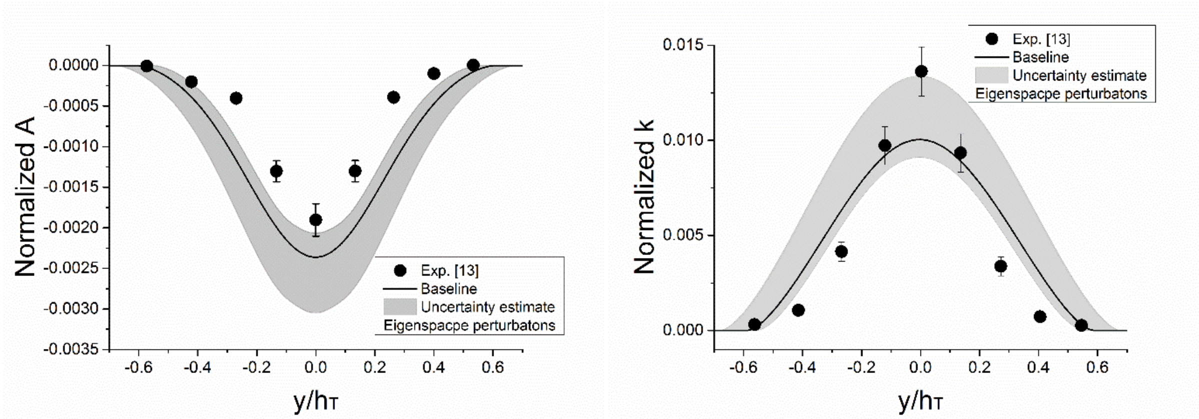
In this test case, we investigate subsonic jets from the NASA Acoustic Response Nozzle. This has been studied experimentally by [11], and extensive particle image velocimetry (PIV) data are available. The PIV data set was generated at the Small Hot Jet Acoustic Rig at NASA Glenn Research Center. The tests were repeated on numerous instances during 2001–2007 with varying PIV configurations. In addition to a robust mean, this corpus provides insight into the data uncertainty.

We outline Mean velocity profiles for the NASA ARN heated Jet at Ma=0.37, delineated at x/D=4,8,12, and 16 respectively. As can be seen, there is a large discrepancy between the experimental measurements (dark circles) and the baseline k-ω SST predictions. However, the uncertainty estimates (shown as grey shaded intervals) account for this discrepancy. Most of the experimental data lies inside the shaded uncertainty estimate regions. Furthermore, the breadth of the intervals mirrors the discrepancy of the turbulence model. Where the discrepancy between turbulence model and experimental data is large, the uncertainty estimates are large. Where the discrepancy between turbulence model and experimental data is small, the uncertainty estimates are correspondingly smaller. This suggests that the uncertainty estimation procedure is accounting for some of the missing physics in the model.

C. 1D Rayleigh-Taylor instability

The BHR *k-S-a* model was first tested for its ability to describe RT instability driven fluid mixing since the experimental data is available in [13]. In the experiment, two gas streams, one containing air and the other containing helium-air mixture, flow parallel to each other leading to the formation of an unstable interface and of buoyancy driven mixing. The numerical simulations were performed with normal gravity g = 9.81 m/s^2 and two fluids with constant densities of ρ_1=1083.3 kg/m^3 and ρ_2=1000 kg/m^3, that matched the experiment as the Atwood number At = 0.04 [12]. We developed the UQFoam for BHR model to simulate the turbulent mixing flow. The model constants are employed in [12], and the model results compared with the numerical and experimental data [12-13].

The normalized turbulence kinetic energy profiles $k{=}k/(At\ g\ t)^2$ at t = 3.5 across the mix are compared in Figure 3 (a). The figure shows that computed and experimentally measured profiles of *k* are approximately parabolic with a peak centered at the geometric centerline of the RT mixing layer. Similar parabolic profiles are observed for the plots of the normalized $a = a\ /(At\ g\ t)$ as seen in Fig. 3 (b). Figure 3 shows the estimation of uncertainty in eigenspace perturbations with the five extreme situations for turbulent mass flux velocity and turbulence kinetic energy. We can see that the uncertainty estimates from eigenspace perturbations are able to account for the discrepancy between model predictions and experimental data. It might be that the turbulent mixing flow is very simple in one dimensional case.



(a) (b)

Fig. 3: Uncertainty estimates of eigenspace perturbations on turbulent mass flux velocity (a) and turbulence kinetic energy (b), comparing with the experimental results of [13].

Section IV. Conclusion

In this work, we built the UQFoam to estimate the structural uncertainty in complex turbulence flows and obtained the interval estimates on the Quantities of Interest. The estimation is quantified by injecting uncertainty into the shape and the orientation of the Reynolds stress tensor in the turbulence model. The performance of the UQFoam has been tested by three cases.

Firstly, we obtained the uncertainty bounds for plane channel flow using k-epsilon model. Although the model overpredicts the flow near the channel center significantly, the structural uncertainty bounds cover the very high fedility DNS data. Second, we simulated the exhaust jet flow of the NASA acoustic response nozzle using k-ω SST model. There is a large discrepancy between the experimental measurements and the baseline k-ω SST predictions, the uncertainty estimates still account for this discrepancy. Lastly, the variable density turbulent mixing flow of Rayleigh-Taylor instability is simulated by the BHR model. The eigenspace perturbations are able to account for the discrepancy between model predictions and experimental data even for this complicated flow. The test cases show that the UQFoam can offer reliable predictions for various turbulence model.

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