Uncertainty Quantification of RANS Closure Models Using Model Error Transport

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In industry, Reynolds-Averaged Navier-Stokes (RANS) is still the standard for simulating turbulent flows in engineering applications [1]. This is due to the relatively cheap computational cost of RANS compared to Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS). However, RANS is still limited by the accuracy of its closure models. RANS closure models introduce multiple kinds of uncertainty, the most important of which are model form uncertainty and parametric uncertainty. In this work the focus will be on model form uncertainty, which arises due to assumptions made regarding physics, either in an effort to reduce the complexity (computational cost) of the physics being modeled or to model physical processes or phenomena that are not well understood. In many RANS models, model form uncertainty is one of the largest forms of uncertainty due to the nature of the physical assumptions made in the closure models.

Previously, the standard for quantifying uncertainty has been to treat the turbulent model variables as random variables and propagate this uncertainty through the model, ultimately obtaining a probability density function (PDF) for the quantity of interest (QoI). This method only captures the uncertainty associated with the parameters, giving the user the optimal value of the model parameters for the given flow. This means that the model form uncertainty is not quantified or it is embedded into the parameter uncertainty [2] so is not well understood in this formulation. More recently, research has addressed this issue and quantified the model form uncertainty using data-driven techniques. These data-driven techniques use high fidelity data from DNS or experiments to aid in closure of the turbulence model [1] [3] [4]. While many of these data-driven methods that address model form uncertainty are less physics-blind than the previously used parametric uncertainty frameworks, they still favor the use of data from experiments and simulations over understanding the physical assumptions in quantifying uncertainty. In this work the focus will be on more physics-based methods that consider the nature of the physical assumptions to quantify model error.

Much of the recent work quantifying model form uncertainty in RANS has been based on the work from the Iaccarino group [5] [6] [7]. Here, the anisotropic Reynolds stress tensor a_{ij} is decomposed into its eigenvalues and eigenvectors, and perturbations are then introduced into the eigenvalues in order to provide error bounds on the base RANS model. The decomposition of a_{ij} results in a direct representation of the magnitude, shape, and orientation of the Reynolds stresses via the turbulent kinetic energy, and eigenvectors and eigenvalues of the anisotropy tensor, respectively. In this way perturbations can be introduced into these three different aspects of the Reynolds stresses, and the uncertainty in the solution can be fully understood. In the framework for uncertainty estimation, they present three main steps: using a marker function the flow field is divided into regions where the model is trusted and regions where it is not. Then, perturbations are introduced into the regions where the model has been marked as untrustworthy, and finally these perturbations are propagated through to the QoIs. Much of the work in [5], [6], and [7] has focused on the injection of uncertainty through perturbations to the magnitude, shape, and orientation of the Reynolds stresses, which ultimately uses the limiting states of the realizable Reynolds stresses as error bounds and does not leverage the physical assumptions. Little attention has also been paid to the marker function that defines where the model deviates from the known flow physics. Some of the marker functions that have been proposed are distance from the wall in channel flow [7] and deviation from parallel shear flow in flow over a wavy wall [5]. These marker functions typically rely on expert knowledge of the flow, as with the example of using deviation from parallel shear flow in cases where separation is anticipated. In the present work, we derive marker functions that are agnostic to the target flow geometry. Building on previous work [8], we introduce a framework for marker functions that relies only on the model assumptions to characterize the model form uncertainty.

The framework for the marker functions is formulated as the transport of the model error. In RANS modeling, closure approximations are used to close the Reynolds stress term. In doing so, model error is introduced. The most basic formulation that represents this error considers the truth, given by $\mathcal{R}$, and a model with physical assumptions resulting in lower fidelity, given by $\mathcal{M}$. The model error e is then represented as

$$\mathcal{R} - \mathcal{M} = e \tag{1}$$

In this work the truth and the model are given by transport equations of physical quantities, which means that we can re-frame Eq. 1 as the transport of the model error given by

$$\frac{D\mathcal{R}}{Dt} - \frac{D\mathcal{M}}{Dt} = \frac{De}{Dt} \tag{2}$$

The significance of deriving a transport equation for the model error is that we can then use this transport equation to propagate the error during a numerical simulation in order to understand where the model is the worst and how the deviation of the model from the truth evolves spatially and temporally.

Presently, this framework has been applied to the Boussinesq assumption and the gradient diffusion hypothesis. For the Boussinesq assumption, we have a general framework given by

$$\mathcal{R} = \overline{u_i'u_j'}, \;\; \mathcal{M} = -2\nu_T S_{ij} + \frac{2}{3}k\delta_{ij} \qquad \frac{D\overline{u_i'u_j'}}{Dt} - \frac{D}{Dt}(-2\nu_T S_{ij} + \frac{2}{3}k\delta_{ij}) = \frac{De}{Dt}, \tag{3}$$

where the truth is the transport of the Reynolds stresses and the model is the transport of the Boussinesq assumption used to model the Reynolds stresses. In order to derive the full model error transport equation we subsequently plug in the model assumption plus the error for all Reynolds stress terms, which will yield an equation with terms that contribute the most to the error. In the final model error transport equation some closure is required due to the introduction of unclosed terms from the Reynolds stress transport equation.

Present work is focused on testing this framework on turbulent channel flow, which is known to produce errors near the channel walls in RANS simulations. Preliminary results have supported this knowledge and more testing will verify this for different two equation RANS models, such as $k - \epsilon$ and $k - \omega$. Additionally, other flow configurations will be tested to verify the validity of these models for a variety of flows and closure models.

Future work will look into benchmarking different methods for UQ and applying the current framework to multi-physics systems, which have multiple sources of model form uncertainty. Understanding the contribution of these sources will be important for application in model adaptive codes, where above some uncertainty threshold the model fidelity is increased. Ultimately, this will be important for increasing the efficiency of model-based computational physics simulations.

References

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