Bayesian calibration of a k-ε turbulence model for predictive jet-in-crossflow simulations

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We propose a Bayesian method to calibrate parameters of a RANS model to improve its predictive skill in jet-in-crossflow simulations. The method is based on the hypotheses that (1) informative parameters can be estimated from experiments of flow configurations that display the same, strongly vortical features of jet-in-crossflow interactions and (2) one can construct surrogates of RANS models for certain judiciously chosen RANS outputs which serve as calibration variables (alternatively, experimental observables). We estimate three k-ε parameters ($C\mu$, C_2, C_1) from Reynolds stress measurements from an incompressible flow-over-a-square-cylinder experiment. The k-ε parameters are estimated as a joint probability density function. Jet-in-crossflow simulations performed with ($C\mu$, C_2, C_1) samples drawn from this distribution are seen to provide far better predictions than those obtained with nominal parameter values. We also find a ($C\mu$, C_2, C_1) combination which provides < 15% error in a number of performance metrics; in contrast, the errors obtained with nominal parameter values may exceed 60%.

Nomenclature

$C\mu$	=	Constant in the expression for eddy viscosity in k-ε models
C_1, C_2	=	Constants in the equation for the evolution of ε
τ^{obs}	=	Experimental observations of Reynolds stress
τ^{m}	=	Surrogate model predictions of Reynolds stress, for a specified ($C\mu$, C_2, C_1)
η	=	Discrepancy between observed and modeled Reynolds stress
$\mathcal{N}(\mu, \sigma^2)$	=	A normal distribution with mean μ and variance σ^2

I. Introduction

K-ε models, due to their robustness and modest resolution demands, are routinely used in RANS modeling of aerodynamic flows. However, they are not particularly accurate in complex flow regimes e.g., separation bubbles and jets-in-crossflow. This lack of accuracy has two causes: (1) sub-optimal values of constants in the empirical models for the generation and dissipation of turbulent kinetic energy and (2) missing physics, due to model approximations inherent in the k-ε model itself. We describe a method by which the first shortcoming can be remedied. The method is demonstrated on a transonic 3D jet-in-crossflow (JIC) problem. JIC problems arise in vortex-fin interactions in finned aerodynamic bodies maneuvered by spin rockets[1].

In principle the sub-optimality of the turbulence model constants can be addressed by calibrating to relevant, realistic flow configurations. A crude estimate of structural/model error in the turbulence models, i.e. the "missing physics", represented as an additive error or multiplicative bias, can also be estimated during the calibration process. However, calibration with an expensive 3D RANS simulator is daunting and largely impractical outside of a few

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"hero" calculations. Also, a deterministic calibration procedure (e.g., based on gradient descent) is hindered by the existence of local minima, leading to a further increase in computational cost.

II. Technical Foundations

We seek to estimate 3 parameters, ($C\mu$, C_2, C_1), that appear in the expression for eddy viscosity and the production and dissipation of ε in k-ε models[2]. Our approach is based on two hypotheses:

1. *Proxy flow configurations:* Turbulence models for predictive JIC simulations can be calibrated from experiments conducted in simpler flow configurations that display the same, strong vortical characteristics as JIC. In our case, we will use flow over a square cylinder, which can be simulated in 2D, as the simpler proxy. Reynolds stress will serve as the calibration variable/observable.
2. *Surrogate models:* The calibration can be performed using surrogates of RANS models. In our case, we will use polynomial surrogates.

The experimental values of Reynolds stress (RS) in the wake region and separation bubble in flow over a square cylinder are obtained from Refs. 3 and 4. The surrogate models are constructed from a set of 14^3 RANS runs, with ($C\mu$-C_2-C_1) parameter samples chosen via Halton sampling. At each experimental probe, the RS is modeled as a quadratic function of the turbulence model constants using regression. Our method, described in detail in Ref. 5, prescribes how one may select a polynomial trend model (i.e., the order and the terms to retain in the polynomial) to ensure accuracy while simultaneously guarding against overfitting. The resulting surrogate model is a close approximation of the RANS simulator and is used in the calibration.

The parameter estimation is performed using an adaptive Markov chain Monte Carlo (MCMC) method, which constructs a joint probability density function (JPDF), called the posterior distribution, for the three turbulence model parameters and an additive error. We examine the quality of the calibration by sampling turbulence model constants and simulating JIC flowfields. This ensemble of simulations provides a probabilistic prediction of experimentally observed quantities, conditioned on the calibrated model.

III. Calibration Results

We performed k-ε simulations for flow over a square cylinder and compared with existing experimental data. Experimental data is collected at 96 probes downstream of the cylinder. We found that the modeled and measured Reynolds stress τ could differ significantly, often by a factor of 5 immediately behind the cylinder, though the discrepancy decreased significantly further downstream in the wake. We found that a surrogate model could only be constructed for about half the probes; for the rest, the variation of τ with the turbulence model parameters was too complex to be captured accurately (i.e., within 10% of RANS simulations) using a computationally inexpensive surrogate. Of the probes that could be so modeled, 80% lay within the vortical, separation zone.

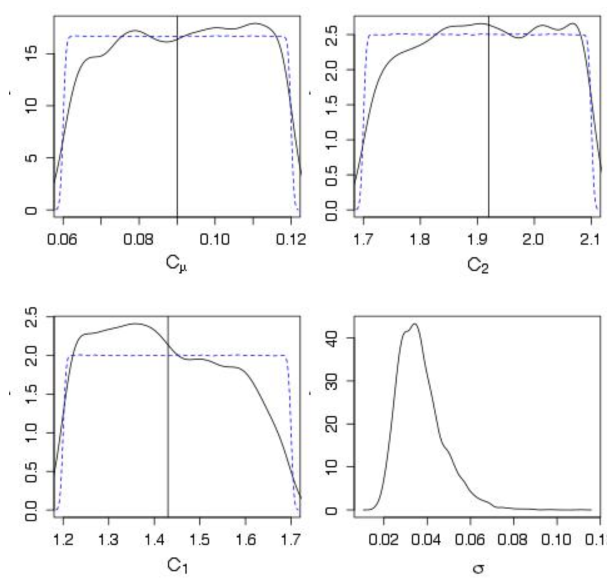

Figure 1. PDFs of $C\mu$, C_2, C_1 and σ. Vertical lines are their nominal values. The dashed lines are uniform priors for ($C\mu$, C_2, C_1).

The parameter estimation problem was modeled as $\tau^{obs} \cong \tau^m(C_\mu, C_2, C_1) + \eta$, where τ^{obs} is the vector of experimental measurements of Reynolds stress and $\tau^m(C\mu, C_2, C_1)$ are the predictions of the surrogate model. η is mostly a measure of the model/structural error in the RANS model, though it includes a very small measurement error. The likelihood, required for Bayesian calibration, is cast in terms of $(\tau^{obs} - \tau^m) = \eta \sim \mathcal{N}(0, \sigma^2)$, where $\mathcal{N}(:,:)$ denotes a normal distribution. The calibration is performed with MCMC and effectively identifies combinations of ($C\mu$, C_2, C_1) and σ which yield $||(\tau^{obs} - \tau^m)/\sigma||_2$ close to 0. The multitude of combinations denotes the uncertainty in the calibrated parameter values; their empirical marginal PDFs

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(Fig. 1) provide a succinct summary. We see that the nominal values of Cμ, C_2, and C_1 (vertical lines in the subfigures) lie in the support of the PDFs but are quite different from the Maximum A Posteriori (MAP) values of the parameters after calibration (the peaks of the PDFs). We also obtain an estimate for σ. The ability of the JPDF to reproduce RS experimental observations in the flow-over-a-square-cylinder configuration is investigated in Ref. 5.

IV. Calibrated Jet-in-Crossflow Simulations

We draw 100 samples of (Cμ, C_2, C_1) from the calibrated JPDF (Fig. 1) and perform JIC simulations. The experiment we seek to match is described in Ref. 6. A supersonic jet interacts with a Mach 0.8 crossflow, rolling up into a counter-rotating vortex pair (CVP) as it evolves downstream. PIV measurements are made on a crossplane 33.6 jet diameters downstream. The figures of merit for judging the accuracy of the RANS simulation are the circulation of the CVP, the location of the centroid of the vorticity distribution, and its radius of gyration.

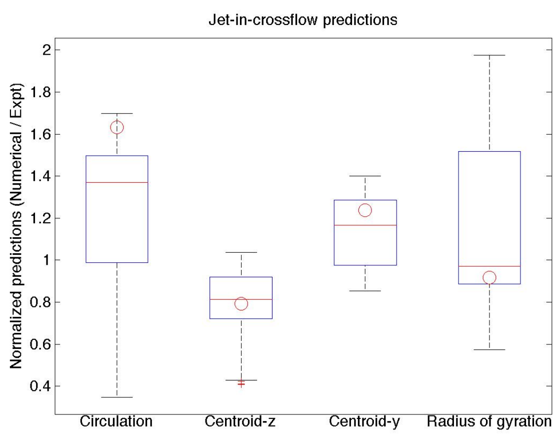

Figure 2. Predictions of circulation, the size and centroidal location of the CVP using (Cm, C2, C1) sampled from the JPDF. The red circles are uncalibrated predictions, and red lines the median prediction. The blue box denotes the IQR range.

The 100 JIC simulations lead to 100 predictions of the figures of merit, which are then normalized by their experimental equivalents. Box-and-whisker plots of these simulations are shown in Fig. 2. The rectangle marks the inter-quartile range (IQR). The (normalized) predictions using the nominal/uncalibrated values of (Cμ, C_2, C_1) are plotted with circles. The red line is the median prediction. We see that the uncalibrated prediction of circulation of the CVP is an outlier in the distribution of post-calibration circulations. The median predicted radius of gyration is very close to the experimental value. The median (y, z) position of the centroid of the vorticity in the crossplane is always closer to the experimental value, post-calibration, compared to the prediction with uncalibrated (Cμ, C_2, C_1). Further, we note that one of the ranges of the IQR is always close to 1 i.e., there might exist a (Cμ, C_2, C_1) combination that might provide figures of merit very close to the experimental values. We search through our 100 samples and find one (heretofore referred to as "Case 79") that provides < 15% error for all four figures of merit.

In Fig. 3 we plot the vorticity field predicted using "Case 79" (Cμ, C_2, C_1) values; the vorticity field using the uncalibrated (Cμ, C_2, C_1) is plotted as a reference. The experimental vorticity distribution is plotted with contours. We see that "Case 79" is an immense improvement over the uncalibrated results; not only is its circulation closer to the experimental value, the extent and location of the vortical region display a better match with the experimental contours.

V. Conclusion, Outline of the Final Paper and Future Work

We have shown that turbulence model parameters can be estimated as PDFs using a Bayesian calibration method. The calibration required 25,000 evaluations of the model to construct converged PDFs; further, the evaluations were strictly sequential. Thus, Bayesian calibration using contemporary MCMC methods cannot be performed using RANS models and we had to take recourse to computationally inexpensive surrogates to do so. This also meant that experimental data from about half the probes could be used; the dynamics of τ at the other half could not be modeled accurately using surrogates. The JPDF obtained from an incompressible flow-over-square-cylinder calibration proved to be predictive in a transonic jet-in-crossflow configuration. The probabilistic (or ensemble) JIC predictions yielded better agreement with JIC experiments on all four figures of merit used in this study. In some cases, the uncalibrated predictions were relegated to the being outliers in the experiment-model comparison.

In the final paper, we will provide the formulation of the surrogate model, details of how they are made, how overfitting is avoided and a test of how well the calibrated ($C\mu$, C_2, C_1, σ) JPDF can reproduce RS measurements in the flow-over-a-square-cylinder problem. In the context of JIC flows, it will also contain a comparison of how well the calibrated ($C\mu$, C_2, C_1) JPDF reproduces measurements in the midplane i.e., the plane of symmetry. It will also contain a description of how our attempts to improve the accuracy of our surrogate models, by using kriging, did not lead to a better calibration. Ref. 5 contains a fairly accurate approximation of the final paper.

One of the shortcomings of our method is the use of a simple additive structural error. This was responsible for our inability to correctly predict τ in the column of probes immediately behind the square cylinder. The structural error could be partially reduced by adopting a more involved model for the eddy viscosity, and calibrating it against experiments. This is underway.

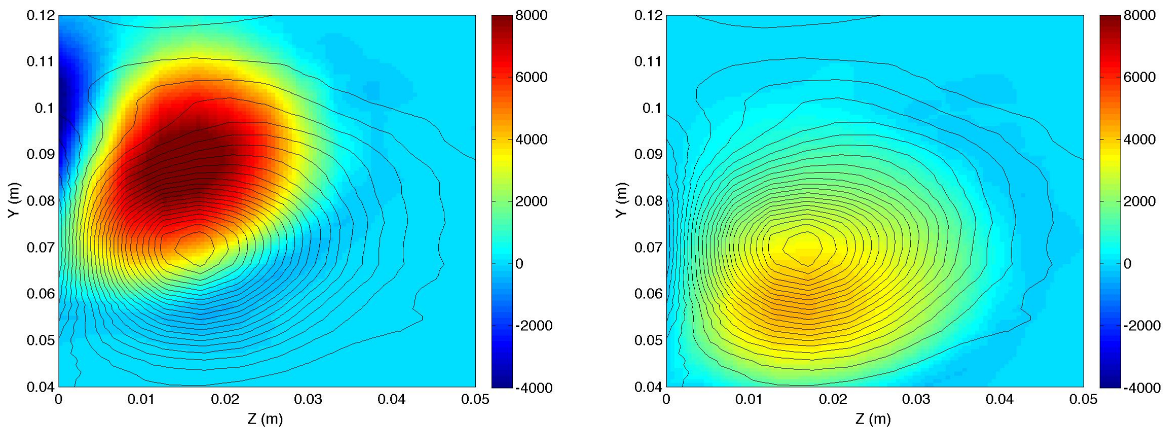

Figure 3. Left: Vorticity field in the crossplane generated using uncalibrated ($C\mu$, C_2, C_1). The black contours are the experimental measurements. The uncalibrated vorticity field is about 60% too strong and in the wrong location. Right: Vorticity field predicted using the “Case 79” values of ($C\mu$, C_2, C_1). The improvement in the agreement vis-à-vis experimental values is quite remarkable.

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