

Augmenting RANS Turbulence Models Guided by Field Inversion and Machine Learning

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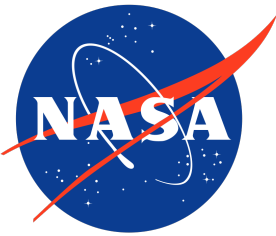
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Abstract

This report investigates the use of a data-driven approach, viz., Field Inversion and Machine Learning (FIML), to improve conventional RANS turbulence models like the Spalart-Allmaras model and the Menter SST $k-\omega$ model. One of the crucial aspects of using an ML-based approach with limited training data to produce corrections that are generalizable to a large range of flow configurations is to design appropriate “features” (inputs to the ML model). A model, based on guidance from the FIML methodology, is presented in analytical form. An additional list of features that have been experimented with during this study is listed at the end of this report. Though these were not utilized in the present correction, they are included to fully document the complete process employed in the present work.

1 Introduction

Reynolds-Averaged Navier-Stokes (RANS) simulations play an important role in the design, analysis and optimization of flow configurations across engineering disciplines. However, these simulations struggle to accurately predict complex phenomena like separated flows, secondary flows, shock/boundary-layer interactions, etc. Over the past decade, several data-driven frameworks have been introduced to attempt to improve the predictive accuracy of RANS. These frameworks leverage machine learning and data from experiments and/or high-fidelity simulations to infer functional corrections to existing phenomenological closure models for RANS equations.

Early developments in the field of data-driven turbulence modeling were inspired by the work of Oliver and Moser [1] and Dow and Wang [2], which focused on quantification of model-form uncertainties as Gaussian random fields. Tracey et al. [3] used machine learning to model numerical fields of model-form inadequacies within the Reynolds-stress tensor as a function of locally available modeled quantities (referred to as features in the machine learning parlance). Tensor Basis Neural Networks [4] were introduced by Ling and Templeton as a framework to design data-driven explicit algebraic Reynolds-stress models. The neural network takes invariants of mean strain rate and mean rotation tensors as inputs and evaluates the coefficients of the Reynolds-stress tensor basis as its outputs. Around the same time, Weatheritt and Sandberg [5] leveraged gene expression programming to approximate the Reynolds-stress anisotropy tensor as an interpretable function of invariants and tensor groups.

The main assumption in all these works is that the amount of data, the chosen features, the function space being explored, and the optimization algorithm being used can ensure that the augmented model mimics the exact Reynolds-stress equations. But it appears extremely unlikely that the augmentation can, in and of itself, overcome the “structural limitations” introduced by the ad hoc approximations constituent in any current turbulence model [6]. Even if appropriate features were to be used, the augmentation will nearly always end up overfitting the data, since it is not able to capture the true underlying structural inadequacies. Thus, while such an augmented closure model would perform well during training (since it overfits the training data), it may result in smaller-than-expected improvements – if not a deterioration – in predictive accuracy when used for flow configurations for which it was not trained. Note that the impact of the aforementioned overfitting will be especially prominent if the function space chosen for the augmentation function is highly nonlinear. Sufficient evidence has been found that this happens even for canonical flows [7]. Another unrelated yet significant shortcoming of such frameworks is that they require full-field data for all variables from an averaged high-fidelity simulation.

Field inversion and machine learning (FIML) [8] was among the first frameworks introduced in the field of data-driven turbulence modeling that emphasized the need for model consistency. A model-consistent augmentation is one where the values of augmentation at all discrete locations within the computational domain (hereafter referred to as the augmentation field) is obtained by solving an inverse problem that seeks to minimize the discrepancy between predictions and available data

for certain quantities of interest, while ensuring that the state variables being used to calculate these predictions satisfy the augmented model equations. The quantities of interest need not be scalars and can instead comprise surface or volumetric data (e.g., skin friction distribution, velocity field, etc.). The FIML framework, in particular, solves the inverse problem by using adjoint-driven gradient-based numerical optimization. Note that in a model-consistent framework, the state variables are no longer constrained to behave like their high-fidelity counterparts and hence the augmentation only needs to make some change within the closure model to accurately predict the quantities of interest. Since the baseline turbulence models are usually calibrated using data from canonical flows, there is a decent chance that well-designed augmentations inferred from high-fidelity data for complex flow configurations (despite its limited availability) can result in improved predictive accuracy for other complex flow configurations with similar physics, without hurting the model accuracy for the canonical flows that the baseline model was calibrated on.

If the degrees of freedom (number of discrete locations in the computational domain) for the augmentation field are significantly greater in number than the quantities of interest, such an inference problem is ill-posed, i.e., there may exist distinct augmentation fields that, when used within the closure model, yield reasonably accurate predictions for the quantities of interest. Different regularizations applied to the inverse problem result in different augmentation fields. These regularizations can be explicit (e.g., Tikhonov regularization, total variation regularization, etc.) or implicit (e.g., discretization of computational domain, choice of optimization algorithm, etc.). A useful implicit regularization technique is to couple the inference of the augmentation field and training of the augmentation function [9–13]. Such a coupled approach constrains the augmentation values to be outputs of an augmentation function that belongs to a pre-determined function space (e.g., a polynomial of a specified degree, a specific neural network architecture, etc.) and takes certain pre-determined model quantities as its inputs (features).

Several works that made use of the aforementioned frameworks [7, 14–16] demonstrated that augmented turbulence models could be applied to unseen flow configurations that are similar to the training flow configurations. However, any improvements offered by such augmentations were lost when applied to configurations that were significantly different from the training ones. Moreover, in several cases, the augmentations resulted in deterioration of model accuracy for canonical flows where the baseline model already performed well [17].

Around 2020, the research in this field started heading in the direction of creating generalizable models, i.e., models that once trained on a few representative flow configurations could improve predictions for a wide range of unseen flows without affecting flows where the baseline model calibrations already result in accurate predictions. This need for generalizability was evident in the collaborative testing challenge at the 2022 Symposium on Machine-Learning Based Turbulence Modeling [18], which was designed to evaluate the capability of such models to generalize predictive accuracy across different flow configurations.

Srivastava and Duraisamy [12, 19] introduced localized learning and hierarchical augmentations and used these techniques to create a data-driven bypass transition model by augmenting the Wilcox k - ω turbulence model. Localized learning is the idea of designing bounded features and then discretizing the bounded feature space to split the augmentation function into several local augmentations. In [12, 19], the local augmentations were chosen as affine transformations of features. Hierarchical augmentation is the strategy of creating successive augmentations for increasingly specialized physical phenomena by using limiters (or blending functions) to activate/deactivate different levels of augmentations. They noted that feature (and limiter) design is among the crucial factors that decide the generalizability of a model augmentation.

Cherroud et al. [20] introduced a space-dependent aggregation of data-driven turbulence models. The process involves first inferring multiple augmentations using different datasets and then training a random forest classifier that, given certain features from converged baseline model solutions, provides weights for each of the inferred augmentations at every location in the computational domain. The final predictions, then, are calculated using weighted means of all augmented model predictions at each spatial location. Though the framework provides an estimate of uncertainty associated with

the predictions, mixing the results from different models can sometimes result in local violations of conservation laws.

Ho et al. [21] used probabilistic machine learning by creating ensembles of augmentation functions (either using Gaussian process regression or deep neural networks). During predictions, a weighted mean of augmentation values calculated from the ensemble members is used to correct the model if the variance of the distribution of these values is within a user-specified tolerance. For locations in the computational domain where this variance is higher than the chosen threshold, the augmentation value is set to unity, i.e., the baseline model is used. Note that since the locations using the augmented model affect those using the baseline model, the converged states observed using the latter will not be identical to their counterparts obtained by using baseline model equations everywhere. Since the RANS solution depends on the ensemble predictions for augmentation values, this method does not result in any violations of conservation laws. The probabilistic framework also provides an uncertainty estimate in the augmentation calculation quite naturally. Ho et al. also noted that the generalizability offered by their probabilistic machine learning framework relies on designing good features.

More recently, Bin et al. [22] used constrained recalibration (also referred to as the rubber-band approach) of the Spalart-Allmaras turbulence model via Bayesian optimization to preserve the model performance for cases for which the baseline model was calibrated on. This approach minimizes any adverse effects of the recalibration on canonical flow configurations where the baseline Spalart-Allmaras model already performs well. However, generalizability to a wide variety of flow configurations from a single model augmentation has not been demonstrated. One such augmented model that they developed for separated flows has been compared with the present augmentation in section 3.

Another relevant recent development is the work by Wu et al. [23], which uses conditioned field inversion and symbolic regression. The conditional field inversion strategy ensures that any augmentation to improve the prediction of separated flows does not activate within attached boundary layers, by using the shielding function that is widely used in detached eddy simulations (DES). They demonstrated that their model generalizes decently by improving the predictive accuracy (by different amounts) for various separated flow configurations while minimizing any spurious effects for attached flow configurations.

A common theme in all these studies is the emphasis on designing features that bolster generalizability of RANS schemes. Recent work by Lozano-Duran and coworkers [24] have explored information-theoretic approaches to create parsimonious sets of features that, when used to create data-driven wall models, seem to provide appreciable generalizability for applications involving wall-modeled large eddy simulations (WMLES). It might be possible to repurpose such techniques to provide data-driven augmentations of RANS models as well.

The present work, which is a follow-up to our preliminary report on the same subject [25], uses FIML to inform the development of an analytic correction that, when introduced into the SST $k-\omega$ and the Spalart-Allmaras turbulence models, improves predictions for reattachment of flows that undergo smooth-body separation. The remainder of the paper is organized as follows. Section 2 describes the development of an analytic augmentation function (derived from ML insights, but codable without any machine learning) for the SST $k-\omega$ turbulence model with a closed-form expression that uses a single feature as input and improves predictions for the point of reattachment of separated flows across different flow geometries and Reynolds numbers. Section 3 presents results obtained when the same augmentation is used within both the SST $k-\omega$ turbulence model, for a range of different geometries. Finally, section 4 presents conclusions and describes various potential improvements that can be pursued in future work.

An appendix is provided that describes the various features (along with some details that the reader may find informative) that were explored in the course of arriving at the presented augmentation function.

2 Methodology

It is often observed that traditional RANS models underpredict the magnitude of Reynolds stresses associated with a separation bubble, resulting in reduced turbulent mixing and hence a delayed reattachment. In other words, such models predict a longer separation bubble compared to high-fidelity simulations and/or experiments. To address this issue, we began by performing a field inversion in FUN3D for the 2D NASA wall-mounted hump (no plenum) case [26].

2.1 Field Inversion on 2D NASA Wall-mounted Hump Case

The field inversion problem can be broken down into two steps: (1) introducing an inadequacy term within the model; and (2) obtaining an optimal field of values corresponding to the inadequacy such that the discrepancy between data and predictions for certain quantities of interest is minimized. Within the Spalart-Allmaras model (SA), an inadequacy field $\beta(\mathbf{x})$ is introduced by multiplying it by the production term in the SA transport equation,

$$\frac{D\tilde{\nu}}{Dt} = \beta(\mathbf{x})c_{b1}(1-f_{t2})\tilde{S}\tilde{\nu} - \left(c_{w1}f_w - \frac{c_{b1}}{\kappa^2}f_{t2}\right)\left(\frac{\tilde{\nu}}{d_w}\right)^2 + \frac{1}{\sigma}\left[\frac{\partial}{\partial x_j}\left((\nu + \tilde{\nu})\frac{\partial\tilde{\nu}}{\partial x_j}\right) + c_{b2}\frac{\partial\tilde{\nu}}{\partial x_i}\frac{\partial\tilde{\nu}}{\partial x_i}\right] \quad (1)$$

(see [27] for notation). The field inversion is then posed as an optimization problem of the form

$$\min_{\beta(\mathbf{x})} [\mathcal{C}(\beta(\mathbf{x})) + \lambda\mathcal{R}(\beta(\mathbf{x}))], \quad (2)$$

where the cost function ($\mathcal{C}$) and regularization function ($\mathcal{R}$) are given as

$$\begin{aligned} \mathcal{C}(\beta(\mathbf{x})) &= \|C_f^{\text{RANS}}(\beta(\mathbf{x})) - C_f^{\text{data}}\|_2^2 \\ \mathcal{R}(\beta(\mathbf{x})) &= \|\beta(\mathbf{x}) - 1\|_2^2, \end{aligned} \quad (3)$$

and the regularization constant λ is chosen in the range between 0.01 and 0.0001. The cost function measures the discrepancy between the data and predictions for the skin-friction distribution (C_f) on the hump geometry. The regularization function, on the other hand, prevents $\beta(\mathbf{x})$ from deviating far from its baseline value of unity. Gradient-based optimization (steepest gradient descent algorithm, in this case), which uses sensitivities $d\mathcal{C}/d\beta(\mathbf{x})$ and $d\mathcal{R}/d\beta(\mathbf{x})$ obtained via the adjoint capability within FUN3D [17, 28], is then used to solve this optimization problem. Contours for the optimized $\beta(\mathbf{x})$ field are shown in figure 1. The different regions labeled in the figure are described as follows:

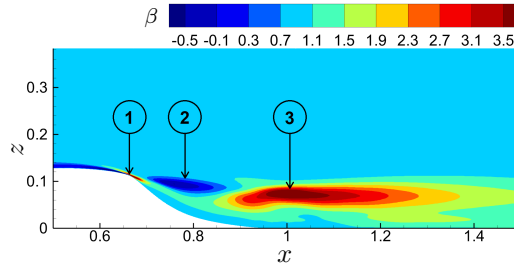


Figure 1: Field Inversion results for SA applied to the NASA wall-mounted hump [26]

1. This $\beta > 1$ region exerts a fine-tuned control over skin friction close to and immediately downstream of the separation location.
2. This $\beta < 1$ region compensates for the increased turbulent diffusion caused by regions 1 and 3 such that skin friction does not become too high in magnitude too soon after separation.

3. This $\beta > 1$ region is primarily responsible for pushing the reattachment location upstream and increasing the skin friction in the recovery region.

Note that there is a low β region upstream of region 1. However, it is observed that this region has almost no influence on where the flow reattaches. Region 3 has the biggest impact on the point of reattachment. Hence, in this work, we attempt to model region 3 and leave regions 1 and 2 for future work. Here we explore features that can generalizably predict region 3 across flows characterized at different Reynolds numbers for different separation-inducing geometries.

2.2 Feature and Limiter Design

For most RANS simulations, the underlying reason for the prediction of a delayed reattachment is an underprediction of Reynolds stresses within the separated shear layer. Thus, the main aim of the augmentation is to identify these regions in the flow and amplify the eddy viscosity such that the shear layer spreads more rapidly, and the flow reattaches earlier compared to what is predicted by the baseline model.

2.2.1 Attempts with the Spalart-Allmaras model

The vorticity Reynolds number $Re_\Omega = d_w^2 \Omega / \nu$ (where d_w is the wall-normal distance, Ω is vorticity magnitude, and ν is the kinematic molecular viscosity) provides crucial information regarding a boundary layer undergoing separation since there are regions of high vorticity farther from the wall in a separated shear layer as compared to an attached boundary layer. Since $Re_\Omega \propto d_w^2$ and because the region corresponding to the highest values of vorticity is further away from the wall in a separated shear layer compared to the attached boundary layer upstream, Re_Ω should have significantly higher values within a separated shear layer. However, the highest values of Re_Ω usually occur above region 3, defined by the field inversion results (figure 1). We found that the product of the square of the turbulence Reynolds number $Re_t = \nu_t / \nu$ and Re_Ω correlates closely with the desired region (compare figures 1 and 2). Let us call this product $\eta_{r,1} = Re_\Omega Re_t^2$.

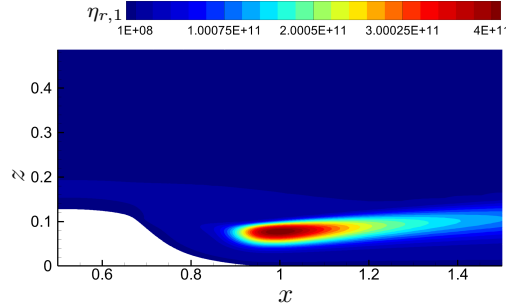


Figure 2: Contours of $\eta_{r,1}$ for the NASA wall-mounted hump

Note that even regions of low vorticity far away from the wall can result in high Re_Ω (when $d_w^2 \gg \nu / \Omega$), and thus produce spurious results. To prevent the augmentation from taking effect outside the turbulent boundary layer, a limiter is designed as

$$\eta_r^\ell = \frac{1}{1 + \exp(100 - 10Re_t)}. \quad (4)$$

Note that by construction, this limiter is close to zero for $Re_t < 9.5$ and smoothly transitions to unity for $Re_t > 10.5$.

While $\eta_{r,1}$ is roughly correlated to region 3 in figure 1, we observed that the range in which its magnitude varies is significantly different for various flow cases (2D NASA wall-mounted hump,

2D curved backstep, 2D periodic hill, etc.). This makes any augmentation inferred from the NASA hump dataset with $\eta_{r,1}$ as a feature useless for other cases. Thus, to make $\eta_{r,1}$ more generalizable, it requires modification using a third non-dimensional quantity such that the resulting feature varies in the same range for different flows. We tried using the Reynolds number based on strain rate magnitude $Re_S = d_w^2 S/\nu$ as this third quantity. However, we did not find any significant improvement using Re_S (in addition to Re_Ω , and Re_t). It quickly became clear that a second transport scalar is required to formulate a Reynolds number independent of Re_S , Re_Ω , and Re_t that can be used to modify $\eta_{r,1}$ to potentially create a generalizable augmentation. Hence, we decided to apply the two-equation Menter SST k - ω model [29], and employ its ‘extra’ variable for this purpose.

2.2.2 Applying lessons from Spalart-Allmaras model to Menter’s SST k - ω model

Similar to the SA model, the standard SST model also overpredicts separation bubble length due to underpredicted Reynolds stresses. A minor difference between the two models is that SST recovers the post-reattachment skin friction faster (and hence more accurately) compared to the SA model. Hence, it may be argued that region 3 from figure 1 need not extend as far downstream for the SST model, as the skin friction recovery is already better for the SST model. Except for this difference, however, the physical arguments that $\eta_{r,1}$ is based on still hold. In the case of the SST model, we observed that using $Re_k = d_w \sqrt{k}/\nu$ as the third quantity to modify $\eta_{r,1}$ helped generalize the augmentation to different flow geometries and Reynolds numbers. Based on trial and error, we chose for the functional form of the single feature

$$\eta_r = \frac{Re_\Omega^{\alpha_\Omega} Re_t^{\alpha_t}}{Re_k} \eta_r^\ell, \quad (5)$$

where α_Ω , α_t and α_k are parameters that need to be set and η_r^ℓ is the limiter described in section 2.2.1. We observed that α_Ω must be greater than α_t to ensure that η_r exhibits large values for a separated shear layer, and not for an attached boundary layer. Please note here that introducing Re_k into the feature significantly changes the region where the augmentation is active as shown in the next section. Introducing the threshold c_{η_r} and the limit $c_\beta^{\max}$ leads to

$$\beta = \begin{cases} 1 & \text{if } \eta_r < c_{\eta_r} \\ c_\beta^{\max} & \text{otherwise} \end{cases}.$$

Multiplying this form of β by the production term in the transport equation for turbulence kinetic energy k tends to improve the reattachment predictions for flows that undergo smooth-body separation. However, the sharp jump in the augmentation value at c_{η_r} can cause convergence issues, and hence the above expression was replaced by a smoothed version, with

$$\beta = 1 + \frac{c_\beta^{\max} - 1}{1 + \exp(100(c_{\eta_r} - \eta_r))}. \quad (6)$$

Optimum values of these constants were found to be $\alpha_\Omega = 0.61$, $\alpha_t = 0.39$, $c_{\eta_r} = 0.9$, and $c_\beta^{\max} = 5$. Note that a further increase in $c_\beta^{\max}$ has minimal effect on the performance of the model. However, the augmentation is sensitive to variations in c_{η_r} , with higher values shrinking the region where the augmentation is active and vice versa.

3 Results and Discussions

3.1 Prediction using augmented SST k - ω model

The SST model was modified within the compressible NASA flow solver FUN3D [17, 28] by using Eqns. 5 and 6 above, then multiplying the production term in the k equation by β . Most of these

cases were also computed independently using the flow solver Joe [30, 31], and the corresponding results were very close, if not identical, to the results obtained by FUN3D.

In the results that follow, this modified form of the SST model is referred to as “SST-SLC” (for “shear layer correction”) in the figure legends. When the augmentation is used for the 2D NASA wall-mounted hump case, the augmentation contours and skin friction profile shown in figure 3 are obtained. While the augmentation contours are very different from the field inversion contours for SA presented in figure 1, the resulting effect on the reattachment location is qualitatively the same, i.e., the reattachment is pushed upstream due to an increase in turbulent diffusivity right after separation occurs. This is evident by the Reynolds-stress plots at different x -locations (see figure 4). It can be seen that the peaks predicted by the baseline model (labeled “SST”) show only small variations with streamwise location when compared to experimental data that exhibit peaks that first increase and then decrease with streamwise location. Qualitatively, the augmented model matches this increasing-then-decreasing trend of peak Reynolds-stress magnitudes observed from experiments. However, the augmented model overpredicts the peaks close to the separation location and underpredicts far from it. This is why the skin-friction magnitudes are overpredicted within the separation bubble compared to the baseline model, thus, increasing the discrepancy/error with respect to experimental data within this region. In this work, our focus was on the reattachment location. Improvement of post-augmentation predictive accuracy within the separation region – which may require introduction of more features to better match the Reynolds stresses – will require further work. It is also important to note that the analytic augmentation does no harm to regions away from separation ($x < 0.6$), as desired.

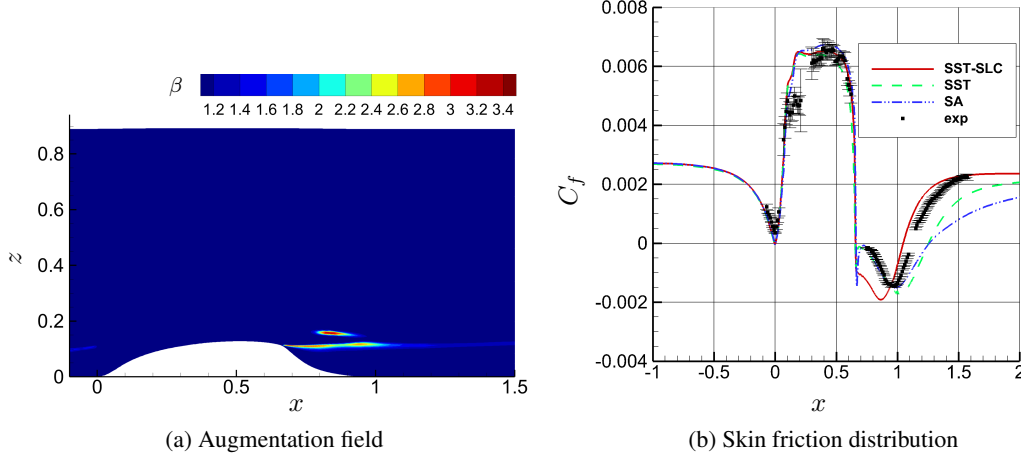


Figure 3: Augmentation results for baseline and modified SST applied to the 2D NASA wall-mounted hump

Similar improvements are observed for the curved backstep (see figure 5) and periodic hill (see figure 6). Note that the flow Reynolds numbers for the hump, curved backstep and periodic hill cases (based on the characteristic lengths of each flow) are quite different. This serves as an a posteriori check that the modification to the feature using Re_k is working as desired. Applying the augmentation to the 2D zero pressure gradient flat plate case (see figure 7), we see a streak of spurious augmented region (with $\beta \approx 2$) in the outer layer. However, the effect of such a streak is minimal on the skin friction predictions, and only the wake region of the boundary layer witnesses a slight change (figure 8). These changes to the predictions for the zero-pressure-gradient flat-plate case are considered to be within acceptable bounds.

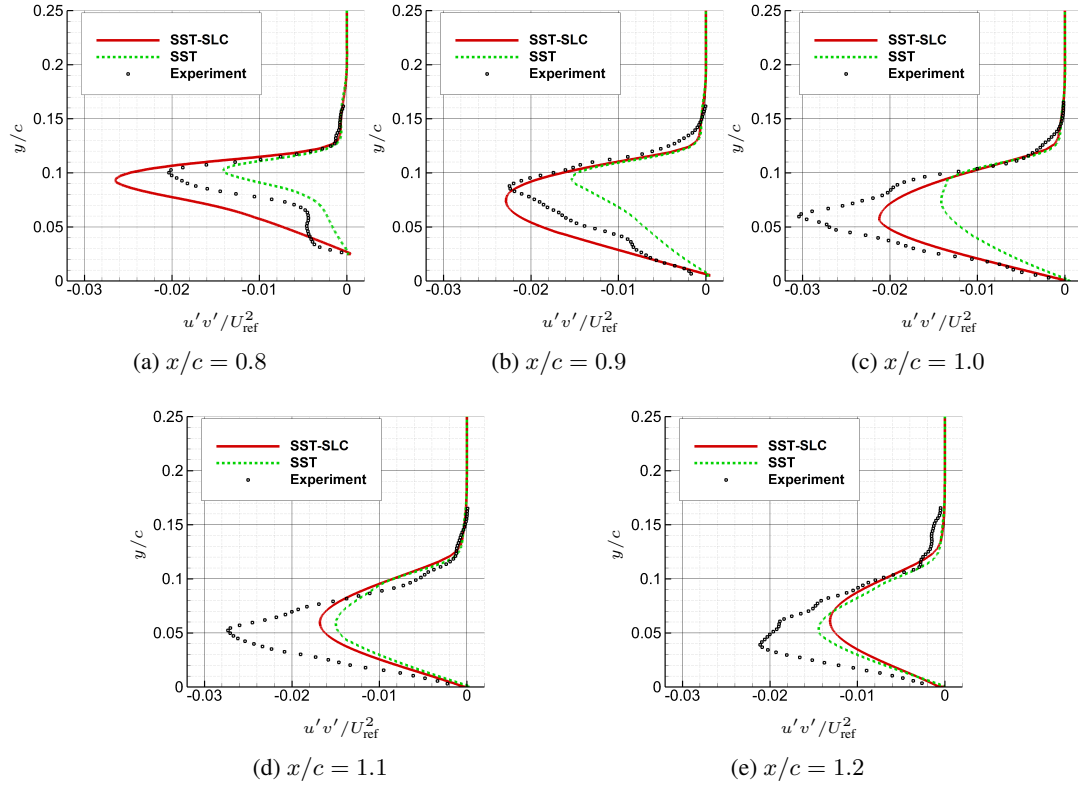


Figure 4: Reynolds stress comparisons for baseline and modified SST applied to the 2D NASA wall-mounted hump

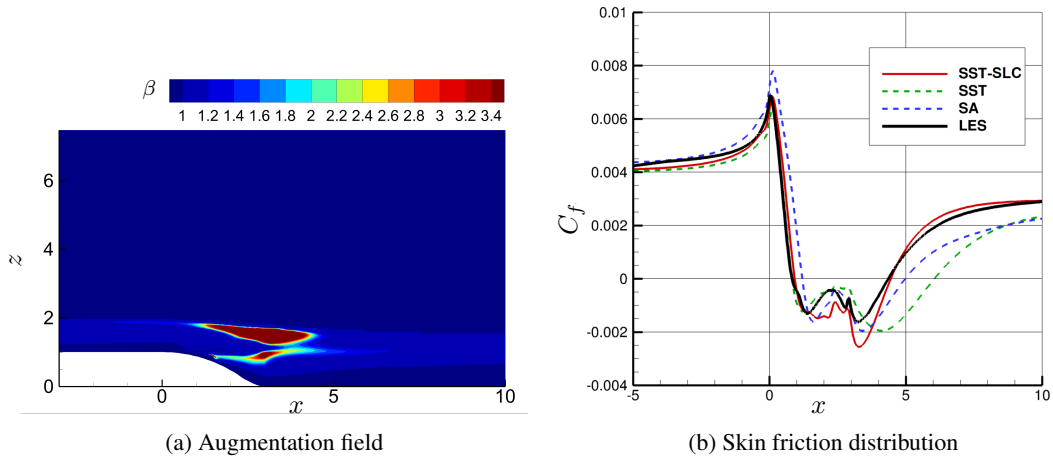


Figure 5: Augmentation results for baseline and modified SST applied to the 2D curved backstep

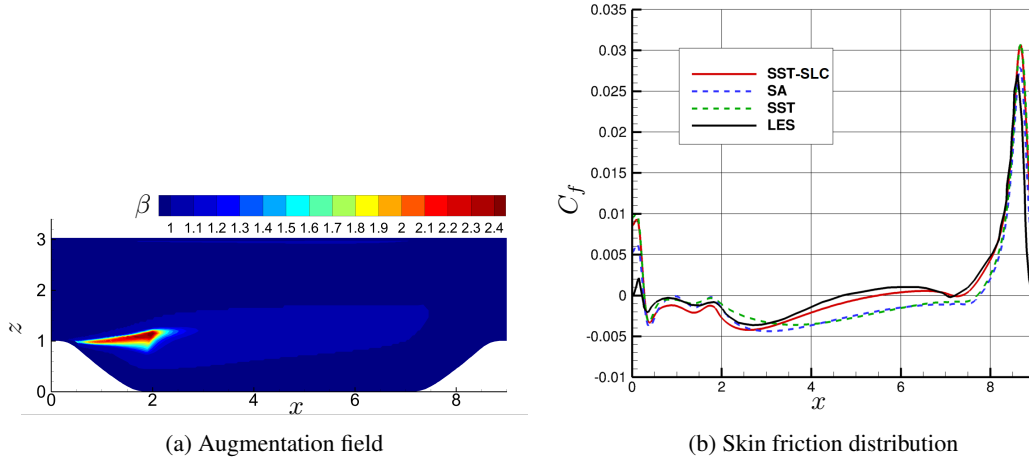


Figure 6: Augmentation results for baseline and modified SST applied to the 2D periodic hill

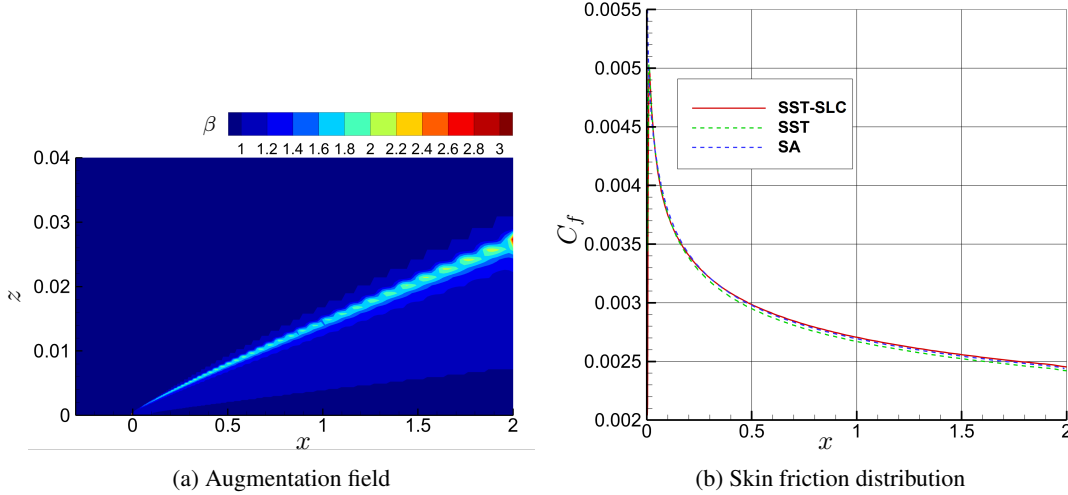


Figure 7: Augmentation results for baseline and modified SST applied to the 2D zero pressure gradient flat plate

3.2 Prediction using augmented SA model

When using the Spalart-Allmaras (SA) model, the turbulence kinetic energy can be approximated using the expression [27]

$$k = \frac{\mu_t \sqrt{2S_{ij}S_{ij}}}{0.31\rho}.$$

Note that the authors initially shifted focus to the two-equation SST model instead of using this approximation because k is an independent scalar in the SST model instead of being a function of local flow quantities in the SA model. However, when the SA model is modified by multiplying the production term for $\tilde{\nu}$ by β calibrated for the SST model (see equation 6), the augmented model performed surprisingly well. The augmentation is also observed to be active in the same regions for both the SST and the SA model. The authors attempted to recalibrate the augmentation to see if better results could be obtained. However, the same calibrations as used for the SST model were found to work the best for the SA model as well. This could be viewed as a weak empirical indication

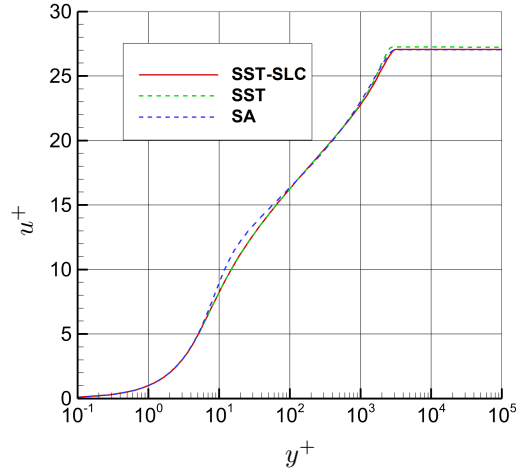


Figure 8: Velocity profiles for baseline and modified SST applied to 2D zero pressure gradient flat plate

that the augmentation contains information of physical significance that is missing from traditional eddy viscosity models, but based on the current observations, the authors cannot make any definite claims in this regard.

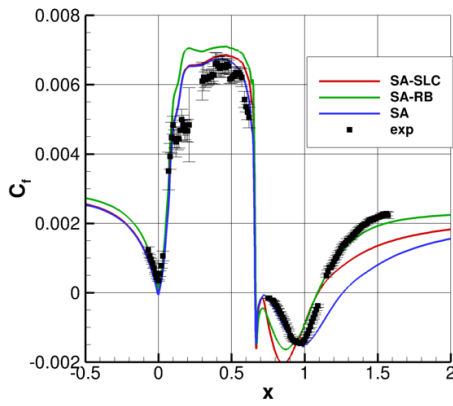
Results obtained using our augmentation function applied to the SA model (labelled as SA-SLC) are presented and compared to another model correction (labelled as SA-RB for “Rubber-Band” model) recently developed by Bin et al. [22]. For the 2D NASA wall-mounted hump case (see figure 9), the two model augmentations are nearly identical as far as the prediction of flow reattachment location is concerned. However, the SA-RB prediction is significantly better than SA-SLC downstream of the reattachment. One should keep in mind when looking at these results that the SA-SLC augmented model was created with the objective to improve predictions for the reattachment location only and hence is not expected to improve the baseline SA model in the post-reattachment region. It should also be noted that the SA-RB model predicts a smaller dip in the skin friction distribution within the separated flow region when compared to the SA-SLC model, which is closer to the dip observed in the experimental results. However, both the augmented models predict this dip somewhat upstream of where it occurs in the experiments. Also, the SA-RB model causes a small increase in the skin friction coefficient upstream and over the hump, where preservation of the original SA results would be preferred.

For the rounded backstep case (figure 10), we see that SA-SLC predicts the reattachment location better than SA-RB (which overcorrects). However, SA-RB once again predicts the post-reattachment skin friction more accurately than SA-SLC.

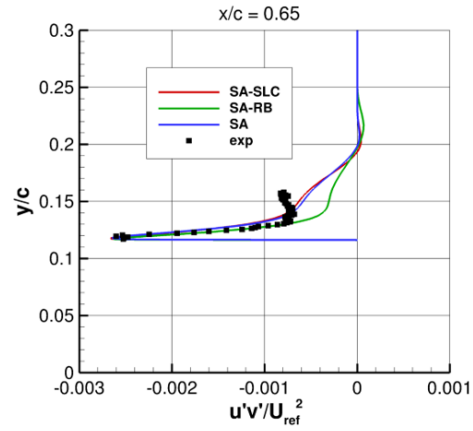
For the zero pressure gradient flat plate boundary layer case (see figure 11), the SA-SLC results are nearly indistinguishable from the baseline SA model (which is a desirable outcome) whereas the SA-RB model predicts a higher skin friction. This is also observed in the law of the wall for this case.

For the sharp backward facing step case (figure 12), both the SA-SLC and SA-RB results predict a much too early reattachment when compared to what is experimentally observed. The SA-SLC shows a more prominent and somewhat more upstream dip in the skin friction predictions than SA-RB, which is consistent with what is observed in other cases.

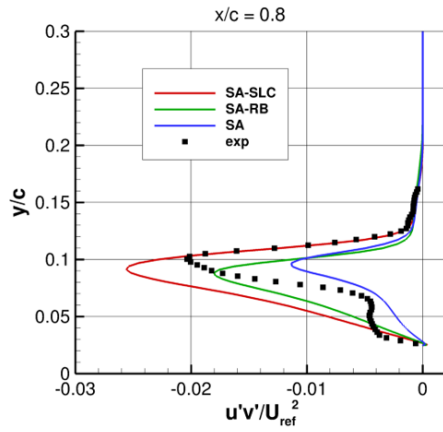
For the 2D periodic hill case (see figure 13), the SA-SLC and SA-RB results are quite close to each other, with SA-RB being slightly better in the separated flow region and SA-SLC being better close to the inflow and outflow boundaries, where it preserves the peaks predicted by the baseline SA model.



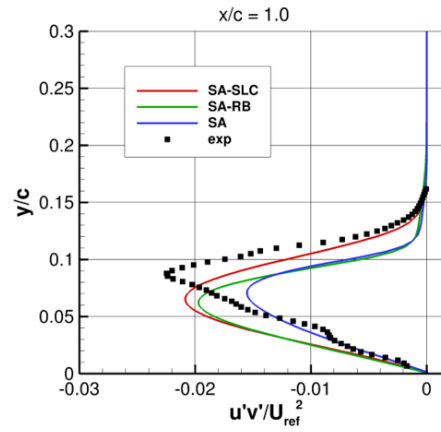
(a) Skin friction coefficient



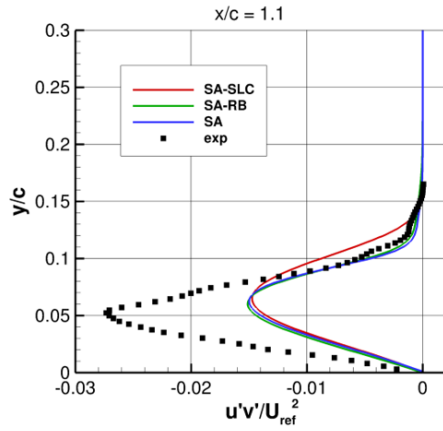
(b) Reynolds stresses ($x/c = 0.65$)



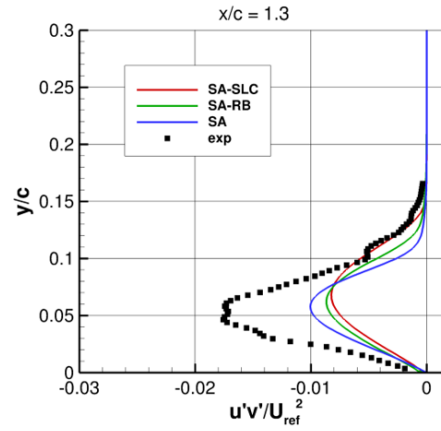
(c) Reynolds stresses ($x/c = 0.80$)



(d) Reynolds stresses ($x/c = 1.00$)



(e) Reynolds stresses ($x/c = 1.10$)



(f) Reynolds stresses ($x/c = 1.30$)

Figure 9: Augmentation results for baseline and modified SA applied to the 2D NASA wall-mounted hump (no plenum)

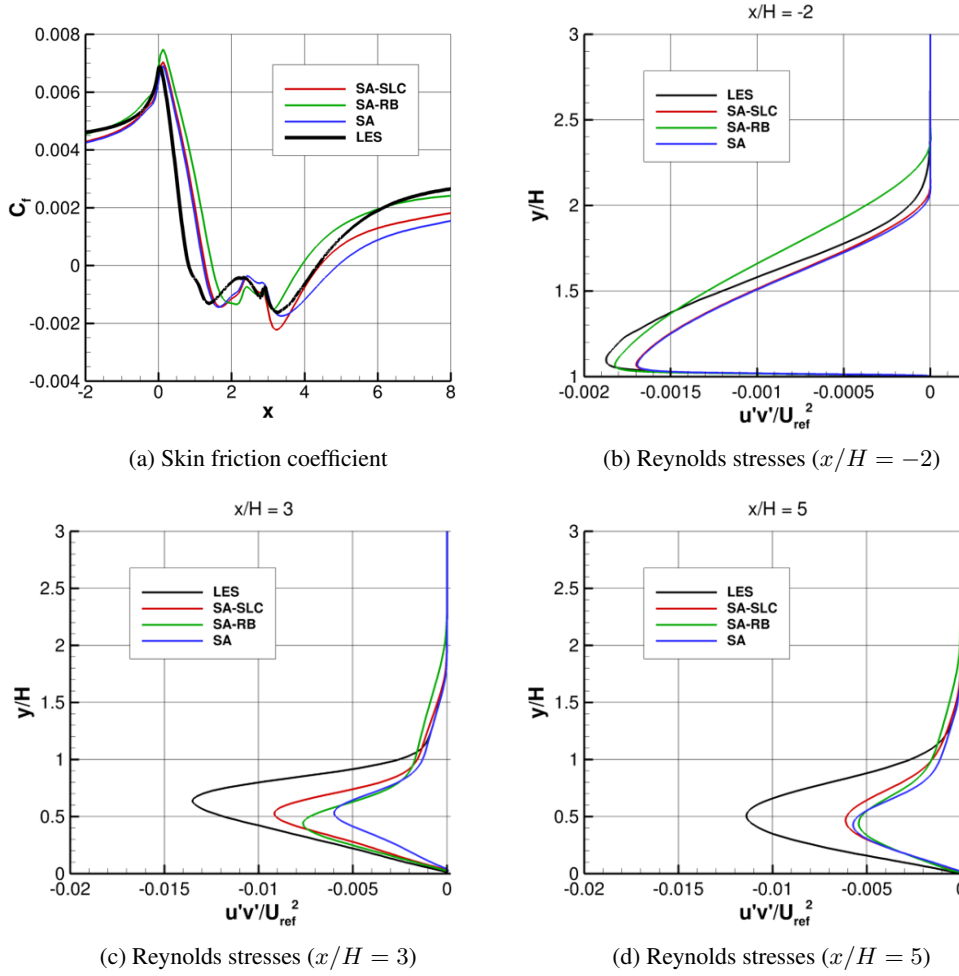


Figure 10: Augmentation results for baseline and modified SA applied to the 2D rounded backstep case

The SLC model was also applied to an axisymmetric flow with smooth-body separation [32] (see figure 14). For this case, the augmented model made only minor differences compared to the baseline and RC versions of the SA model. Only a very slight reduction in the length of the separation bubble was observed. It is also noteworthy that different turbulence models show different sizes of separation bubbles. From the available surface pressure coefficient data, it seems that the SST $k-\omega$ model provides the best estimates for this case.

The augmented model was also applied to a few 3D flow cases. For the ONERA M6 wing cases (see figures 15, 16, and 17), the two augmented models predicted very similar results to the those obtained using the baseline SA model. This is viewed as a favorable outcome, in that the augmentation did not lead to spurious results. Among the few locations where the predictions among the three models vary, there are some where the SA-SLC seems to be less erroneous than SA-RB. However, it is difficult to draw any solid conclusions from these instances.

For the high-lift Common Research Model (CRM-HL) case from the Fifth High-Lift Prediction Workshop [33] (see figure 18), the augmented model results from SA-SLC are virtually identical to those obtained using the baseline SA model.

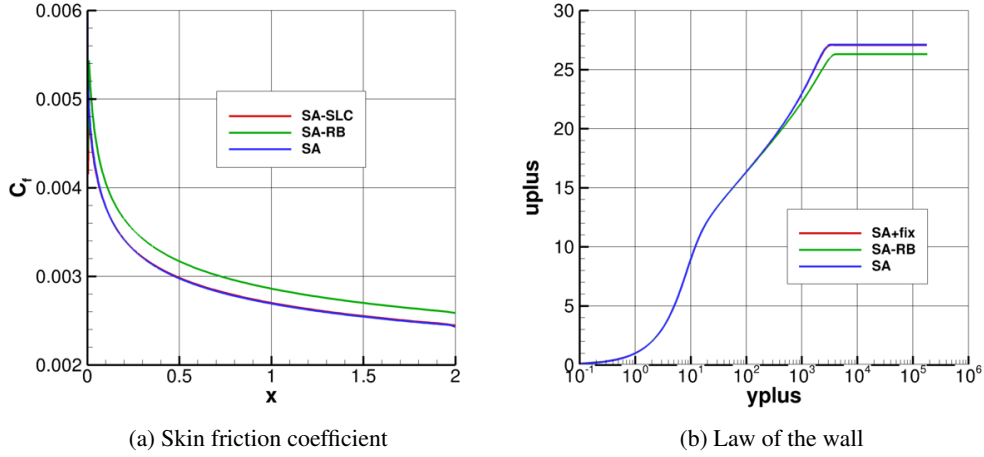


Figure 11: Augmentation results for baseline and modified SA applied to the zero pressure gradient flat plate

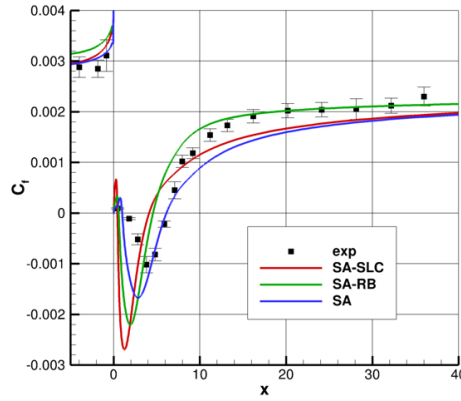


Figure 12: Augmentation results (skin friction) for baseline and modified SA applied to the 2D sharp backward facing step

4 Conclusions

A closed-form augmentation is presented that improves the predictive accuracy for reattachment locations of flows that have undergone smooth-body separation. The simple formulation of the augmentation makes it interpretable and intuitive for the user, thus resulting in convenient fine-tuning for a specific application, if required. The augmentation, while developed for Menter's SST $k-\omega$ model, performed surprisingly well for the Spalart-Allmaras model without needing any recalibration. The augmentation was tested on a variety of different 2D and 3D flow configurations mainly with its implementation within the SA model. Among these configurations, the augmentation improved the result for 2D configurations where smooth-body separation is observed, and leaves the other configurations virtually unaffected. In all our tests, the numerical solver had similar iterative convergence behavior for both augmented and baseline models. While this success is encouraging, more work is required to improve the current augmentation and introduce new corrections that can improve the prediction of incipient flow separation due to adverse pressure gradients: (1) more

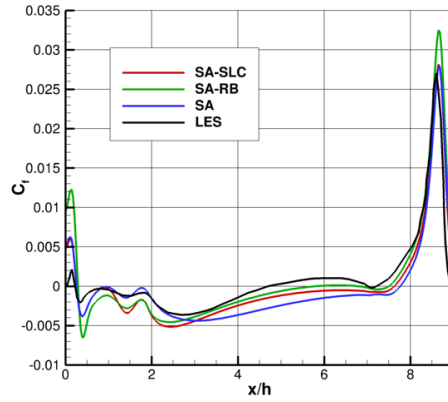


Figure 13: Augmentation results (skin friction) for baseline and modified SA applied to the 2D periodic hill

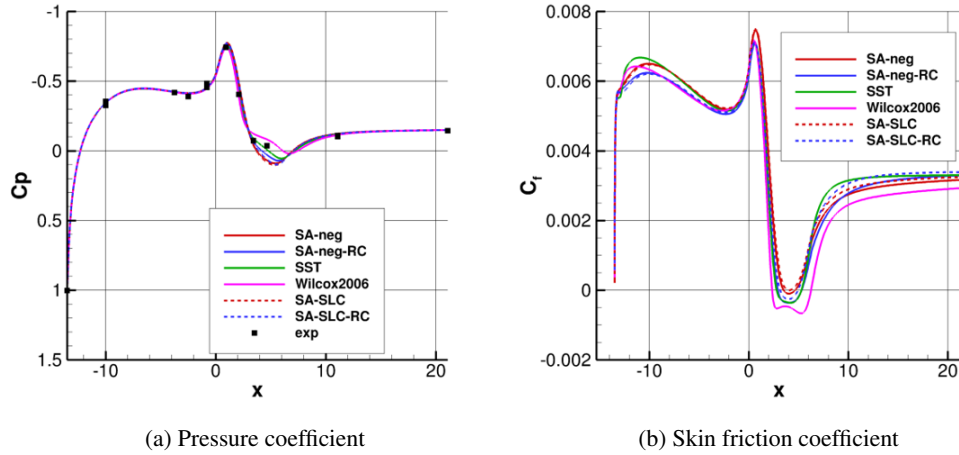


Figure 14: Augmentation results for baseline and modified SA applied to an axisymmetric case with flow separation

features/limiters need to be introduced to prevent the augmentation from taking effect in the outer layer of attached flows (as is seen in the case of zero-pressure-gradient boundary layer); (2) unlike smooth-body separation, the effect of the augmentation needs to be attenuated for cases where the flow is separated off a sharp corner; and (3) details such as excessively negative skin friction within the separation bubble for the NASA hump case need to be resolved.

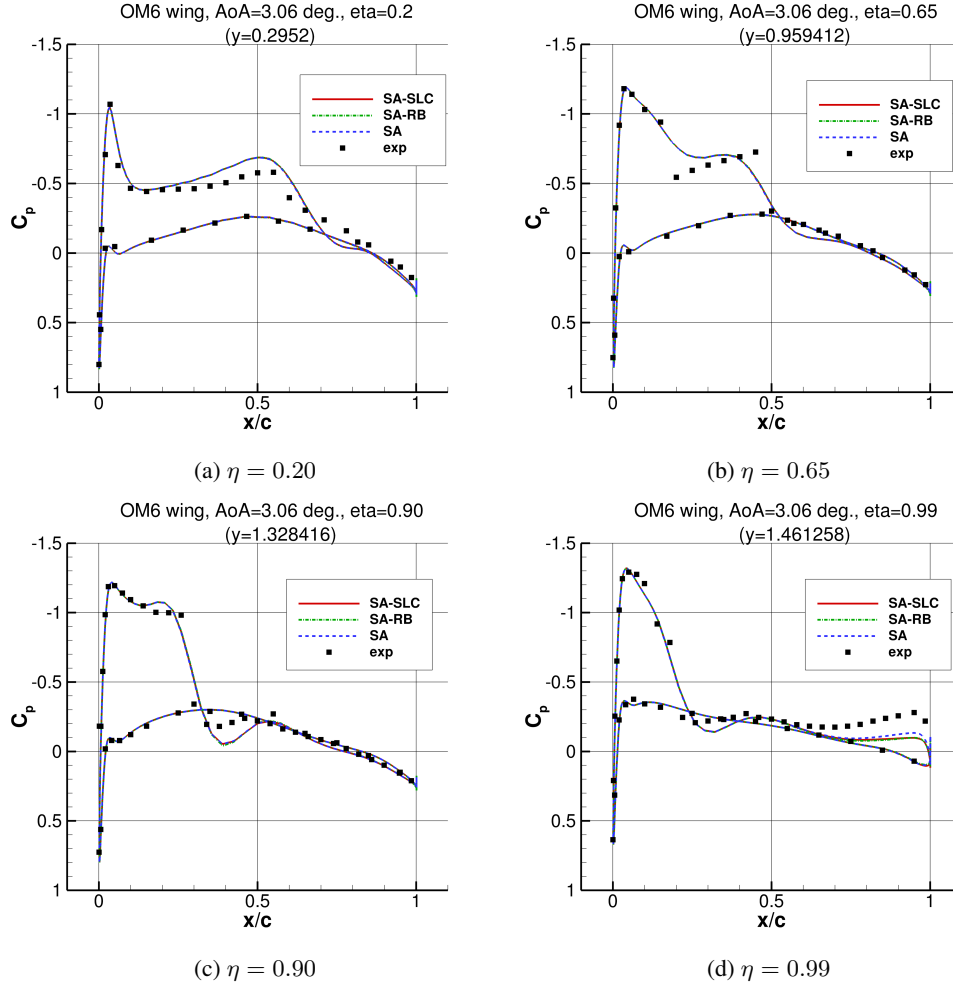


Figure 15: Results for baseline and modified SA applied to the ONERA M6 wing (angle of attack = 3.06°)

Appendix 1: Feature Exploration

To obtain generalizable augmentations, one needs to carefully design features that have the following properties:

- **Nondimensionality:** The feature values must not change if the measurement units are changed. For example, velocity is poor candidate for being a feature as its value will change depending upon whether it is measured in m/s or ft/s. Another equally important reason (mentioned later) is that it is not Galilean invariant.
- **Rotational invariance:** The feature values must not change if the model equations are solved in a rotated frame of reference. For instance, using an appropriately nondimensionalized velocity derivative in the x -direction is a poor feature candidate as the “ x -direction” is itself subject to change when the frame of reference is rotated by 90° . Please note that a “rotated” frame of reference is different from a “rotating” (non-inertial) frame of reference and that derivatives in the wall-normal direction are invariant to a rotation of the coordinate system and can hence be used.

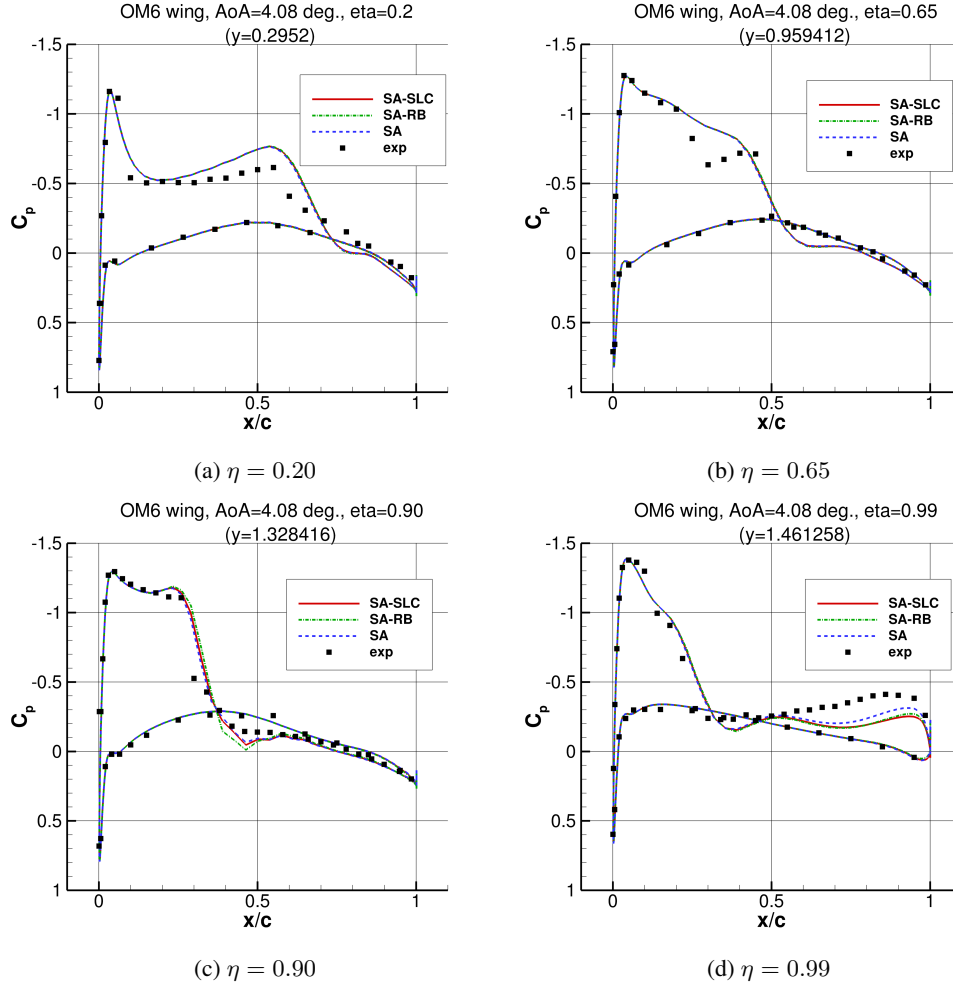


Figure 16: Results for baseline and modified SA applied to the ONERA M6 wing (angle of attack = 4.08°)

- Galilean invariance: The feature values must be agnostic to the velocity of any inertial frame of reference that may be chosen to solve the model equations. For instance, using an appropriately nondimensionalized velocity value would still constitute a poor feature, as such a value is subject to change when measured from a moving frame of reference.
- No use of pressure gradients: As mentioned by Spalart [34], pressure gradients are not a good feature candidate. To illustrate this point, he often uses the example of how flow over an oscillating flat plate (under no pressure gradients) is identical to the flow over a stationary flat plate under oscillating pressure gradients, and also how the pressure gradient term is absent from the vorticity transport equation for incompressible flows.
- Physics-based scaling: It is desirable that appropriate scaling is included within the features such that the variations in their value does not have a strong dependence on flow parameters like Reynolds numbers. Note that simply scaling a non-dimensionalized feature based on the mean and variance of the samples in the training dataset is often insufficient to ensure such invariance.

This section lists some of the features considered in this study of data-driven turbulence mod-

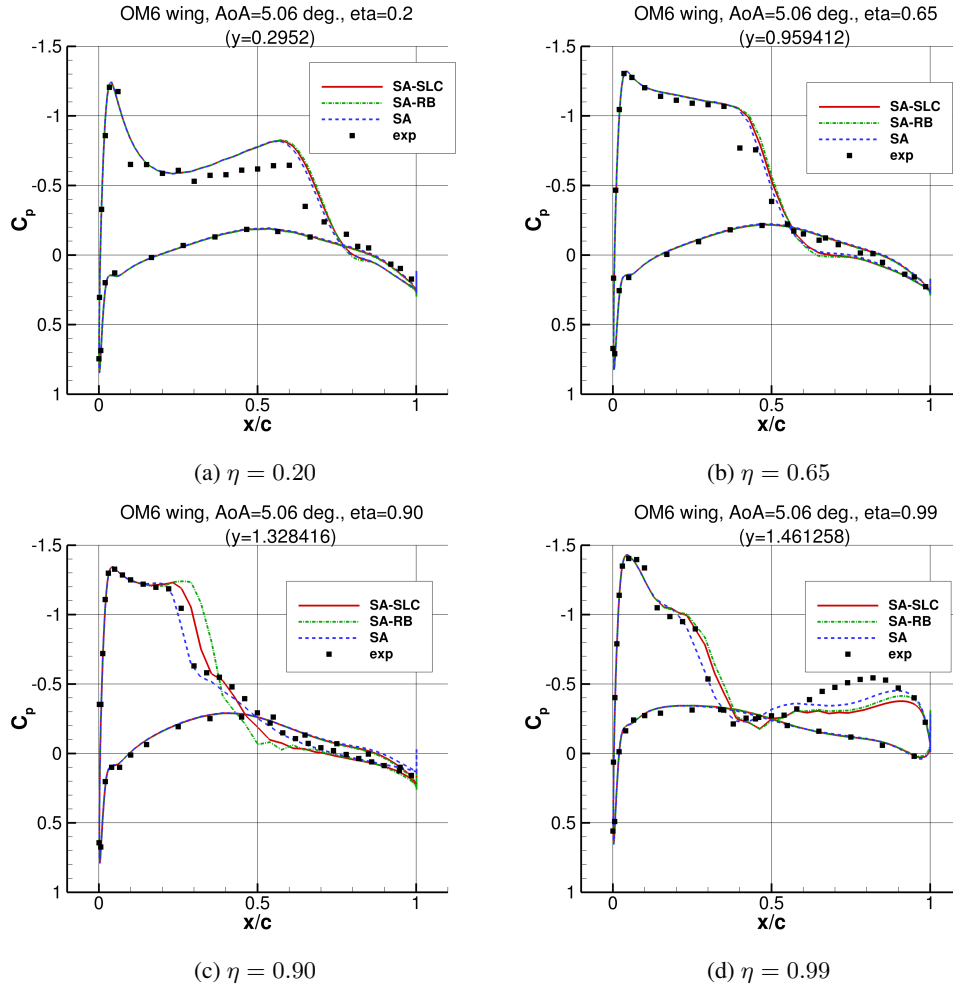


Figure 17: Results for baseline and modified SA applied to the ONERA M6 wing (angle of attack = 5.06°)

eling, and some general observations. As will be clear from the illustrated arguments, different functional forms of the same features can exhibit very different variations in the physical space and hence are useful to provide an (implicit) inductive bias for appropriate applications.

1. Turbulence Reynolds Number: $Re_t = \nu_t/\nu$

Available in: all models

Useful to isolate: turbulent boundary layers and free shear layers

Observations:

- The freestream value of Re_t (denoted here as $Re_{t,\infty}$) is generally small ($Re_{t,\infty} < 1$).
- Given some value $Re_{t,1} > Re_{t,\infty}$, there is one location in the outer layer and one location in the inner layer within a fully turbulent attached boundary layer where $Re_t = Re_{t,1}$ (see figure 19). Noting the existence of multiple locations that correspond to the same feature value is important because any augmentation that uses Re_t to introduce model corrections in the outer layer will affect the inner layer and vice versa. Hence, another feature (or limiter) will be required to prevent any unintended augmentations.

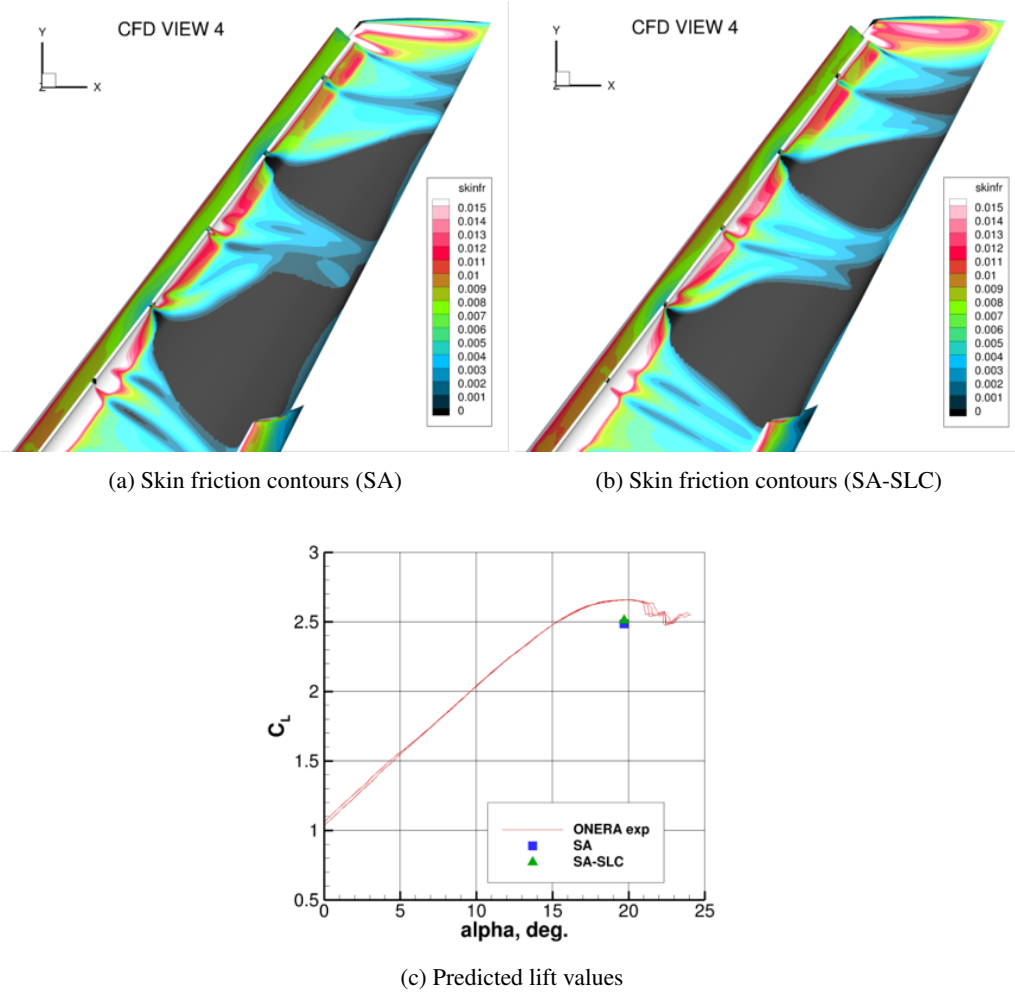


Figure 18: Results for baseline and modified SA applied to a high-lift configuration of the Common Research Model

Notable transformations (see figure 19):

- $1/(\text{Re}_t + 1)$ specifically focuses (and show variations) over the buffer layer and the outermost parts of the wake region in a turbulent boundary layer.
- In the SA model, the variable $\chi = \tilde{\nu}/\nu$ is similar to Re_t . The most prominent dissimilarity between Re_t and χ is in their behaviors within the viscous sublayer and the inner layer.
- We have observed that a transformation like $100/(\text{Re}_t + 100)$ is very useful when the one desires to resolve variations in Re_t within the boundary layer.
- A simple sigmoid function like $1/(1 + \exp(s \cdot (t - \text{Re}_t)))$ results in a limiter that is close to zero for $\text{Re}_t < t$ and close to unity for $\text{Re}_t > t$, given that a sufficiently high sharpness s is chosen. Hence, such a limiter helps isolate regions strictly within a boundary layer (or a shear layer). For some features that follow, we shall use such a limiter $\text{Re}_{t,\text{lim}} = 1/(1 + \exp(100 - 10\text{Re}_t))$

2. Vorticity Reynolds Number: $\text{Re}_\Omega = d_w^2 \Omega / \nu$

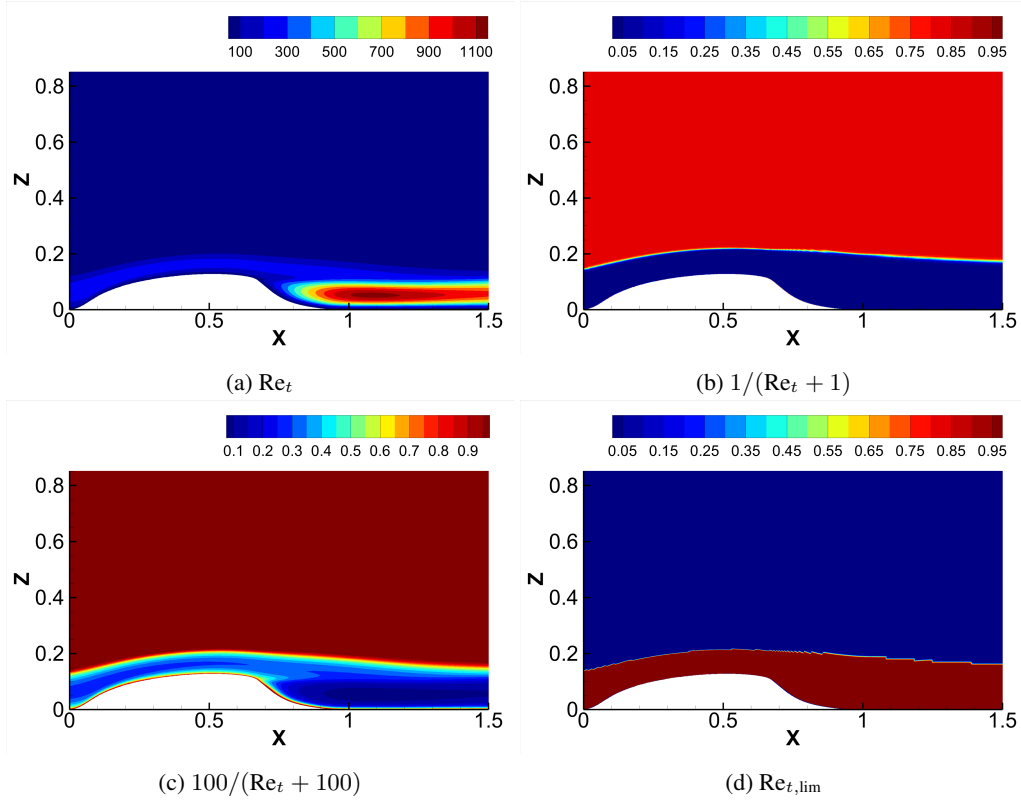


Figure 19: Feature variations of Re_t for 2D wall-mounted hump flow

Available in: all models

Useful to isolate: separated boundary layers and outer regions of attached boundary layers

Observations:

- The maximum value of Re_Ω along the wall normal direction is roughly linearly correlated to the momentum thickness Reynolds number (Re_θ) for attached boundary layers [35]. Note that this correlation also has a weak dependence on the pressure gradient.
- Contrary to what is assumed in the theory, the value of Re_Ω rarely asymptotes to zero in the freestream for most practical applications. Instead the d_w^2 part of this quantity amplifies even very small values of vorticity away from the wall, resulting in a noisy field outside the boundary layer. This quantity should, thus, be used with an appropriate limiter that can suppress this undesirable behavior outside the boundary layer.

Notable transformations (see figure 20):

- A variation of Re_Ω is Re_S which behaves very similarly but can assume slightly different values under regions of non-zero pressure gradients (see figure 20b).
- Within the SA model, one can use $Re_{\tilde{S}} = d_w^2 \tilde{S} / \nu$ instead of Re_Ω . The major difference between the two quantities is observed within the inner layer of an attached turbulent boundary layer where $Re_{\tilde{S}}$ is observed to be slightly less than Re_Ω .
- Other transformations like $Re_\Omega / (Re_\Omega + 3000)$ can also be useful especially for modeling bypass transition and determining incipient flow separation.

- The transformation $\text{Re}_t/(\text{Re}_\Omega + \text{Re}_t)$ can be useful to isolate regions with free shear layers.

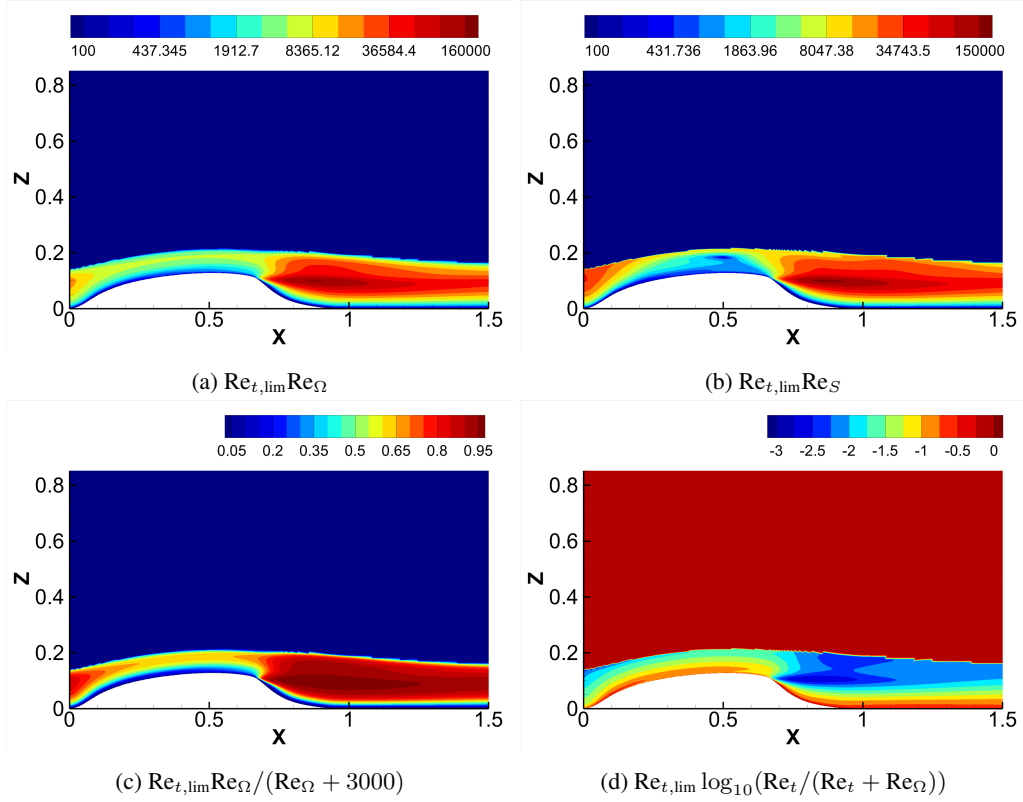


Figure 20: Feature variations of Re_Ω for 2D wall-mounted hump flow

3. Turbulence kinetic energy (TKE) Reynolds Number: $\text{Re}_k = d_w \sqrt{k}/\nu$

Available in: almost all models (approximations are available for one-equation models)

Useful to isolate: close-to-wall regions, high turbulence production regions

Observations:

- This feature can be thought of as a scaling for the wall distance to isolate regions in the inner layer of a turbulent boundary layer.
- The behavior is similar to that of Re_t , however some variations exist as is shown in figure 21c.

Notable transformations (see figure 21):

- Two interesting transformations are $\text{Re}_\Omega/(\text{Re}_\Omega + \text{Re}_k)$ and $\text{Re}_t/(\text{Re}_t + \text{Re}_k)$. Both of them are bounded between 0 and 1. The first transformation simplifies to $d_w \Omega/(d_w \Omega + \sqrt{k})$. This quantity is close to 1 within the viscous sublayer (since k is small). It decreases along the wall-normal direction, reaches a minimum, and then increases slowly in the outer layer. This is useful to find regions of relatively high vorticity and/or low turbulence kinetic energy in the outer layer (where the value will be close to 1). The second transformation simplifies to $\ell_t/(\ell_t + d_w)$ where ℓ_t is the turbulent length scale $\nu_t/\sqrt{k}$. Hence, it provides a comparison between the wall distance and the local turbulence length scale. This quantity is usually smaller for some regions in separated shear

layers since they are farther from the wall compared to regions in attached boundary layers that exhibit a similar local turbulence length scale.

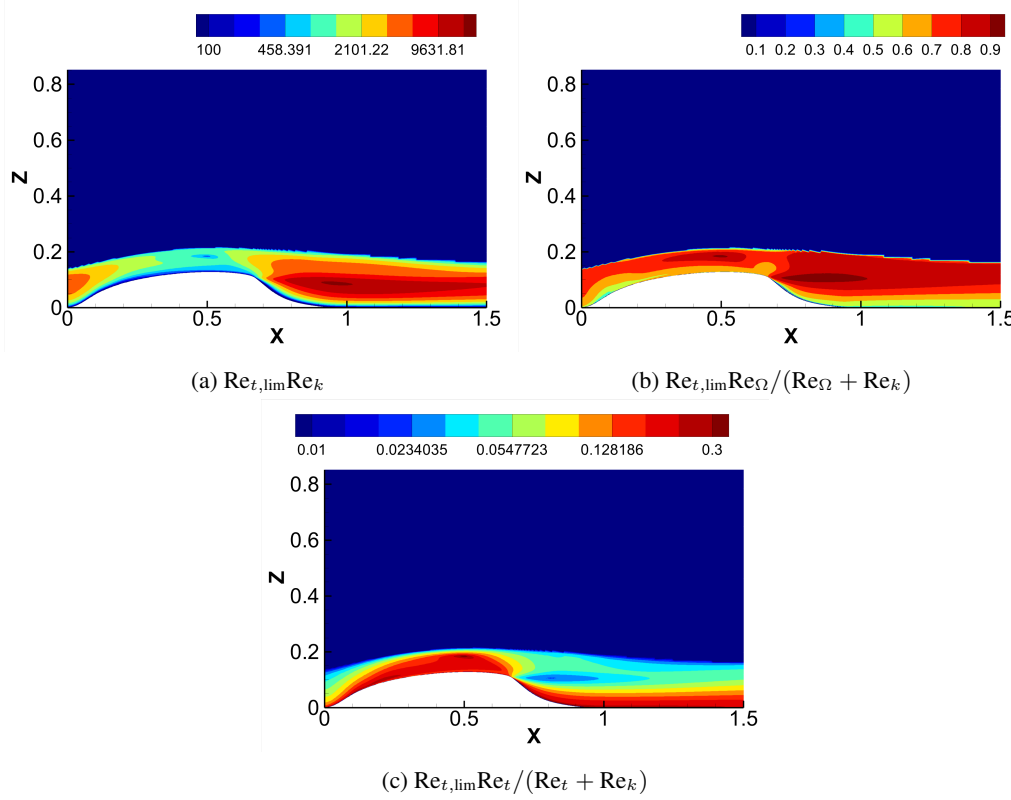


Figure 21: Feature variations of Re_k for 2D wall-mounted hump flow

4. Ratio of strain rate and vorticity: $r^* = S/\Omega$

Available in: all models

Useful to isolate: changes in streamline curvature and/or pressure gradients

Observations:

- This feature can be also thought of as a ratio between Re_S and Re_{Ω} .
- This feature can cause floating point overflow errors for regions with vorticity very close or equal to zero. It is, hence, recommended that a very small number is added to the denominator.
- The scaled Q-criterion $(\Omega^2 - S^2)/(\Omega^2 + S^2) = (1 - r^{*2})/(1 + r^{*2})$ is a transformation of this feature. Note that the Q-criterion is the second invariant of the velocity gradient tensor.

Notable transformations (see figure 22):

- One of the known transformations which is also used in the SA-RC model is $2r^*/(1 + r^{*2})$.

5. Shielding function used in detached-eddy simulations: f_d

Available in: all models

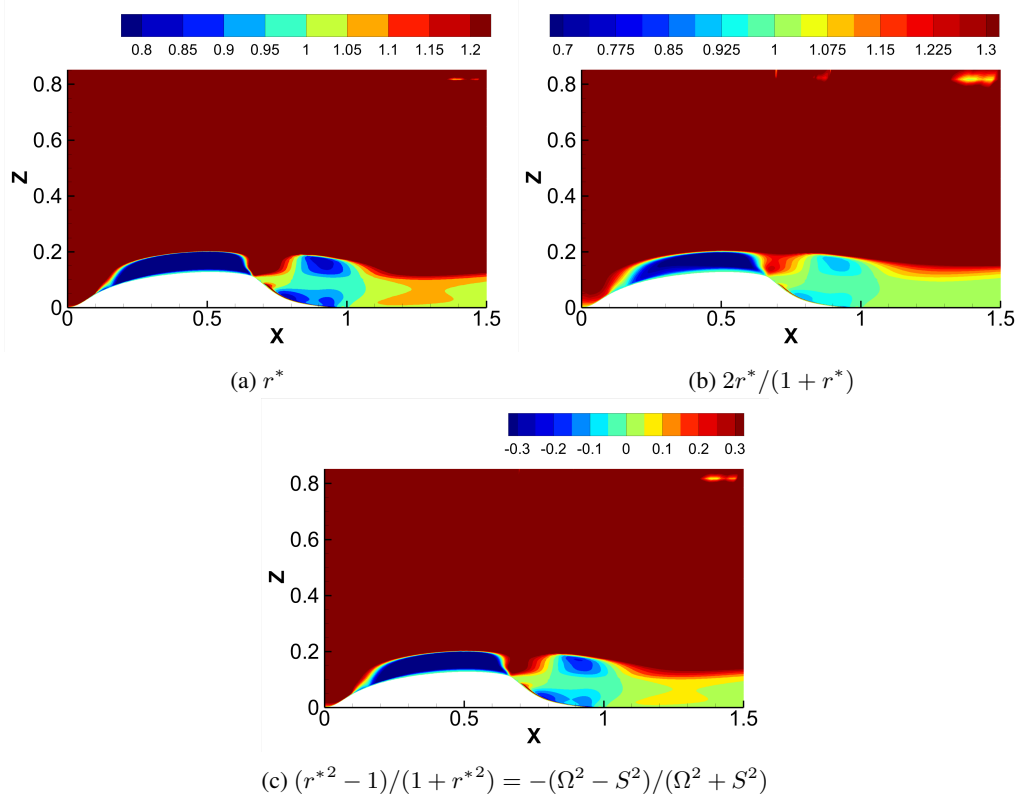


Figure 22: Feature variations of r^* for 2D wall-mounted hump flow

Useful to isolate: attached boundary layer regions

Observations:

- This feature depends on another quantity that can be considered a feature on its own: $r_d = (\nu + \nu_t) / (\kappa^2 d^2 \max(\sqrt{\text{tr}([\nabla \mathbf{U}][\nabla \mathbf{U}]^T)}, 10^{-10}))$ (where $\nabla \mathbf{U}$ is the mean velocity gradient tensor), which is analogous to the functions r (from the 1992 version of the SA model that is used to calculate model functions g and f_w) and $(1 + \text{Re}_t)/\text{Re}_\Omega$.

Notable transformations (see figure 23):

- The feature $\text{Re}_{t,\text{lim}} f_d$ can be used to isolate only the outermost regions of a turbulent boundary layer (including separated shear layers regions).
- The feature $\text{Re}_{t,\text{lim}} r_d$ can be very useful in detecting regions of separated turbulent shear layers with the highest values of Re_Ω .

We also tried out material derivatives of most of the feature variations mentioned above, since the material derivative of a Galilean invariant quantity also satisfies Galilean invariance. In many cases (e.g., $D\mathbf{S}/Dt$, $D\Omega/Dt$, etc.), the variation of the quantity in the separation region aligns well with what is desired from the augmentation. However, the main challenge with using a material derivative is proper non-dimensionalization. For instance, $D\Omega/Dt$ could be nondimensionalized with Ω^2 . However, for regions close to the edge of the boundary layer with small values of Ω , $D\Omega/Dt$ values get undesirably amplified. If one nondimensionalizes with ν_t^2/d_w^4 instead of Ω^2 , regions outside the boundary layer (far from the wall) with a small value of ν_t may get undesirably amplified. Moreover, using these nondimensionalization strategies modifies the behavior of the

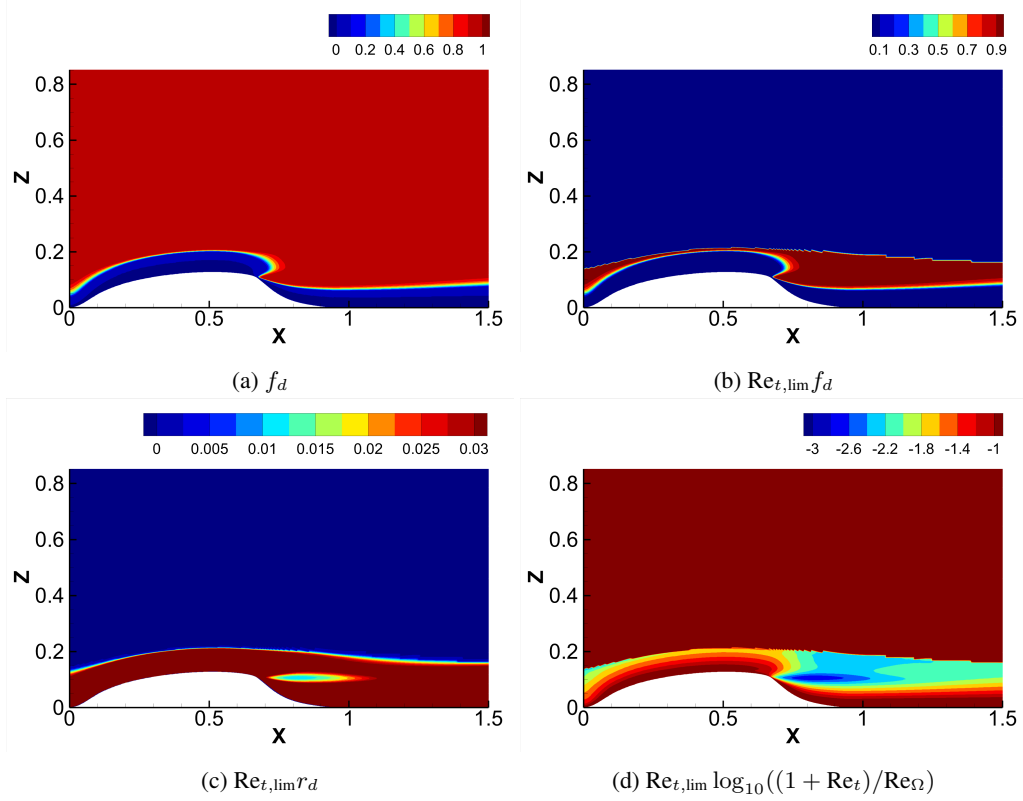


Figure 23: Feature variations of f_d for 2D wall-mounted hump flow

material derivative in the separated region, often deteriorating effectiveness. Hence, it is not trivial to choose a functional form that does the intended job well. Also note that calculating material derivatives of quantities that are spatial derivatives involves calculating second derivatives and hence may pose an inconvenience for some flow solvers.

Since it might be a good idea for the augmentation to be active in the entire separation bubble, another option that was explored made use of an auxiliary transport equation for the modified augmentation term $\beta' = \beta - 1$ similar to other turbulence variables, where the source term is zero everywhere except in the separated shear layer and the destruction term is designed to slowly dissipate β' . Since the streamlines form a loop within a separation bubble, the hope in choosing such a framework is that the production term would reinforce a positive feedback mechanism that will result in an amplification of the augmentation values within a separation bubble. On the other hand, for streamlines outside a separation bubble, any local increment in the augmentation value will be eventually dissipated and hence the effects should not carry too far from where the production term would be active. The time scale for such an augmentation is either chosen to be Ω , S , ω , or ν_t/d_w^2 (time scaling similar to that used in the destruction term of the Spalart-Allmaras model). Other combinations of these quantities (e.g., $\sqrt{S\Omega}$) may also serve as valid time scales in the transport equation. Note that the choice of the time scale may shield some flow regions from the effects of the production/destruction terms (e.g., zero vorticity regions) and attention should be paid to such shielding effects during modeling and validation. When taking the time scale to be the specific dissipation ω , the transport equation can be given as:

$$\frac{D\beta'}{Dt} = \omega(\phi_{\beta'} - c_{\beta'}\beta') + \nabla \cdot ((\nu + \nu_t)\nabla\beta') \quad (7)$$

where $c_{\beta'}$ is an appropriate constant, and $\phi_{\beta'}$ is a function of nondimensionalized modeled quan-

ties that has a positive value within a separated shear layer and zero otherwise. Note here that if one wishes to attenuate the values of β' even faster, one could take inspiration from the dissipation used in transport equations for ω from $k-\omega$ models and use β'^2 instead of β' in the destruction term. Several attempts were made to use the aforementioned features as candidates for $\phi_{\beta'}$. Different calibrations of such production terms were tried. Most of these trials showed that either the dissipation overpowered the production such that the augmentation was rendered ineffective, or the stability of the auxiliary transport equation was compromised. For the cases when stability was achieved without excessive dissipation, the results were virtually the same as or worse than using a corresponding algebraic formulation for the augmentation, and/or the stability was compromised for unseen configurations during testing. Note that despite our experience, there might exist candidates for $\phi_{\beta'}$ that result in superior results compared to algebraic augmentation functions.

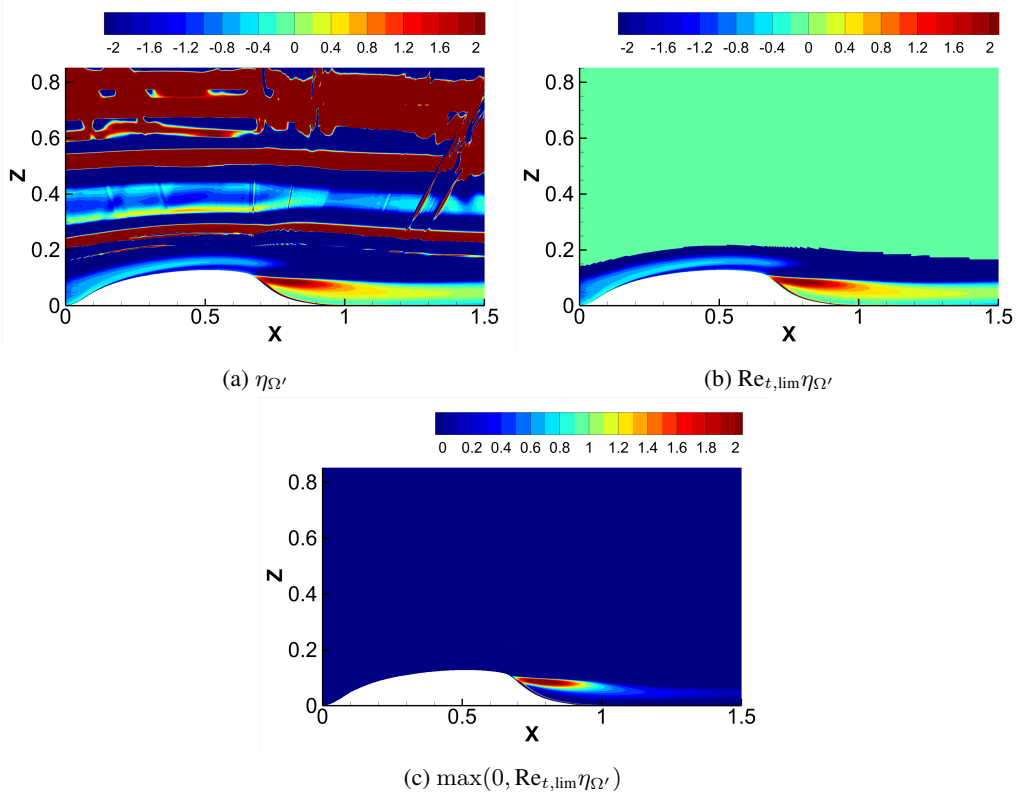


Figure 24: Feature variations of $\eta_{\Omega'}$ for 2D wall-mounted hump flow

We also considered the derivatives of the aforementioned feature candidates in the wall-normal direction, since derivatives of Galilean invariant quantities in the wall-normal direction are also Galilean invariant quantities. There are two minor issues that may cause some inconvenience when using wall-normal derivatives:

- The vector field of wall-normal directions is discontinuous if the wall has a concave sharp corner.
- Computing the gradient of a gradient (e.g., $\nabla\Omega$) may or may not be trivial in some flow solvers.

One such nondimensional quantity that we are currently exploring is $\eta_{\Omega'} = d_w \mathbf{n}_w \cdot (\nabla\Omega) / \Omega$ where $\mathbf{n}_w$ is the unit vector in the wall-normal direction. A convenient method to compute $\mathbf{n}_w$ is by setting

it to ∇d_w . For an attached boundary layer under zero/favorable pressure gradients, vorticity monotonically decreases away from the wall, and $\eta_{\Omega'}$ is negative. Under sufficiently adverse pressure gradients, attached boundary layer profiles exhibit an inflection point. Thus, vorticity starts increasing as one moves away from the wall ($\eta_{\Omega'}$ is positive close to the wall), then changes direction and starts decreasing into the freestream. For separated flows, as one moves away from the wall, the vorticity magnitude first decreases, then changes sign and increases for a while, and finally changes sign again and keeps on decreasing into the freestream. Hence, the region where $\eta_{\Omega'}$ is positive in such cases is no longer adjacent to the wall but away from it. The range in which the magnitude of $\eta_{\Omega'}$ varies depends on the local Reynolds number. Thus, making a feature out of $\eta_{\Omega'}$ will require some kind of normalization to ensure that the feature can be used across different flows. Note that for separated flows, there could be a location in the discretized domain within the boundary-layer profile where the vorticity is close to zero. The value of $\eta_{\Omega'}$ at this point may be extremely high (if not infinity – in the case where the value of vorticity is exactly zero). Also, a filter needs to be appropriately used to avoid large fluctuations outside the boundary layer, since the d_w in the numerator (and Ω in the denominator) will amplify even small values of $\mathbf{n} \cdot \nabla \Omega$ in this region. From our observations, the filter $\text{Re}_{t,\text{lim}}$ works reasonably well (see figure 24). Despite all these issues, $\eta_{\Omega'}$ can be reliably used to at least classify regions of separated flow and regions of adverse pressure gradients that lead up to incipient separation. Some other useful feature candidates based on wall-normal derivatives that we have explored are

- $d_w \mathbf{n}_w \cdot (\nabla S) / S$ behaves similar to $\eta_{\Omega'}$ except that it is active in some non-separated regions close to the edge of the boundary layer.
- $d_w \mathbf{n}_w \cdot (\nabla r^*)$ tends to be positive for regions within the boundary layer that are characterized by favorable pressure gradients.
- $d_w \mathbf{n}_w \cdot (\nabla \mu_t) / \mu_t$ and $d_w \mathbf{n}_w \cdot (\nabla k) / k$ behave similar to f_d .

Quite recently, along the lines of the work by Lozano-Duran and coworkers [24], we are exploring products of nondimensional feature candidates raised to fractional exponents. Our initial experience with such techniques indicates that the method of obtaining the optimal number of features (and exponent values) is not trivial and requires some additional work in the context of RANS modeling.

As should be clear by now, any function of the quantities listed above (when nondimensionalized properly) is also a feature candidate. Thus, it is not possible to prepare an exhaustive list of all features. However, we hope this discussion benefits the reader in understanding features can be created that are appropriate for a given application in turbulence modeling.

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