Towards LES wall models using optimization techniques

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1. Introduction

Large-eddy simulations (LES) of high Reynolds number flows are difficult to perform due to the need to include a large number of grid points in the near wall region. While LES models the small scales of the flow and resolves the large, dynamically important scales, near the wall, eddies scale with the distance from the wall and move increasingly nearer to the wall as the Reynolds number increases. These eddies are dynamically important despite their small size. Unfortunately, the eddy viscosity sub-grid scale (SGS) models only make a small contribution to the total Reynolds stress. This makes these models invalid near the wall (Jimenez & Moser 2000), unless the LES grid is sufficiently refined to resolve the near-wall vortical structures. Therefore, the number of grid points for an LES scales as Re_τ^2 in an attached boundary layer (Baggett, Jimenez & Kravchenko 1997). This is only a slight improvement on the scaling for a full direct numerical simulation (DNS) of $Re^{9/4}$.

The technique of wall modeling was developed to reduce the Reynolds number scaling of LES resolution so that LES could be applied in practical situations. For recent reviews, see Cabot & Moin (1999) and Piomelli & Balaras (2002). The approach has a long history dating back to atmospheric science and oceanographic applications. Limited by the computational power of the time, Deardorff (1970) was the first to implement a model for the wall layer in an LES of a channel flow at infinite Reynolds number. He implemented constraints on wall-parallel velocities in terms of the wall-normal second derivatives to ensure the LES satisfied the log-law in mean. The wall transpiration velocity was set to zero. The first "modern" wall model was developed by Schumann (1975). It is a modern wall model in the sense that the wall stresses are determined directly by an algebraic model. The wall stresses were found by assuming that they were in phase with the velocity at the first off wall grid point and that the deviation from their mean was proportional to the deviation of the velocity from its mean. Since the flow was in a channel, both the mean wall stresses and mean velocities were known. The transpiration velocity was set to zero. Many improvements to this basic model have been proposed and tested, see e.g. Piomelli *et al.* (1989), Mason & Callen (1986), Grötzbach (1987), and Werner & Wengle (1991), although none of these attempts produced a wall model robust enough for use in most engineering flows.

To address this robustness issue in wall modeling, several investigators used more elaborate near-wall flow models to compute the wall stresses (see e.g. Balaras *et al.* (1996) and Cabot & Moin (1999)). This type of approach divides the computational domain into two regions: one near the wall and one away from the wall. A simplified set of equations based on turbulent boundary-layer (TBL) approximations are solved on a near wall grid separate from the outer LES grid, subject to boundary conditions determined from the outer LES velocity together with the no-slip wall. The computed wall stress is then provided to the LES as a boundary condition. While this method does require the solution of an extra set of equations, the simplifications made in these equations makes its cost much less than the evaluation of the LES equations. This method was tested in a plane channel, square duct, and rotating channel by Balaras *et al.* (1996) and in a plane channel and backward-facing step by Cabot & Moin (1999). More recently, Wang & Moin (2002) used a variant of this method to perform an LES of an airfoil trailing edge flow. The results are generally better than those of the algebraic models, since the TBL equations can account for more of the physics of the flow. However, there is insufficient evidence of robustness of this approach, particularly on coarse meshes and at high Reynolds numbers.

The difficulty of formulating a robust wall model was highlighted by Cabot (1996). In that work, a backward facing step LES was performed using the "exact" time series of the wall stress from a resolved LES as the wall model. The results of this approach were not satisfactory and in fact not an improvement over the other types of wall models previously mentioned. This indicates that SGS and numerical errors play an important role in the coarse grid LES, which has not been accounted for by the previous wall models. To investigate this hypothesis and determine what information a wall model must provide to the LES, Nicoud *et al.* (2001) used optimal control techniques to compute the wall stresses in a channel LES at $Re_\tau = 4000$. A cost function was defined to be the difference between the plane-averaged LES streamwise and spanwise velocity fields and their known mean values (log-law in the streamwise direction and zero in the spanwise direction). Adjoint equations were used to determine the cost function derivatives, and iterations were performed at each time step to determine the best wall stress. Since the iterations were not performed over a large time window, this approach was sub-optimal. Linear stochastic estimation (LSE) was then used to determine a feedback law for the wall stresses based on their correlation with LES velocities obtained from the sub-optimal control algorithm.

Many important lessons were learned from this work involving wall models based on optimal control theory. Unfortunately, this approach proves to be impractical due to the high computational cost required for the suboptimal control since it requires both the solution of adjoint equations and many iterations to achieve convergence in the wall stresses. Furthermore, the cost function is based on known target data, making the model non-predictive. Baggett *et al.* (2000) also demonstrated that the LSE models generated from such computations are too sensitive to the numerical parameters to construct a universal LSE coefficient database. The objective of the present work is to develop a low-cost, robust wall model to achieve the accuracy of the sub-optimal control technique without an *a priori* target solution. A cost function based on a Reynolds-averaged Navier Stokes (RANS) solution will be constructed in Section 2 to make the model predictive, and in Section 3, the problem will be formulated in an optimal shape design setting in an attempt to reduce the computational cost. Some test results and discussions are presented in Sections 4 and 5.

2. Cost function

In order to make the wall model predictive, an easy to evaluate cost function near the wall using quantities not known *a priori* must be defined. To this end, a RANS model is used to provide the target velocity. This is motivated by the recognition that the near-wall region of a high Reynolds number boundary layer is more appropriately modeled by

RANS than by a coarse grid LES with filter length larger than the integral scale of the turbulence.

In the present work, the RANS model is obtained from a simplified version of the TBL equation model used by Wang & Moin (2002):

$$\frac{d}{dy}\left[\left(\nu+\nu_t\left(y\right)\right)\frac{du_i}{dy}\right]=\frac{1}{\rho}\frac{\partial p}{\partial x_i}\bigg|_{\mathrm{LES}}, \quad i=1,3 \tag{2.1}$$
$$\nu_t\left(y\right)=\kappa\nu y^+\left(1-e^{-y^+/A}\right)^2, \quad y^+=yu_\tau/\nu.$$

These equations model all Reynolds stresses through a damped mixing length eddy viscosity, and explicitly account for the pressure gradient which is assumed constant across the wall layer and is imposed by the LES. To complete the model, a no slip condition is applied at the wall and the outer boundary is set to be the LES velocity. The resulting velocity profile should be interpreted as the ensemble averaged velocity profile given the local LES state. It can therefore be expected that, on average, the resolved LES should match the RANS solution near the wall. Note that this model is chosen for simplicity in this initial attempt, and there are likely better models for this application that will be explored in future work.

In an overlapped region consisting of N LES grid points in the wall-normal direction, cost functions are devised to match the LES and RANS solutions on average. An attractive method in a statistically stationary flow would be to use a running time average to provide the target velocities. However, if the control authority is restricted to the current time, this approach becomes impractical since the flow at the current time would contribute only a small fraction of the total cost function. This makes it difficult to determine the control since the cost function is insensitive to it. If the control is explicitly computed as a function of time, then adjoint equations have to be integrated backward in time to find a correct solution over a sufficiently large time window which contains enough statistical samples.

An alternative is to use the current state as the statistical sample. Thus, the first cost function is defined to be the $\mathcal{L}_2$ difference between the LES and RANS states:

$$J_{\mathcal{L}_2}=\int_S\sum_{n=1}^{N}\left(\left(u_{\mathrm{RANS},1}|_{y_n}-u_{\mathrm{LES},1}|_{y_n}\right)^2+\left(u_{\mathrm{RANS},3}|_{y_n}-u_{\mathrm{LES},3}|_{y_n}\right)^2\right)dS, \tag{2.2}$$

where S is the surface and y_n are the locations of the n overlap points. In this way, a sufficient number of samples of the flow state are used to make a meaningful average. Also, the cost function is based only on quantities at the current time step, so no history information is required. This type of cost function is also compatible with the gradient evaluation methods used in this work (see Section 3).

Other cost functions can also be formulated for this problem. A cost function based on the average deviation of the LES and RANS is:

$$J_A=\left(\int_S\sum_{n=1}^{N}\left(\left(u_{\mathrm{RANS},1}|_{y_n}-u_{\mathrm{LES},1}|_{y_n}\right)+\left(u_{\mathrm{RANS},3}|_{y_n}-u_{\mathrm{LES},3}|_{y_n}\right)\right)dS\right)^2. \tag{2.3}$$

This cost function is similar to that used by Nicoud *et al.* (2001). However, as shown in Section 4, this cost function performs quite poorly. Analysis of its gradients indicates that they do not capture the sign information correctly in some regions (gradient computation will be discussed in the next section). In order to retain more information and move in the direction of feedback control, a signed cost function has also been used:

$$J_S = \int_S \sum_{n=1}^{N} \left(\left(u_{\mathrm{RANS},1}|_{y_n} - u_{\mathrm{LES},1}|_{y_n} \right) + \left(u_{\mathrm{RANS},3}|_{y_n} - u_{\mathrm{LES},3}|_{y_n} \right) \right) dS. \qquad (2.4)$$

When this cost function is used, the control strategy is shifted to force the cost function to zero rather than minimizing it. It was thought that this approach might better take advantage of the method being used for gradient evaluation, but it only resulted in a moderate improvement (see Section 4)

The choice of N in (2.2) - (2.4) should be made to include as many matching layers as possible while remaining in the region where the RANS model is a reasonable approximation for the given local flow. Furthermore, the LES velocity too close to the wall may involve large errors (Cabot 1996) and thus is not suitable as a RANS boundary condition. In the calculations presented in this article, N has been chosen to be three.

Two important points should now be noted. First, while all the cost functions here are based on matching RANS and LES velocities, other quantities could also be used. These could include matching vorticity or energy fluxes with suitable models. Second, it may not be possible or desirable to reduce the cost function to zero. Doing so could artificially reduce the turbulence fluctuations of the flow. Also, if an inexpensive scheme is required, it may not be possible to fully optimize the solution. Thus, the cost function must act as a suitable quantity for feedback regulation, rather than for minimization.

3. Optimization using shape design techniques

Optimal shape design consists of a set of techniques for optimizing a shape to achieve an engineering objective (e.g. Mohammadi & Pironneau 2001). Several approaches have been developed in this field that have had some success in reducing the computational expense of the optimization procedure. In an attempt to bring these techniques to bear, the wall modeling problem is formulated in this framework.

In general, the formulation is to consider a partial differential equation $A\,(U, q, a) = 0$ in a region Ω satisfying boundary conditions $b\,(U, q, a) = 0$ on $\partial\Omega$. The optimization is performed to determine

$$\min_a \left\{ J\,(U, q, a) : A\,(U, q, a) = 0\; \forall x \in \Omega, b\,(U, q, a) = 0\; \forall x \in \partial\Omega \right\} \qquad (3.1)$$

for some cost function $J\,(U, q, a)$. In this formulation, U is the state, q the shape, and a are the control variables. The gradient of the cost function with respect to the control variables is then:

$$\frac{dJ}{da} = \frac{\partial J}{\partial a} + \frac{\partial J}{\partial q}\frac{\partial q}{\partial a} + \frac{\partial J}{\partial U}\frac{\partial U}{\partial q}\frac{\partial q}{\partial a}. \qquad (3.2)$$

The standard technique for solving this equation is to use an adjoint method interfaced with a gradient minimization technique. But, as previously noted, this can be expensive and present data storage difficulties in time-accurate computations. Since it is the last term in (3.2) that requires the adjoint evaluation, Mohammadi & Pironneau (2001) suggest the following assumption when the controls and the cost function share the same support:

$$\frac{dJ}{da} \approx \frac{\partial J}{\partial a} + \frac{\partial J}{\partial q}\frac{\partial q}{\partial a}. \qquad (3.3)$$

This assumption is called the method of incomplete sensitivities since the sensitivity to the state gradient is ignored. The use of this method has been explored in this work since it has produced positive results in the optimization of aerodynamic shapes. For examples, see Mohammadi (1999), Mohammadi *et al.* (2000), and Mohammadi & Pironneau (2001), although these are all steady, two-dimensional applications. Since no rigorous proof on the applicability of this technique exists and its usefulness is based on purely empirical studies, it was not known how well it would perform in a full LES. Furthermore, the present cost function is not defined exactly on the support of the control, although it is defined in a small neighborhood of the control. While these factors will produce errors, the gradient evaluation needs only accurately predict the sign of the gradient and capture to some degree the difference in magnitudes of the derivatives with respect to different control parameters. A goal of this work is to determine if the amount of information contained in this gradient is sufficient for application to wall boundary conditions.

In order to apply the incomplete sensitivity assumption, the control must be related to shape design parameters. B-splines spaced evenly along the surface (although not enough to form a complete basis) are used to parameterize deformations normal to the surface. The control parameters, a_i, are then the spline amplitudes. The gradient of the cost function with respect to these parameters can be computed using finite differences by perturbing each parameter by a small value, ϵ, and then using (3.3) to evaluate the gradient based on the current state information. It is not necessary to recompute the actual geometry or grid because all the state variables of interest can be stored and matched to the new surface. The parameter ϵ is chosen *a priori* by making it small enough such that the gradient values are independent of it.

Once the cost function gradient is known, the new spline amplitudes can be computed by

$$a_i^{k+1} = a_i^k - \rho \frac{\partial \mathcal{J}}{\partial a_i}, \tag{3.4}$$

where ρ is a descent parameter set in advance and k is the iteration count. The new shape is computed by adding the surface perturbations to the previous shape. To relate this to the wall stresses, the RANS model is used to compute the correction to the equivalent slip velocity on the original surface:

$$u_{w,i}^c = f_{\mathrm{RANS},i}\left(y_{new}\right), \quad i = 1, 3, \tag{3.5}$$

where f stands for the RANS model given by (2.1). This approach is inspired by a Taylor series expansion about the wall (Mohammadi & Pironneau 2001). In this way, it is not necessary to change the computational geometry of the LES.

The total slip velocity is given by adding the correction $u_{w,i}^c$ to the old wall slip velocity. Corrected wall stresses can then be computed directly by definition

$$\tau_{w,i} = \tau_{w,i}^o + \frac{1}{Re} \frac{-u_{w,i}^c}{\Delta x_2}, \tag{3.6}$$

where Δx_2 is the local wall normal grid spacing.

While this approach avoids the evaluation of a set of adjoint equations, iterations are still required to converge the solution. Additional function evaluations are also often used to determine an optimal choice for ρ at each iteration. In order to make the wall model practical, these costs must be avoided. Therefore, no iterations are performed at each time step. The cost function gradients are computed and used in a feedback manner to provide a correction. Every a_i is reset to zero at each time step. Also, ρ is taken to be a fixed parameter similar to the gain in a feedback controller. To make up for some of this

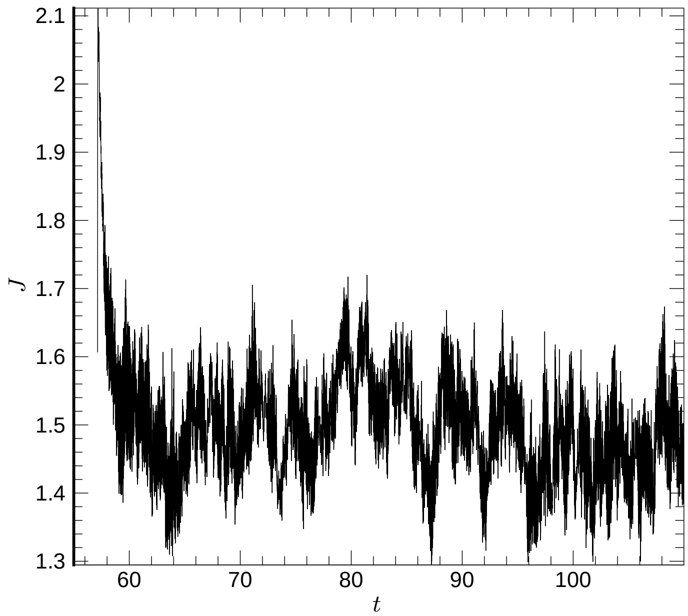

FIGURE 1. $\mathcal{L}_2$ cost function history.

lost information, a predictor-corrector approach to the control algorithm is used. This is done by using (2.1) to compute a prediction of the wall stress before the optimization is used. It is expected that the prediction will account for the missing physics in the coarse grid LES while the optimization will correct for the numerical and SGS modeling errors. While this approach must be classified as sub-optimal, it is still reasonable to expect a cost function reduction if at each time step the LES velocity is forced in the direction of the reduced cost function.

4. Results

The application of this method to the trailing edge flow simulated previously by Wang & Moin (2000, 2002) has produced mixed results. The first goal is to justify the incomplete sensitivities assumption. The $\mathcal{L}_2$ cost function history is shown in Figure 1. While the average value is reduced approximately 15% from the inital value, this is not completely out of the range of the cost function fluctuations. It is therefore inconclusive regarding the validity of the assumption. As shown in Figure 2, the predicted wall stress matches the full LES wall stress quite well in some regions for the $\mathcal{L}_2$ and signed cost functions, but performs poorly in other regions. The separation point is predicted reasonably accurately for both these cost functions. As previously indicated, the average cost function performed more poorly. Figure 3 contains a comparison between the $\mathcal{L}_2$ cost function results and the predictor alone. The new results are much better in the region near the skin friction peak, although they produce a less smooth skin friction profile, and rather large errors remain in part of the adverse pressure gradient region. Overall, the model demonstrates

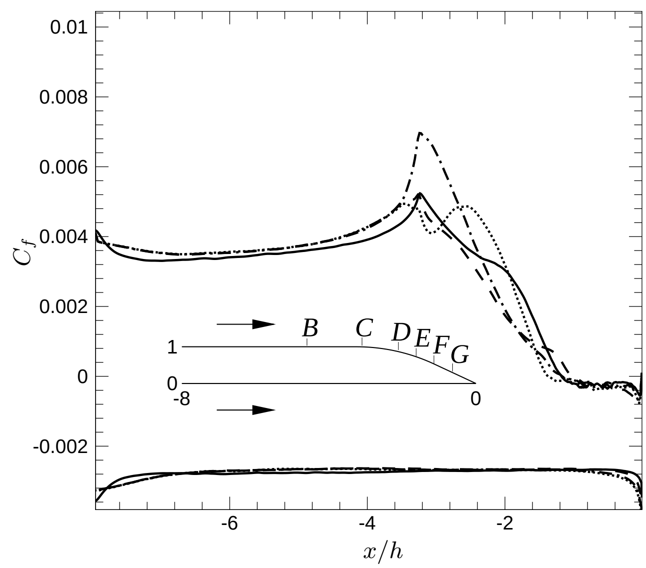

FIGURE 2. Time averaged skin friction over the airfoil surface: ---- , $\mathcal{L}_2$ cost function; —·— , average cost function; ········ , signed cost function; ——— , full LES of Wang & Moin (2000).

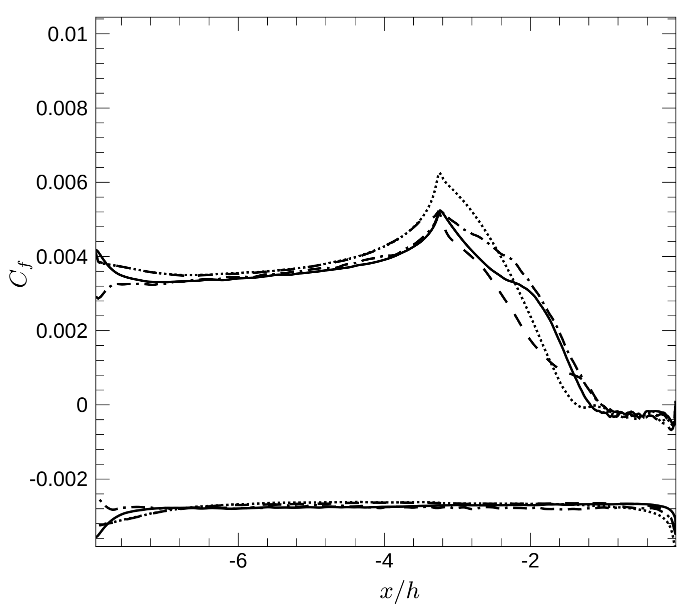

FIGURE 3. Time averaged skin friction over the airfoil surface: ---- , $\mathcal{L}_2$ cost function; ········ , predictor only; ——— , full LES of Wang & Moin (2000); —·— , TBL model of Wang & Moin (2002).

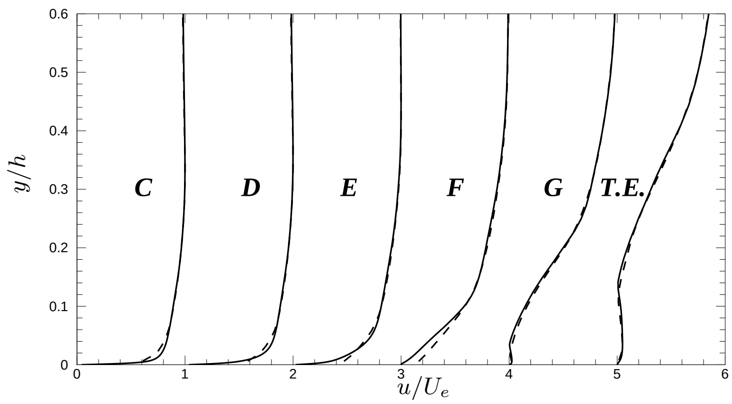

FIGURE 4. Mean velocity magnitude profiles at several trailing edge stations: ---- , $\mathcal{L}_2$ cost function; ——— , full LES of Wang & Moin (2000). Locations are those indicated in Figure 2. T.E. is the trailing edge point.

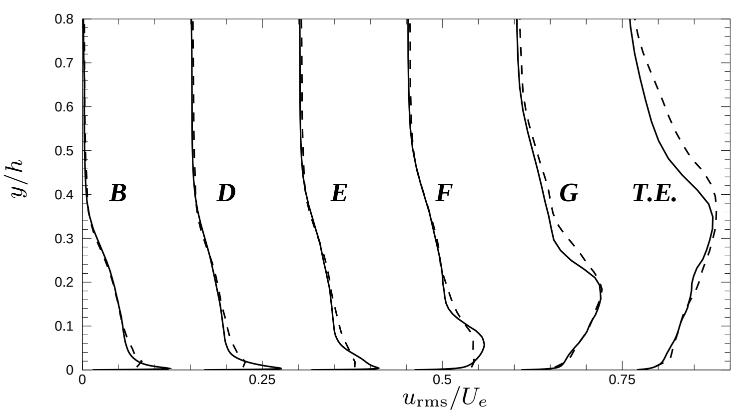

FIGURE 5. Streamwise component of turbulence intensities at several trailing edge stations: ---- , $\mathcal{L}_2$ cost function; ——— , full LES of Wang & Moin (2000). Locations are those indicated in Figure 2. T.E. is the trailing edge point.

some improvement over the simple wall model used as a predictor, but is less accurate than the full TBL equation model used in Wang & Moin (2002).

Comparison of the velocities between the full LES and wall modeled LES (based on the $\mathcal{L}_2$ cost function, which produced the best results) are quite good. As shown in Figures 4 and 5, the coarse grid LES is able to match the resolved LES very closely. The main (moderate) discrepancy occurs in the turbulent intensities near the wall. This is not unreasonable since these quantities were not included in the cost function and it may in fact not be possible to capture these regions accurately because the LES grid does not resolve the intensity peak. When compared to the results of Wang & Moin (2002) using only the predictor, the results are found to be comparable and in fact are worse for the two cost functions not shown. Therefore, it is difficult to draw definitive conclusions about the effect of the gradient based optimization procedure on the velocity field.

5. Channel flow analysis

In order to evaluate the proposed wall model in a more controlled environment, the algorithm has been implemented in the plane channel LES of Nicoud *et al.* (2001). This is a simpler and well known case, so the model can be more readily analyzed. It was immediately noticed that, unlike the trailing edge case, the cost function gradients could not be made independent of the small parameter ϵ used in the finite-difference computation. The gradients monotonically decreased with ϵ until they reached a value of zero. This result indicated that the incomplete sensitivity approach did not accurately capture the gradients in the channel since Nicoud *et al.* (2001) observed non-zero gradients in the sub-optimally controlled channel. The following analysis is used to explain these results, as well as the difficulties encountered with this method in the trailing edge geometry.

Consider a cost function of form

$$J(a) = \int_S f(u(a))dS. \tag{5.1}$$

Since in the current framework, the shape and shape deformations are defined in two dimensions, the surface can be parameterized by taking the y coordinates as a function of x, i.e. $y = g(x)$. Then the cost function becomes

$$J(a) = \int_0^l f(u(x;a))\sqrt{1 + (g'(x))^2}dx. \tag{5.2}$$

Consider a perturbation to this surface parameterized by $\epsilon h(x)$. In the current context, $h(x)$ would correspond to the spline and ϵ to the small change in the control parameter. The new cost function is computed by considering its sensitivity to geometry only, so

$$J(a+\epsilon) = \int_0^l f(u(x;a))\sqrt{1 + (g'(x) + \epsilon h'(x))^2}dx. \tag{5.3}$$

By using a Taylor series expansion, one obtains to $O(\epsilon)$:

$$\sqrt{1 + (g'(x) + \epsilon h'(x))^2} \approx \sqrt{1 + (g'(x))^2} + \epsilon(1 + (g'(x))^2)^{-1/2}g'(x)h'(x). \tag{5.4}$$

When the gradient is computed by taking $(J(a+\epsilon) - J(a))/\epsilon$, the resulting term is

$$\frac{\partial J}{\partial a} \approx \int_0^l f(u(x;a))(1 + (g'(x))^2)^{-1/2}g'(x)h'(x)dx. \tag{5.5}$$

This expression explains the observed cost function gradients. First, it has been demonstrated in both the trailing edge and channel flows that in regions where the surface is flat, the gradients are zero. This is clear since in these regions, $g'(x) = 0$. A similar observation occurs in areas where the surface is a straight line. This is because $g'(x)$ is constant and, in this case, $h(x)$ is symmetric, meaning that whenever $h'(x) > 0$, there is a corresponding x_1 such that $h'(x_1) = -h'(x)$. Thus, unless $f(u(x;a))$ has a very large change between x and x_1, since $g'(x)h'(x) + g'(x_1)h'(x_1) = 0$ the gradient will be very small.

Finally, it has been observed that in regions of curvature away from the direction of perturbation and for a positive definite $f(u(x;a))$ (such as the $\mathcal{L}_2$ cost function), the gradient is always positive. This can be seen by examining the product $g'(x)h'(x)$. In these regions, $g'(x)$ is always negative and increases monotonically in magnitude. By the symmetry of $h(x)$, the regions where $h'(x)$ is positive correspond to $g'(x)$ having a smaller magnitude, and the regions where $h'(x)$ is negative correspond to $g'(x)$ having a greater magnitude. Thus, the positive contribution is greater in magnitude than the negative contribution, and hence the gradient is positive since $f(u(x;a))$ is positive and varies less than the curvature.

The sensitivity computed by this method is then almost exclusively dependent on the curvature of the function whose information is contained in $g'(x)$. It is difficult to determine how this information could be useful in changing the state u such that the given cost function is minimized in a rigorous and well defined manner. For any cost function defined as above, the incomplete sensitivity method will act in a way directly related to the curvature of the surface. If a correlation exists between reducing this curvature and reducing the cost function, the method may produce reasonable results. However, there is no reason to believe that, in general, reducing surface curvature will be helpful in wall modeling. In fact, as experience in the channel has demonstrated, a region of no curvature still requires control to obtain an accurate solution. Therefore, it is likely that an alternative method must be found for the general application of a wall model.

6. Conclusions and future work

Wall modeling using control theory is a promising new approach for developing robust wall models which account for not only the unresolved flow physics but also numerical and SGS modeling errors. In the present work, a methodology has been proposed to overcome the deficiencies of the model of Nicoud *et al.* (2001) and make the control-based wall model predictive and practical in terms of computational expense. Two critical components, namely the use of RANS velocity profiles as the near-wall LES target in the cost function and the incomplete sensitivity method for gradient evaluation have been examined and tested in a turbulent trailing edge flow.

Based on the results, it is clear that the assumption of incomplete sensitivities is not appropriate for LES wall models with the type of cost function considered in this work. This is at least partly due to the cost function measuring the LES state in the flow and not at the wall. A cost function that is more sensitive to the geometry could be better suited, but it is unclear how to formulate such a cost function for a wall model. Furthermore, there is evidence suggesting that in applications similar to this, the gradient calculated with incomplete sensitivities may have not only incorrect magnitude but also incorrect sign (Marsden *et al.* 2002). Clearly, a more accurate means is needed to compute the gradient.

The use of a cost function matching a RANS profile near the wall may however prove useful in LES wall modeling. It has a solid physical basis, although the RANS model used here is rather rudimentary. More robust RANS models, such the k-ω model are being considered. In addition to choosing an appropriate RANS model, the choice of matching quantities is also an important factor in the performance of the model. Matching LES and RANS velocities may prove not to be the best quantity to minimize for optimal performance of the model. Cost functions based on vorticity or energy could better account for dynamics that are more important to the large scales in the LES. An investigation of these cost functions and implementation of a RANS model is underway in a channel flow.

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