Building-block-flow wall model for large-eddy simulation

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A wall model for large-eddy simulation (LES) is proposed by devising the flow as a collection of building blocks. The core assumption of the model is that a finite set of simple canonical flows contains the essential physics to predict the wall stress in more complex scenarios. The model is constructed to predict zero/favorable/adverse mean-pressure-gradient wall turbulence, separation, statistically unsteady turbulence with mean-flow three-dimensionality, and laminar flow. The approach is implemented using two types of artificial neural networks: a classifier, which identifies the contribution of each building block in the flow; and a predictor, which estimates the wall stress via combination of the building-block flows. The training data are directly obtained from wall-modeled LES optimized to obtain the correct mean quantities. This approach guarantees the consistency of the training data with the numerical discretization and the gridding strategy. The output of the model is accompanied by a confidence score in the prediction. The latter aids the detection of areas where the model underperforms, such as flow regions that are not representative of the building blocks used to train the model. The model is validated in canonical flows (laminar/turbulent boundary layers, turbulent channels, turbulent Poiseuille-Couette, turbulent pipe) and two realistic aircraft configurations: the NASA Common Research Model High-lift and NASA Juncture Flow Experiment. It is shown that the building-block-flow wall model outperforms (or matches) the predictions by an equilibrium wall model. It is also concluded that further improvements in WMLES should involve advances in SGS modeling.

I. INTRODUCTION

The use of computational fluid dynamics (CFD) for external aerodynamic applications has been a key tool for aircraft design in the modern aerospace industry. However, flow predictions from state-of-the-art solvers are still unable to comply with the stringent accuracy requirements and computational efficiency demanded by the industry. In recent years, wall-modeled large-eddy simulation (WMLES) has gained momentum as a high-fidelity tool for routine industrial design. In WMLES, only the large-scale motions in the outer region of the boundary layer are resolved, which enables a competitive computational cost compared with other CFD approaches [17, 18, 71]. As such, NASA has recognized WMLES as an important pacing item for “developing a visionary CFD capability required by the notional year 2030” [64]. In the present work, we introduce a wall model based on the flow-state classification that also provides a confidence score for the classification.

Several strategies for modeling the near-wall region have been explored in the literature, and comprehensive reviews can be found in Cabot & Moin [16], Piomelli & Balaras [56], Spalart [65], Larsson et al. [39], and Bose & Park [12]. One of the most widely used approaches for wall modeling is the wall-flux modeling approach (or approximate boundary conditions modeling), where the no-slip and thermal wall boundary conditions are replaced with stress and heat-flux boundary conditions provided by the wall model. This category of wall models utilizes the large-eddy simulation (LES) solution at a given location in the LES domain as input and returns the wall fluxes needed by the LES solver. Examples of the most popular and well-known approaches are those computing the wall stress using either the law of the wall [20, 57, 61], the full/simplified Reynolds-Averaged Navier-Stokes (RANS) equations [7, 8, 10, 19, 35, 54, 69, 72] or dynamic wall models [5, 11].

In recent years, advances in data science and machine learning have incited new efforts to complement the existing turbulence modeling approaches in the fluids community. The reader is referred to Duraisamy et al. [21] and Brunton et al. [15] for a literature review on machine learning for fluid mechanics. Supervised learning, i.e., the machine-learning task of learning a function that maps an input to an output based on provided training input-output pairs, was first introduced in turbulence modeling in the form of subgrid-scale (SGS) modeling for LES. Early approaches used artificial neural networks to emulate and speed up a conventional, but computationally expensive, SGS model [60].
More recently, SGS models have been trained to predict the (so-called) perfect SGS terms using data from filtered direct numerical simulation (DNS) [27, 70]. Other approaches include deriving SGS terms from optimal estimator theory [67] and deconvolution operators [e.g., 26, 31, 52]. One of the first attempts at using supervised learning for wall models in LES can be found in Yang et al. [73]. These authors noted that a model trained on channel flow data at a single Reynolds number could be extrapolated to higher Reynolds numbers and similar configurations. Similar approaches for data-driven wall models using supervised learning were developed for various flow configurations such as a spanwise rotating channel [33], flow over periodic hills [76], turbulent flows with separation [74], and boundary layer flow in the presence of shock-boundary layer interaction [9] with mixed results in a posteriori testing. First attempt at a semi-supervised learning approach for WMLES can be found in Bae & Koumoutsakos [1], where the authors used reinforcement learning to train on channel flow at relatively low Reynolds numbers. The model based on reinforcement learning was able to extend to higher Reynolds numbers for channel flow and zero-pressure-gradient turbulent boundary layers. The reinforcement learning wall model has been extended to account for pressure gradient effects [75]. However, some of the models cited above rely on information about the flow that is typically inaccessible in real-world applications, such as the boundary-layer thickness and most are limited to simple canonical flow configurations.

Currently, the major challenge for WMLES of realistic external aerodynamic applications is achieving robustness and accuracy necessary to model the myriad of different flow regimes that are characteristic of these problems. Examples include turbulence with mean-flow three-dimensionality, laminar-to-turbulent transition, flow separation, secondary flow motions at corners, and shock wave formation, to name a few. The wall-stress generation mechanisms in these complex scenarios differ from those in flat plate turbulence. However, the most widespread wall models are built upon the assumption of statistically-in-equilibrium wall-bounded turbulence without mean-flow three-dimensionality, which only applies to a handful number of flows. The latter raises the question of how to devise models capable of seamlessly accounting for such a vast and rich collection of flow physics in a single unified approach, which is the aim of the present effort.

In this work, we develop a wall model for LES using building-block flows. A preliminary version of the method can be found in Lozano-Durán & Bae [44]. The model is formulated to account for various flow configurations, such as wall-attached turbulence, wall turbulence under favorable/adverse pressure gradients, separated turbulence, statistically unsteady turbulence, and laminar flow. The model comprises two components: a classifier and a predictor. The classifier is trained to place the flows into separate categories along with a confidence value, while the predictor outputs the modeled wall stress based on the likelihood of each category. The output of the model is also accompanied by confidence in the prediction. The training data are directly obtained from wall-modeled LES with an ‘exact’ model for mean quantities to guarantee consistency with the numerical discretization and grid structure. The model is validated in canonical flows outside the training set and complex flows. The latter includes two realistic aircraft configurations, namely, the NASA Common Research Model High-lift and NASA Juncture Flow Experiment.

This paper is organized as follows. The formulation of the new model is discussed in Section II. The numerical approach and traditional model to compare in Section III. The model is validated in Section IV and compared with the equilibrium wall model. Finally, conclusions are offered in Section VI.

II. MODEL FORMULATION

The working principle of the proposed model is summarized in Figure 1. The model is referred to as the building-block-flow wall model (BFWM) and was first introduced by Lozano-Durán & Bae [44]. The BFWM is comprised of two elements: a classifier and a predictor. First, the classifier is fed with data from the LES solver and quantifies the similarities of the input with a collection of known building-block flows. The predictor leverages the information of the classifier together with the input to generate the wall-stress vector prediction via interpolation of the building-block database. Each building block is dedicated to modeling different flow physics (e.g., wall-attached turbulence, adverse/favorable pressure-gradient effects, separation, laminar flow, etc.) and the model provides a blending between flows using information from the classifier. A confidence score is generated based on the similarity between the input data and the building-block flows. If the input data looks extraneous, the model provides a low confidence score, which essentially means that the flow is unknown and do not match any knowledge from the database. In the following, we elaborate on the model assumptions, requirements, input/output data, training data, and artificial neural network (ANN) architecture.

A. Model assumptions

The main modeling assumptions are:

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FIG. 1: Schematic of the building-block flow wall model (BFWM). Details are provided in Section II.

1. There is a finite set of simple flows (referred to as building-block flows) that contains the essential flow physics to formulate generalizable wall models.

2. The effect of the (missing) near-wall subgrid scales in WMLES of complex flows is representable by a linear combination of the near-wall behavior of the building-block flows.

3. The number of model inputs to correctly predict the wall stress is, at least, equal to the number of non-dimensional groups required to completely characterized all the building-block flows.

4. The non-dimensional form of the model inputs/outputs that provides the best predictive capabilities (i.e., interpolation/extrapolation between training cases) is obtained by scaling the variables with the kinematic viscosity and the distance to the wall.

5. Flow information from two contiguous wall-normal locations is enough to predict the wall stress in the vicinity of those locations.

6. History effects for the subgrid-scale flow are captured using instantaneous accelerations without the need for additional information from past times.

B. Model requirements

We consider the following model requirements:

1. The wall model should be able to account for different flow physics (i.e., laminar flow, wall-attached turbulence, separated flow,...) in a unified manner (i.e., the input and output structure of the model must be identical regardless of the case).

2. The model must be scalable to incorporate additional building-block flows if needed in future versions.

3. The model must provide a confidence score in the prediction at each point at the wall.

4. The model formulation must be directly applicable to complex geometries (e.g., realistic aircraft configuration) without any additional modifications. This requirement will constrain the allowable input variables (i.e., they will need to be local-in-space) and the parameters used for their non-dimensionalization.
5. The model must account for the numerical errors of the schemes employed to integrate the LES equations. This implies that the input data used to train the model must be consistent with data obtained from the actual LES solver rather than from filtered DNS.

6. The inputs and outputs of the model must be given in non-dimensional form to comply with dimensional consistency.

7. The model must be invariant under constant space/time translations and rotations of the frame of reference.

8. The model must be Galilean invariance under uniform velocity transformations of the frame of reference.

C. Building-block flows

Seven building-block flows are considered and examples are shown in Figure 2. All the cases entail an incompressible flow confined between two parallel walls with the exception of freestream flow. Cases with additional complexity, such as airfoils, wings, bumps, etc, are intentionally avoided. The rationale behind this choice is that building blocks should encode the key flow physics to predict more complex scenarios. Hence, we aim at avoiding case overfitting, i.e., correctly predicting the flow over a wing merely because the model was also trained on similar wings instead of faithfully capturing the flow physics.

For the building blocks, the streamwise, wall-normal, and spanwise spatial coordinates are denoted by $x$, $y$, and $z$, respectively. The walls are separated by a distance $2h$. The density is $\rho$ and the dynamic and kinematic viscosities of the fluid are $\nu$ and $\nu$, respectively. In the following, we discuss the configuration and physical motivation behind each building block. We also include in parenthesis the label for each building-block flow.

- Freestream (‘Freestream’). A uniform and constant velocity field is used as representative of freestream flows. The main role of this building-block flow is to identify near-wall regions with zero points per boundary-layer thickness. In these situations, BFWM applies a ‘ZPG’ model to estimate the wall stress. The prediction is accompanied by a low confidence score.

- Wall-bounded laminar flow (‘Laminar’). The near-wall region of a laminar flow is modeled using Poiseuille flow (i.e., parabolic mean velocity profile). The goal of this building block is to allow the prediction of the wall stress in wall-attached laminar scenarios. The case is characterized by the friction Reynolds numbers $Re_\tau = u_\tau h/\nu$, where $u_\tau$ is the friction velocity at the wall and $h$ is the channel half-height. The range of Reynolds numbers considered is from $Re_\tau = 5$ to $10^4$. A parabolic mean velocity profile is used to analytically predict the stress at the wall.

- Wall-bounded turbulence under zero mean-pressure-gradient (‘ZPG’). Canonical wall turbulence without mean pressure gradient effects is modeled using turbulent channel flows as a building block. The wall-stress predictions are provided by an ANN trained for $Re_\tau = 100$ to $Re_\tau = 10,000$ using numerical data [32, 48].

- Wall-bounded turbulence under favorable/adverse mean-pressure-gradient and separation (‘FPG’, ‘APG’, and ‘Separation’, respectively). We utilize the turbulent Poiseuille-Coetue flow as a simplified representation of wall-bounded turbulence subject to favorable and adverse mean-pressure-gradient effects. The bottom wall is set at rest and the top wall at a constant velocity equal to $U_t > 0$. A streamwise mean-pressure-gradient, denoted by $dP/dx$, is applied to the flow. Favorable pressure gradient effects are obtained for values of $dP/dx$ accelerating the flow in the same direction as the top wall. Adverse pressure gradient conditions are achieved for values of $dP/dx$ that accelerate the flow in the opposite direction as the top wall. Flow separation is represented by values of $dP/dx$ at which the wall stress at the bottom wall is zero. The different flow regimes are characterized by the two Reynolds numbers $Re_P = \pm \sqrt{(dP/dx)/\rho h/\nu}$ and $Re_U = U_t h/\nu$. The wall-stress predictions are provided by an ANN trained for $Re_P$ from $-1.2 \times 10^3$ to $1.2 \times 10^3$ and $Re_U = 5 \times 10^3$ to $2 \times 10^4$. New DNSs were conducted for these cases using the same numerical solver as in previous investigations by our group [42, 47].

- Statistically unsteady wall turbulence with 3-D mean flow (Unsteady). The last building-block flow considered is a turbulent channel flow subject to a sudden spanwise mean pressure gradient $dP/dz$. The role of this case is to capture out-of-equilibrium effects due to strong unsteadiness and mean-flow three-dimensionality, such as the decrease in the magnitude of the wall stress and the misalignment between the wall-stress vector and mean shear vector. Only the initial transient of the flow, where non-equilibrium effects manifest, is considered. The different flow regimes are characterized by the streamwise friction Reynolds number $Re_\tau = u_\tau h/\nu$ before the imposition of $dP/dz$ and the ratio of streamwise to spanwise mean pressure gradients $\Pi = (dP/dz)/(dP/dx)$. 


FIG. 2: Examples of the building block units taken as representative of the flow configurations. (a) Freestream, (b) laminar channel flow, (c) turbulent channel flow, (d) turbulent Poiseuille-Couette flow for zero wall stress, (e) turbulent Poiseuille-Couette flow with a strong adverse mean pressure gradient, and (f) turbulent channel flow with the sudden imposition of spanwise mean-pressure-gradient.

The wall-stress predictions are provided by an ANN trained for $Re_T = 100$ to 1000 and $Π = 5$ to 100 using data from Lozano-Durán et al. [46].

Figure 3 contains examples of the DNS mean velocity profiles for a selection of building-block flows. An advantage of the present building-block setup is that it allows for continuously generate data from one flow regime to another without modifying the geometry but only varying the non-dimensional numbers defining the case (e.g., from FPG to ZPG to APG to separation by just changing the mean pressure gradient). This facilitates the generation of training data filling the non-dimensional space of inputs, which translates into a more reliable model.

**D. Input and output variables**

The input variables are acquired using a two-point stencil as shown in Figure 1. The stencil contains the center of the control volume attached to the wall (where the wall stress is to be predicted) and the second control volume off the wall along the wall-normal direction. Given that the model is intended to be used in complex geometries, the centers do not need to perfectly align along the wall-normal direction. This misalignment is considered during the model training. The information collected from the flow is

$$\{u_1, u_2, γ_{12}, a_1, \dot{γ}_1, k_1, k_{m1}\},$$

where $u_1 = |\vec{u}_1|$ and $u_2 = |\vec{u}_2|$ are the magnitude of the wall-parallel velocities relative to the wall at the first and second control volumes, respectively, $γ_{12}$ is the angle between $\vec{u}_1$ and $\vec{u}_2$, $a_1$ is the magnitude of the acceleration at the first control volume, $\dot{γ}_1$ is the time derivative of the angle of $\vec{u}_1$ in the wall-parallel direction, $k_1$ and $k_{m1}$ are the turbulent kinetic energy and mean kinetic energy, respectively at the first control volume and relative to the wall. The mean velocity to compute $k_1$ and $k_{m1}$ is obtained via an exponential average in time (denoted by $\bar{\cdot}$) with time scale $10\Delta/\sqrt{k_{m1}}$, where $\Delta$ is the characteristic grid size based on the cube-root of the control volume. The quantities predicted by the model are

$$\{τ_w, γ_{1w}, p_{class}, p_{conf}\},$$
FIG. 3: Mean velocity profiles for a selection of building-block flows. (a) Turbulent channel flows for (from left to right) $Re_{\tau} = 180, 550, 950, 2000, 4200, \text{ and } 10,000$ (ZPG). (b) Turbulent Poiseuille-Couette with favorable mean-pressure-gradient (FPG) at $Re_U = 6500$ (dashed) $Re_P = 0, 100, 150, 200, 250, 300$ (from left to right) and $Re_U = 22,360$ (solid) for $Re_P = 0, 380, 550, 750, 800, 1000$ (from left to right). (c) Turbulent Poiseuille-Couette with adverse mean-pressure-gradient (APG) and separation at $Re_U = 6500$ (dashed) $Re_P = 0, -100, -150, -200, -250, -300$ (from right to left) and $Re_U = 22,360$ (solid) for $Re_P = 0, -380, -550, -750, -800, -1000$ (from right to left). (d) Turbulent channel flow with the sudden imposition of spanwise mean-pressure-gradient for increasing time (from light to dark color) for the streamwise (in blue) and spanwise (in red) mean velocity profiles at $Re_{\tau} = 550$ (solid) and $Re_{\tau} = 950$ (dashed) for $\Pi = 60$. In all cases, $u_{\tau,ZPG}$ is the friction velocity of the case without adverse/favorable/spanwise mean-pressure-gradient.

where $\tau_w = |\vec{\tau}_w|$ is the magnitude of the wall-stress vector, $\gamma_{1w}$ is the angle between $\vec{u}_1$ and $\vec{\tau}_w$, $p_{\text{class}}^i \in [0,1]$ for $i = 1, ..., 7$ is the probability of the flow corresponding to each building-block category, and $p_{\text{conf}} \in [0,1]$ is the model confidence score.

The input to the wall model comprises the non-dimensional groups formed by the set

$$\left\{ \frac{u_1 y_1}{\nu}, \frac{u_2 y_2}{\nu}, \gamma_{12}, \frac{a_1 y_1^3}{\nu^2}, \frac{\gamma_{1w} y_1^2}{\nu}, \frac{k_1}{k_{m1}} \right\}. \tag{3}$$

The model applies the exponential averaged ($\overline{\cdot}$) to the input variables, and this is accounted for in the training. The non-dimensional output of the wall model is

$$\left\{ \frac{\tau_w y_1}{\mu u_1}, \gamma_{1w}, p_{\text{class}}^i, p_{\text{conf}} \right\}. \tag{4}$$
We have explicitly avoided the use of flow parameters such as freestream velocity, bulk velocity flow, etc., as they are not unambiguously identifiable for arbitrary geometries.

The non-dimensional groups in (3) are devised to enable the classification and wall-stress prediction according to the building-block flows considered. The first two inputs, $u_1 y_1 / \nu$ and $u_2 y_2 / \nu$, represent the local Reynolds numbers at the first and second control volumes. They are key drivers for the prediction of the wall stress in all cases by detecting the shape of the mean velocity profile. They aid the distinction between freestream, turbulent channel flow, and turbulence with favorable or adverse mean pressure gradient. The relative angle $\gamma_{12}$ is used to detect three-dimensionality in the mean velocity profile. The non-dimensional acceleration $a_{ij} y_i^2 / \nu^2$ and the angular rate-of-change $\gamma_{1} y_{1i}^2 / \nu$ facilitates the prediction of the magnitude and direction of statistically unsteady effects in the wall stress. Finally, $k_1/k_{m1}$ is leveraged to discern between turbulent and non-turbulent flows (i.e., freestream and laminar flow). The wall stress at the output is non-dimensionalized using the pseudo-wall-stress $\mu u_1 / y_1$, as it was found to minimize the spread of the data between cases. This improved the generalizability of the model and facilitated learning the trends in the data by the ANNs.

E. Training data: WMLES with optimized SGS/wall model

The training data is generated using WMLES with SGS/wall models optimized to obtain the exact values for the mean velocity profiles and wall stress distribution in order to attain consistency with the numerical discretization and gridding strategy of the solver. This approach was preferred over filtered DNS data, as it is known that the SGS tensor in implicitly filtered LES ($\tau_{ij}^\text{SGS}$) does not coincide with the Reynolds stress terms resulting from filtering the Navier-Stokes equations. The ambiguity in the filter operator renders DNS data inadequate for the development of SGS models because of inconsistent governing equations [2–4, 49, 50]. This limitation is particularly relevant in the present work, as the typical grid sizes utilized in WMLES of external aerodynamics are orders of magnitude larger than the characteristic Kolmogorov length-scale of the near-wall turbulence. Consequently, numerical errors are comparable to modeling errors, and the former must be accounted for in order to yield accurate predictions.

We introduce an exact-for-the-mean SGS model (ESGS) given by

$$\tau_{ij}^\text{SGS} = \tau_{ij}^\text{base} + \Delta \tau_{ij}^\text{SGS},$$

where $\tau_{ij}^\text{base}$ is SGS stress provided by the baseline (imperfect) SGS model (in this case, the dynamic Smagorinsky model, albeit another model could have been selected), and $\Delta \tau_{ij}^\text{SGS}$ is the SGS model correction such that the WMLES mean velocity profiles match the DNS counterparts. In this approach, instantaneous DNS flow fields are not needed and neither is a specific LES filter shape. The correction $\Delta \tau_{ij}^\text{SGS}$ is numerically calculated on the fly as the instantaneous force, $\partial \Delta \tau_{ij}^\text{SGS} / \partial x_j$, required for $\langle u_i \rangle_{xz} = \langle u_i^\text{DNS} \rangle_{xz}$, where $\langle \cdot \rangle_{xz}$ denotes average over the homogeneous directions $x$ and $z$, and $\langle u_i^\text{DNS} \rangle_{xz}$ is the DNS mean velocity profile for the $i$-th velocity component. The boundary condition at the wall is also modified to reproduce the probability density function of the wall stress from DNS and it is referred to as EBC (exact boundary condition).

WMLES of all the building-block flows was conducted using ESGS with EBC (hereafter, E-WMLES). The simulations were carried out in the same flow solver later used to implement the BFWM. This guarantees consistency of the training data with the actual numerical errors of the solver and gridding structure under the assumption of an SGS model able to accurately predict the mean velocity profiles. The E-WMLES database comprises the building-block flows cases discussed in §II C at isotropic grid resolutions $\Delta = h/N$ with $N = 5, 10, 20, 40, 80, 160$ and $380$, which cover (by a wide margin) the grid resolution encountered in external aerodynamic applications. For finer grid resolutions, BFWM was trained with DNS data to ensure convergence to the no-slip boundary condition.

F. Neural network architecture, classification, and training method

The classifier is an ANN with 5 hidden layers and 20 neurons per layer. The layers are connected with rectified linear units (ReLUs) as the activation function. The input to the classifier is the set of non-dimensional groups from Eq. (3). The last layer of the classifier is followed by the softmax activation function, which provides the probabilities of belonging to each building-block flow category ($p^\text{class}_{i, \text{test}}$, $i = 1, ..., t$) such that $\sum p^\text{class}_{i, \text{test}} = 1$. The network is trained using the Broyden-Fletcher-Goldfarb-Shanno quasi-Newton algorithm [14, 23, 24, 30, 62]. A confidence score $p_{\text{conf}} \in [0,1]$ is inferred from the distance of the input to its nearest neighbor in the training set. In particular, the confidence is based on the ratio $d_\text{r}/d_i$ (clipped to be less than one), where $d_i$ is the distance of the input to the closest sample in the training set, and $d_\text{r}$ is the average distance of the latter to its ten closest samples in the training set. The performance of the classifier after training is evaluated in figure 4, which shows the normalized confusion matrix. The
diagonal of the matrix contains the percentage of inputs that are correctly classified, whereas off-diagonal values show the amount of misclassification among cases. The matrix shows that most samples are correctly classified. There are a few misclassifications (off-diagonal values) which are intended to ensure a smooth transition between building blocks. This is caused by the overlap between contiguous building blocks, such as ‘Separation’ and strong ‘APG’, mild ‘APG’ and ‘ZPG’, ‘ZPG’ and mild ‘FPG’, and ‘ZPG’ and ‘Unsteady’. The only unintentional misclassification is the larger number of ‘ZPG’ samples classified as ‘FPG’. However, this did not impact the performance of BFWM, as the wall-stress prediction for ‘FPG’ and ‘ZPG’ are comparable. There is no ambiguity in the distinction between ‘Freestream/Laminar’ and turbulent cases, which is important as their predictions vary considerably.

A dedicated ANN is responsible for predicting the wall stress for each turbulent building-block flow. The predictions are obtained via a deep feed-forward neural network with 5 hidden layers and 30 neurons per layer. The activation functions selected for the hidden layers are hyperbolic tangent sigmoid transfer functions and ReLU activation transfer functions. Predictions of the ANN are calculated for each building-block category and added together weighted by the probability of belonging to the \( i \)-the category: \( \tau_w = \sum p_{\text{class}} \tau_{iw} \) (similarly for \( \gamma_{1w} \)). The neural networks are trained using Bayesian regularization backpropagation by dividing the training data into two groups: the training set (80% of the data) and the test set (20% of the data). The test set includes full cases for Reynolds numbers (and II’s) that are not part of the training set. This was found to improve the predictive capability of the network when interpolating and extrapolating among unseen cases. Figure 5 shows the performance plot of the ANN trained for the ‘Unsteady’ building-block flow.

The training set for both the classifier and predictors is augmented by performing arbitrary rotations of the frame of reference. The inputs and outputs are standardized using the mean and standard deviation of the training set. A parametric study was performed in terms of the number of layers and neurons per layer and the present layouts were found to give a fair compromise between neural network complexity and predictive capabilities. Finally, the computational overhead in the full flow solver using BFWM is between \( \times 1.1 \) and \( \times 1.3 \) compared to using the algebraic equilibrium wall model from §III B. However, no effort was done to optimize the current implementation of BFWM.
FIG. 5: Joint probability density function of the predicted output and actual output for (a) magnitude of the wall stress $\tilde{\tau}_w$ and (b) relative angle $\tilde{\gamma}_{1w}$. The tilde denotes values standardized by the mean and standard deviation of the training set. The results are for the statistically unsteady turbulent flow (Unsteady).

III. NUMERICAL METHODS

A. Flow solver and grid generation

The simulations are conducted with the high-fidelity solver charLES developed by Cascade Technologies, Inc [13, 25]. The code integrates the compressible LES equations using a kinetic-energy conserving, second-order accurate, finite volume method. The numerical discretization relies on a flux formulation which is approximately entropy preserving in the inviscid limit, thereby limiting the amount of numerical dissipation added into the calculation. The time integration is performed with a third-order Runge-Kutta explicit method.

The mesh generation follows a Voronoi hexagonal close-packed (HCP) point-seeding method, which automatically builds locally isotropic meshes for arbitrarily complex geometries. First, the water-tight surface geometry is provided to describe the computational domain. Second, the coarsest grid resolution in the domain is set to uniformly seeded HCP points. Additional refinement levels are specified in the vicinity of the walls if needed. Ten iterations of Lloyd’s algorithm to smooth the transition between layers with different grid resolutions.

B. Traditional SGS/wall models

Three SGS models are considered: the dynamic Smagorinsky model [28] with the modification by Lilly [40] (DSM), the Vreman model [68] (VRE), and the ESGS. The latter aims at assessing the performance of the BFWM in the absence of SGS modeling errors for the mean flow. For the wall, we use a traditional equilibrium wall model (EQWM). The no-slip boundary condition at the walls is replaced by a wall-stress boundary condition. The walls are assumed adiabatic and the wall stress is obtained by an algebraic equilibrium wall model derived from the integration of the one-dimensional stress model along the wall-normal direction [20, 57],

$$u_2^+(y_\perp^+) = \begin{cases} y_\perp^+ + a_1(y_\perp^+)^2 & \text{for } y_\perp^+ < 23, \\ \frac{1}{\kappa} \ln y_\perp^+ + B & \text{otherwise} \end{cases}$$

where $u_2$ is the model wall-parallel velocity at the second grid point off the wall, $y_\perp$ is the wall-normal direction to the surface, $\kappa = 0.41$ is the Kármán constant, $B = 5.2$ is the intercept constant, and $a_1$ is computed to ensure $C^1$ continuity. The superscript $+$ denotes inner units defined in terms of wall friction velocity and $\nu$. 

IV. MODEL VALIDATION

The BFWM is first validated in canonical flows: laminar and turbulent boundary layers with zero mean-pressure-gradient, turbulent pipe flow, turbulent Poiseuille-Couette flows, and statistically unsteady turbulent channel flow. These cases are intended to test the predictive capabilities of BFWM in flows that are comparable (but not identical) to the training and test sets. The performance of BFWM to predict the wall-shear stress in complex scenarios is evaluated in two realistic aircraft configurations: the NASA Common Research Model High-lift and the NASA Juncture Flow Experiment.

The validation cases are conducted by combining BFWM with two SGS models: DSM and VRE. The simulations performed with DSM and VRE together with BFWM are denoted by DSM-BFWM and VRE-BFWM, respectively. The results are compared with WMLES using DSM and VRE in conjunction with the equilibrium wall model (EQWM). The last two cases are referred to as DSM-EQWM and VRE-EQWM, respectively.

A. External and internal wall-modeling errors

Two sources of errors can be identified in a wall model [45]: errors from the outer LES input data, referred to as external wall-modeling errors, and errors from the model physical assumptions referred to as internal wall-modeling errors. In the former, errors by the SGS model at the matching locations propagate to the value of $\tau_w$ predicted by the wall model. These errors can be labeled as external to the wall model inasmuch as they are present even if the wall model provides an exact physical representation of the near-wall region. The second source of errors represents the intrinsic wall-model limitations: even in the presence of exact values for the input data, the wall model might incur errors when the physical assumptions of the model do not hold. In BFWM, errors may come from the inadequacy of the building-block flows to represent the physics of the near-wall region (e.g., compressibility effects, heat transfer effects, separation differing from the physics modeled by Poiseuille-Couette flows, etc). A consequence of internal errors is that WMLES might not converge to the DNS solution with grid refinements until the grid is in the DNS-like regime, when the contribution of the wall model is negligible. The combined external plus internal error is referred to as total error. We use BFWM with ESGS (labeled as ESGS-BLWM) to isolate the internal wall-modeling errors when possible.

B. Laminar boundary layer

The setup for the laminar boundary layer is the flow over a flat plate with zero mean-pressure-gradient and imposed inflow velocity from the Blasius solution. At the top boundary, the freestream velocity is $U_\infty$ and the vertical velocity is also calculated from the Blasius solution. A convective boundary condition is used at the outflow. The range of Reynolds numbers is $\text{Re}_x = U_\infty L_0/\nu = 10^4$ to $\text{Re}_x = 10^6$, where $L_0$ is the distance of the inlet to the leading edge of the plate. The streamwise, wall-normal, and spanwise sizes of the domain are $150L_0 \times 2L_0 \times 1L_0$, respectively. The grid resolution is uniform in the three directions with $\Delta/\delta_i \approx 1/2$ at the inlet, which corresponds to $\Delta/\delta_o \approx 1/20$ at the outlet, where $\delta_i$ and $\delta_o$ are the boundary layer thickness based on 99% of $U_\infty$ at the inlet and outlet, respectively. The reference solution was computed by DNS of the same setup.

The streamwise mean velocity profiles are captured within to 5% error for DSM-EQWM, VRE-EQWM, DSM-BFWM, and VRE-BFWM as shown in figure 6(a). Figure 6(b) reveals that the flow is correctly classified as ‘Laminar’ with confidence near 100%. The only exception is a small region close to the inlet, where the flow is labeled as ‘Freestream’ with lower confidence owing to the lack of grid resolution in that region (there are only two points per boundary layer in the inlet). The internal wall-model errors are included in figure 6(c), which shows a clear improvement in performance by BFWM compared to EQWM. After the initial transient from the inflow, errors for BFWM are below 1% and decay faster than the errors for EQWM, which are always above 20%. The total wallstress error is evaluated in figure 6(d). The performance of BFWM is still superior to that of EQWM. However, the accuracy of BFWM is severely diminished due to the external wall-modeling errors from DSM and VRE. Figure 6(d) also reveals that DSM-EQWM and VRE-EQWM are subjected to internal/external error cancellation (i.e., predictions may improve despite the fact that input values differ from ESGS). The degraded accuracy of BFWM due to SGS model errors and the presence of error cancellation using the EQWM are recurrent observations in the following validation cases.
C. Zero mean-pressure-gradient turbulent boundary-layer

For the zero-mean-pressure-gradient turbulent boundary layer case, the range of Reθ for the turbulent boundary layer is from 800 to 2,000, where Reθ is the Reynolds number based on U∞ and the momentum thickness (θ). The length, height, and width of the simulated box are Lx = 106θavg, Ly = 18θavg, and Lz = 35θavg, where θavg denotes θ averaged along the streamwise coordinate. The boundary conditions at the top plane are u = U∞, w = 0, and v is estimated from the known experimental growth of the displacement thickness for the corresponding range of Reynolds numbers as in Jiménez et al. [34]. This controls the average streamwise pressure gradient, whose nominal value is set to zero. The turbulent inflow is generated by the recycling scheme of Lund et al. [51], in which the velocities from a reference downstream plane, xref, are used to synthesize the incoming turbulence. The reference plane is located well beyond the end of the inflow region to avoid spurious feedback [53, 63]. In our case, xref/θi = 890, where θi is the momentum thickness at the inlet. A convective boundary condition is applied at the outlet with convective velocity U∞ [55] and small corrections to enforce global mass conservation [63]. The spanwise direction is periodic. The grid resolution at the inlet is ∆/δi ≈ 1/5 and at the outlet ∆/δo ≈ 20. The reference DNS solution is from Towne et al. [66], which follows an identical numerical setup.

To facilitate the comparison between DNS and WMLES, we use as independent variables Rez and x/L0, as these are free from modeling errors. The streamwise mean velocity profiles (figure 7a) deviate about 10% to 30% from the DNS profile. The flow is correctly classified by BFWM as ‘ZPG’ with almost 100% confidence across the vast majority of the domain (figure 7b). Close to the inlet, the flow is labeled as ‘Unsteady’ and ‘APG’, probably because it is still recovering from the artificial inlet boundary condition. The internal wall-modeling errors are quantified in figure 7(c), which shows moderate improvements in the performance of BFWM compared to EQWM. In particular, the averaged wall-stress error is below 0.5% for BFWM and about 2% for EQWM once the effect of the inlet condition is forgotten.
FIG. 7: Validation case: zero mean-pressure-gradient turbulent boundary layer. (a) The streamwise mean velocity profiles at Re = 6 × 10^5, 8 × 10^5, 10 × 10^5, and 12 × 10^5, for DSM-EQWM (blue squares), VRE-EQWM (blue crosses), DSM-BFWM (red squares), VRE-BFWM (red crosses), and DNS (solid line). The mean velocity profiles are shifted by ∆u = (x/L0 − 1)/5. (b) Flow classification (solid blue) and confidence score (solid red) by DSM-BFWM as a function of the streamwise distance. (c) Internal wall-modeling error of the wall-stress prediction for ESGS-BFWM (diamonds) and ESGS-EQWM (circles) as a function of the streamwise distance. (d) Total wall-modeling error for DSM-EQWM (dashed square), DSM-BFWM (solid square), VRE-EQWM (dashed crosses), and VRE-BFWM (solid crosses) as a function of the streamwise distance.

This case demonstrates that BFWM is able to successfully interpolate among grid resolutions and Reynolds numbers. In terms of total wall-stress error (figure 7d), BFWM and EQWM exhibit comparable performance with errors between 5% and 15%. Similar to the previous case, the accuracy of BFWM worsens due to the external wall-modeling errors when the wall model is coupled with DSM and VRE.

D. Turbulent pipe flow at Reτ = 40,000

The next validation case is a turbulent pipe flow at Reτ ≈ 40,000 with reference data obtained from experiments by Baidya et al. [6]. The flow is driven by a mean streamwise pressure gradient that fixes the Reynolds number based on the centerline velocity to the correct experimental value. The radial coordinate is r. The length of the pipe is 100R, where R is the radius of the pipe, and the streamwise direction is periodic. Four grid resolutions are considered: R/∆ ≈ 5, 10, 20, and 40.

Figure 8(a) shows that the streamwise mean velocity profile for DSM-BFWM and VRE-BFWM approaches the reference data with grid refinement. The flow is accurately classified as ‘ZPG’ for all the grid resolutions (figure 8b). BFWM correctly identifies the flow as ‘ZPG’ with high confidence (>95%) for R/∆ > 5. For the coarsest grid (R/∆ ≈ 5), the flow is also labeled as ‘ZPG’ but with lower confidence (<60%). The internal wall-modeling errors are shown in figure 8(c). Overall, both BFWM and EQWM perform satisfactorily with errors below 5% even at the coarsest grid resolution. This validation case demonstrates that BFWM successfully extrapolates to high Reynolds numbers for different grid resolutions. The total wall-stress error (figure 8d) ranges from 4% and 12% for BFWM and EQWM regardless of the SGS model, with a mildly improved accuracy for BFWM. The results also exhibit the non-monotonic convergence typically observed for WMLES in the range of grid resolution considered. This effect can be ascribed to the interplay between numerical errors and SGS model errors as previously discussed in Lozano-Durán.
FIG. 8: Validation case: turbulent pipe flow at $Re_\tau = 40,000$. (a) The streamwise mean velocity profiles non-dimensionalized by the centerline mean velocity ($U_c$) for DSM-BFWM (squares) and VRE-BFWM (crosses) for $R/\Delta \approx 5$ (blue), 10 (red), and 20 (yellow). The dashed line is the experimental mean velocity profile from Baidya et al. \[6\]. (b) Flow classification (solid blue) and confidence score (solid red) by DSM-BFWM as a function of the grid resolution. (c) Internal wall-modeling error of the wall-stress prediction for ESGS-BFWM (diamonds) and ESGS-EQWM (circles) as a function of the grid resolution. (d) Total wall-modeling error for DSM-EQWM (dashed square), DSM-BFWM (solid square), VRE-EQWM (dashed crosses), and VRE-BFWM (solid crosses) as a function of the grid resolution.

& Bae \[43\] and Lozano-Durán et al. \[45\] and remains a key issue of WMLES.

E. Adverse/favorable mean-pressure-gradient Poiseuille-Couette turbulence

Turbulent Poiseuille-Couette flows at $Re_U = 14,000$ are tested for adverse mean-pressure-gradients until separation and beyond for $Re_p \times 10^{-3} = -1.40, -1.32, -1.23, -1.13, -1.02, -0.90, -0.76$ and $Re_U = 14,000$ and for favorable mean-pressure-gradients for $Re_p \times 10^{-3} = 1.02, 1.13, 1.23, 1.32, 1.41, 1.49$. In all cases, the mean streamwise pressure gradient ensures that the Reynolds number based on the centerline velocity matches the correct value. The grid resolution is $h/\Delta = 10$. The reference solutions were obtained by DNS. It is worth remarking that these validation cases are not included in the training or testing set discussed in § II E. Hence, the current cases assess the predictive capabilities of BFWM when both $Re_p$ and $Re_U$ are simultaneously varied.

The results for APG/Separation cases and FPG cases are shown in figures 9 and 10, respectively. There are noticeable deviations in the prediction of the mean velocity profiles for both DSM-EQWM and VRE-EQWM. Similar results are obtained for their BFWM counterparts. Nonetheless, the flow classification (panel (b) in figures 9 and 10)
FIG. 9: Validation case: turbulent Poiseuille-Couette low with adverse mean-pressure-gradient. (a) The streamwise mean velocity profiles non-dimensionalized by the centerline mean velocity \( U_{cl}^{ZPG} \) of the case with zero mean-pressure-gradient for DSM-EQWM (blue squares), VRE-EQWM (blue crosses), DSM-BFWM (red squares), and VRE-BFWM (red crosses) for different \( Re_P \). The dashed lines are mean velocity profiles from DNS. (b) Flow classification (solid blue) and confidence score (solid red) by DSM-BFWM as a function of the adverse pressure gradient \( Re_P \). (c) Wall-stress prediction in the absence of external errors for ESGS-BFWM (diamonds) and ESGS-EQWM (circles) as a function of \( Re_P \). (d) Total wall-stress prediction for DSM-EQWM (dashed square), DSM-BFWM (solid square), VRE-EQWM (dashed crosses), and VRE-BFWM (solid crosses) as a function of \( Re_P \). In panels (c) and (d), the wall-stress prediction is non-dimensionalized by the DNS wall stress for the case with zero mean-pressure-gradient.

is accurate with a high confidence score (> 90%). The internal wall-modeling errors for APG/Separation and FPG cases are shown in figures 9(c) and 10(c), respectively. For the APG/Separation cases, we report the value of the wall-shear stress (rather than the relative error) to avoid dividing by zero close to separation. BFWM outperforms EQWM for APG/Separation cases, whereas ZPG cases are all accurately predicted by both wall models with errors below 3%. The total wall-stress error for APG/separation and FPG cases is shown in panel (d) of figures 9 and 10, respectively. For APG/Separation, EQWM provides more accurate predictions than BFWM, but these are subjected to error cancellation: EQWM underpredicts the wall-shear stress; however, the mean velocities close to the wall are overpredicted. The combination of both effects results in better predictions for EQWM, but for the wrong reasons. For FPG, the total error rises from 5% and 20% for increasing favorable pressure gradient. This trend applies to both BFWM and EQWM, although BFWM still outperforms EQWM.
FIG. 10: Validation case: turbulent Poiseuille-Couette flow with favorable mean-pressure-gradient. (a) The streamwise mean velocity profiles non-dimensionalized by the centerline mean velocity ($U_{ZPG}^{2}$) of the case with zero mean-pressure-gradient for DSM-EQWM (blue squares), VRE-EQWM (blue crosses), DSM-BFWM (red squares), and VRE-BFWM (red crosses) for different $Re_P$. The dashed lines are mean velocity profiles from DNS. (b) Flow classification (solid blue) and confidence score (solid red) by DSM-BFWM as a function of $Re_P$. (c) Internal wall-modeling error of the wall-stress prediction for ESGS-BFWM (diamonds) and ESGS-EQWM (circles) as a function $Re_P$. (d) Total wall-modeling error for DSM-EQWM (dashed square), DSM-BFWM (solid square), VRE-EQWM (dashed crosses), and VRE-BFWM (solid crosses) as a function of $Re_P$.

F. Turbulent channel flow with the sudden imposition of spanwise pressure gradient

The last canonical validation case is a turbulent channel flow with the sudden imposition of a mean spanwise pressure gradient. The ratio of spanwise to streamwise mean pressure gradient is $\Pi = 80$. The grid resolution is $h/\Delta = 10$. The simulation is started from a turbulent channel flow at a statistically steady state with $Re_\tau = 700$ for $t < 0$ and the lateral pressure gradient is imposed at time $t = 0$.

Figures 11(a) and (b) show the history of the streamwise and spanwise mean velocity profiles for all cases. Predictions of the mean flow remain accurate within 5% error for the second grid point off the wall. More acute errors are observed for the first grid point off the wall. The classifier accurately detects the change of regime from ‘ZPG’ to ‘Unsteady’ at $t = 0$ with high confidence (figure 11c). The internal wall-modeling errors for the streamwise ($\tau_{w,x}$) and spanwise ($\tau_{w,z}$) wall stress are shown in figures 11(d) and (e), respectively. As expected, BFWM performs better than EQWM, with errors below 1% for all times. Additionally, BFWM is able to predict the mild drop in $\tau_{w,x}$ as a function of time, which is completely missed by EQWM. A similar conclusion applies to the relative angle between $\vec{u}_1$ and $\vec{\tau}_w$ (namely, $\gamma_{1w}$). BFWM correctly predicts the increase and decrease of $\gamma_{1w}$, whereas $\gamma_{1w}$ remains zero for EQWM essentially by construction of the model. Finally, BFWM still improves the predictions compared to EQWM.
in terms of the total wall stress and $\gamma_{1w}$ errors (figures 11g, h, and i), but with lower accuracy than before due to the presence of external wall-modeling errors.
The NASA Common Research Model High-Lift (CRM-HL) is a geometrically complex aircraft that includes the bracketry associated with deployed flaps and slats as well as a flow-through nacelle mounted on the underside of the wing. The simulations are performed in free air at the Reynolds number of 5.49 million based on the mean aerodynamic chord and freestream velocity. The freestream Mach number is 0.20. The results are compared with wind tunnel experimental data from Evans et al. corrected for free air conditions. Further details of the set-up can be found in Lacy & Sclafani.

We follow the computational setup from Goc et al. A semi-span aircraft geometry is simulated and the symmetry plane is treated with free-slip and no penetration boundary conditions. Uniform plug flow is used as the inlet. A non-reflecting boundary condition with specified freestream pressure is imposed at the outlet. The total number of grid points is 30 million and the number of grid points per boundary layer thickness range from zero to twenty. The reader is referred to Goc et al. for more details about the gridding strategy. Figure offers one example of the grid topology. The SGS model is the DSM. A summary of previous WMLES of the CRM-HL can be found in Kiris et al. using traditional SGS and wall models. Here, we re-run the simulations using DSM-EQWM and perform new simulations for DSM-BFWM at angles of attack of 7 and 19 degrees.

The lift ($C_L$), drag ($C_D$), and pitching moment ($C_M$) coefficients are shown in figure. It is worth remarking that BFWM has never ‘seen’ an aircraft-like flow or been trained in a case that resembles an airfoil or a wing. DSM-BFWM provides moderate improvements with respect to DSM-BFWM, especially close to the stall. The improvements are more clearly manifested in the pitching moment, which is a marker of the accuracy in the force distribution along the wing. The exception is $C_L$ at low angles of attack, where DSM-EQWM outperforms DSM-BFWM. However, it has been reported that the good predictions by DSM-EQWM at low angles of attack is coincidental and due to error cancellation, so this should not be taken as a failure of DSM-BFWM. Despite the improvements by DSM-BFWM, the results suggest that a superior wall model alone does not suffice to further boost the performance of WMLES unless the SGS model is also accordingly improved.

Figure shows the confidence map of BFWM over the surface of the aircraft. Two types of low confidence (<20\%) regions are identified. The first region is located at the leading of the nacelle, slats, and flaps and is probably related to the lack of grid resolution in those locations (i.e., zero points per boundary layer thickness). The second low confidence region is related to separation at the wing tip and close to the wing root. This may hint at a lack of grid resolution, the inadequacy of the building block flows to model separation, or a combination of both. It is worth mentioning that confidence values of 20\% still indicate that the flow features detected resemble the building blocks up to some reasonable extent. For example, the presence of completely unknown flow (i.e. random values of the model inputs) will result in confidence scores of 0\%. The confidence map is a key feature of BFWM which enables further evaluation of the model performance. As such, the information from figure might aid grid refinement in poor confidence regions and/or inform future developments of the model, for example, by suggesting alternative building-block flows
FIG. 13: Validation case: NASA Common Research Model High-Lift. (a) The lift, (b) drag, and (c) pitching moment coefficients as a function of the angle of attack (AoA) for DSM-BFWM (red circles) and DSM-EQWM (blue circles). The dashed lines are experimental results.

or the necessity of new ones.

H. NASA Juncture Flow

The NASA Juncture Flow experiment consists of a full-span wing-fuselage body configured with truncated DLR-F6 wings and has been tested in the Langley 14- by 22-foot Subsonic Tunnel. The case has been proposed as a validation experiment for generic wing-fuselage junctions at subsonic conditions [59]. The Reynolds number is \( Re = \frac{LU_{\infty}}{\nu} = 2.4 \) million, where \( L \) is the chord at the Yehudi break. We consider an angle of attack of 5 degrees. The experimental dataset comprises a collection of local-in-space time-averaged measurements [36], such as velocity profiles and Reynolds stresses which aid the validation of BFWM in more detail. The frame of reference is such that the fuselage nose is located at \( x = 0 \), the \( x \)-axis is aligned with the fuselage centerline, the \( y \)-axis denotes the spanwise direction, and the \( z \)-axis is the vertical direction. The associated instantaneous velocities are denoted by \( u \), \( v \), and \( w \).

The SGS model is the DSM and we perform simulations for DSM-EQWM and DSM-BFWM. We use a boundary-layer-conforming grid [45], such that the control volumes are distributed to achieve five points per boundary layer thickness. Figure 15 contains a visualization of Voronoi control volumes for the boundary-layer-conforming grid. The reader is referred to Lozano-Durán et al. [45] for an in-depth description of the computational setup, numerical methods, and grid generation.

The prediction of the mean velocity profiles is shown in figure 16 and compared with experimental measurements. Three locations are considered: the upstream region of the fuselage, the wing-body juncture, and the wing-body juncture close to the trailing edge. Table I contains information about the flow classification and confidence in the solution at each location. In the first region, the flow resembles a ZPG turbulent boundary layer. Hence, the DSM-EQWM and DSM-BFWM perform accordingly (i.e., errors below 2%). The flow is identified by BFWM as 88% ‘ZPG’ and 12% ‘FPG’ with 98% confidence. The outcome is expected as BFWM was trained in turbulent channel flows and we have argued that the boundary layer at the fuselage resembles a ‘ZPG’.

On the contrary, there is a decline in accuracy by DSM-EQWM in the wing-body juncture and trailing-edge region, which are dominated by adverse pressure gradient effects in the corner and flow separation at the trailing edge. Lozano-Durán et al. [45] have shown that not only DSM-EQWM exhibits larger errors in the wing-body juncture and trailing-edge region, but that the rate of convergence of DSM-EQWM by merely refining the grid is too slow to compensate for the modeling deficiencies at a reasonable computational cost.

DSM-BFWM improves the predictions in the juncture location by augmenting the value of the wall stress, which alleviates the overprediction of \( u \) and \( w \) using EQWM. The flow in the juncture is classified as 52% ‘APG’ and 41% ‘ZPG’. The confidence in the prediction is above 80%. The performance of DSM-BFWM in the separated region is the poorest of all three locations, but also the most interesting. There is a quantitative improvement in the mean velocity prediction by DSM-BFWM with respect to DSM-EQWM, but this is still far from satisfactory. Interestingly, DSM-BFWM classifies the flow as a mix of ‘ZPG’, ‘APG’, and ‘Separation’, the latter being the most dominant class (56%). Moreover, despite the erroneous prediction by DSM-BFWM, the model prompts a warning about its poor performance, which is evidenced by the low confidence in the wall-stress prediction (~20%). The deficient performance
FIG. 14: Validation case: NASA Common Research Model High-Lift. Visualization of the instantaneous wall-shear stress (left) and confidence map (right) by DSM-BFWM.

| Location (a) | Location (b) | Location (c) |
|--------------|--------------|--------------|
| Freestream   | 0%           | 0%           | 0%           |
| Laminar      | 0%           | 0%           | 0%           |
| FPG          | 12%          | 0%           | 0%           |
| Classification | ZPG         | 88%          | 41%          | 13%          |
| APG          | 0%           | 52%          | 31%          |
| Separation   | 0%           | 7%           | 56%          |
| Unsteady     | 0%           | 0%           | 0%           |

Confidence 98% 82% 22%

TABLE I: Validation case: NASA Juncture flow. The flow classification and confidence in the solution by BFWM. The locations are (a) upstream region of the fuselage, (b) wing-body juncture, and (c) wing-body juncture close to the trailing edge.

of DSM-BFWM and DSM-EQWM is not surprising if we note that the separation zone has a wall-normal thickness of 0.3δ, where δ is the boundary layer thickness, whereas the WMLES grid size is Δ ≈ 0.2δ. Thus, there is only one grid point across the separation bubble. Despite the fact that the model was trained in separated flows, the external SGS model errors dominate the LES solution in this case. These errors hinder the capability of BFWM to correctly classify and predict the flow. Nonetheless, the ability of BFWM to assess the confidence in the prediction is a competitive advantage with respect to traditional wall models.
V. MODEL LIMITATIONS

We close this work by discussing some of the limitations of BFWM.

- First, the identification of meaningful building-block flows and the minimum number of blocks required to make accurate predictions remains an open question. The present version of the model uses seven building blocks, which is far from being representative of the rich flow physics that might occur in all complex scenarios (i.e., compressibility effects, shock waves, chemical reactions, multiphase flows, different mean-flow three-dimensionalities and separation patterns, etc). Additionally, there is no specific mechanism in BFWM to faithfully capture the laminar-to-turbulent transition, which is of paramount importance in many applications.

- The confidence score offered by BLWM is based on the similarities between the input flow features and the building-block flows. This implies that low confidence scores may still result in accurate wall-stress predictions and vice versa. Moreover, the confidence score does not provide an error bound on the value of the prediction, which would be more representative of the model performance.

- Consistency between the model and the numerical/gridding schemes is solver-dependent. As such, BFWM must be re-trained to yield accurate predictions in different flow solvers. However, this inconvenience seems inevitable
FIG. 16: Validation case: NASA Juncture flow. The mean velocity profiles at (a) upstream region of the fuselage at $x = 1168.4$ mm and $z = 0$ mm, (b) wing-body juncture at $x = 2747.6$ mm and $y = 239.1$ mm, and (c) wing-body juncture close to the trailing edge at $x = 2922.6$ mm and $y = 239.1$ mm. Solid lines with open symbols are for DSM-EQWM and closed symbols are for DSM-BFWM. Dashed lines are experiments. Colors denote different velocity components. The distances $y$ and $z$ are normalized by the local boundary-layer thickness $\delta$ at each location.

considering the intimate relationship between numerics, gridding, and modeling in implicitly filtered LES.

- A key conclusion of this work is that the main limiting factor in the accuracy of BFWM predictions originates from external modeling errors due to the poor performance of SGS models. This hints at the necessity of a unified SGS/wall model approach where the building-block flow model is also used to devise a numerically consistent SGS model (referred to as BFSGS). Steps in that direction are already been undertaken by our group and Ling et al. [41] have shown that the prediction of the lift, drag, and pitching moment coefficients for the CRM-HL in §IVG are greatly improved in the first version of BFSGS combined with BFWM.

- The prediction and classification tasks in BFWM rely on ANNs. In this work, it was found that feedforward ANNs with 5 hidden layers and roughly 20 to 30 neurons per layer enabled accurate results. However, the neural network architectures utilized here may be far from optimal. Moreover, there was no attempt to optimize the computational efficiency of the ANNs, for example via GPUs, and further work should be devoted in this direction.
VI. CONCLUSIONS

The prediction of aerodynamic quantities of interest remains among the most pressing challenges for computational fluid dynamics, and it has been highlighted as a Critical Flow Phenomena in the NASA CFD Vision 2030 [64]. The aircraft aerodynamics are inherently turbulent with mean-flow three-dimensionality, often accompanied by laminar-to-turbulent transition, flow separation, secondary flow motions at corners, and shock wave formation, to name a few. However, the most widespread wall models are built upon the assumption of canonical flat-plate statistically-in-equilibrium wall turbulence and do not faithfully account for the wide variety of flow conditions described above. This raises the question of how to devise models capable of accounting for such a vast and rich collection of flow physics in a feasible manner.

In this work, we have developed a wall model for large-eddy simulation by devising the flow as a collection of building blocks whose information enables the prediction of the wall stress. The concept was first introduced by Lozano-Durán & Bae [44] and it is referred to as building-block-flow wall model (BFWM). The model relies on the assumption that simple flows contain the essential flow physics to formulate generalizable wall models. Seven types of building-block units were used to train the model accounting for zero/favorable/adverse mean-pressure-gradient wall turbulence, separation, statistically unsteady turbulence with 3-D mean flow, and laminar flow. The approach is implemented using two types of artificial neural networks: a classifier, which identifies the contribution of each building block in the flow; and a predictor, which estimates the wall stress via a combinations of building-block units. The output of the model is accompanied by the confidence score. The latter value aids the detection of areas where the model underperforms, such as flow regions that are not representative of the building blocks used to train the model. This a critical component of BFWM and is considered a key step for developing reliable models. For example, the present model will provide a low confidence score in the presence of a flow that has never seen before (e.g., a shock wave), or when the wall-model input is located in the freestream. Finally, the model is designed to guarantee consistency with the numerical scheme and the gridding strategy. This was attained by training the model using WMLES data obtained with an optimized SGS model that accounts for the numerical errors of the solver.

The BFWM has been validated in laminar and turbulent boundary layers, turbulent pipe flow, turbulent Poiseuille-Couette flows mimicking favorable/adverse mean-pressure-gradient effects, and statistically unsteady turbulent channel flow with 3-D mean flow. The performance of BFWM in complex scenarios was evaluated in two realistic aircraft configurations: the NASA Common Research Model High-lift and the NASA Juncture Flow Experiment. The validation cases were conducted by combining BFWM with two SGS models: Dynamic Smagorinsky model and Vreman model. BFWM outperforms the traditional equilibrium wall model in canonical cases and the two realistic aircraft scenarios. The only exceptions are the coincidental accurate predictions by the equilibrium wall model due to error cancellation. Despite the improved performance of BFWM, its accuracy deteriorates considerably owing to external errors from the SGS model. This suggests that additional wall-model improvements will not suffice to further boost the performance of WMLES unless the SGS model is also improved.

The modeling capabilities demonstrated by BFWM, and the ability to extend the model to a richer collection of flow conditions, makes the building-block flow approach a realistic contender to overcome the key deficiencies of current CFD methodologies. We have argued that truly revolutionary improvements in WMLES will encompass advancements in numerics, grid generation, and wall/SGS modeling. Here, we have focused on wall modeling and its consistency with the numerics and the grid. However, work remains to be done on the SGS modeling front. In a recent work by our group, Ling et al. [41] extended the building-block flow methodology to the SGS model and showed that the prediction of the lift, drag, and pitching moment coefficients in the CRM-HL are greatly improved compared to BFWM combined with traditional SGS models. There is also a data science component to the problem, such as the need for efficient and reliable machine-learning techniques for data classification and regression. However, in our experience the model performance is mainly controlled by the physical assumptions rather than by the details of the neural network architecture at hand.

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