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DATA-DRIVEN WALL SHEAR STRESS MODEL FOR LARGE EDDY SIMULATIONS APPLIED TO FLOW SEPARATION

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INTRODUCTION

RANS simulations are the reference in the industry for turbomachinery design due to their low computational cost. Even if progress has been made towards more accurate closure models for RANS, they still fail at off-design conditions due to their inherent assumptions. At those conditions, different flow regimes occur in blade passages where complex flow features coexist, including secondary flows and flow separation.

Direct Numerical Simulations (DNS) provide a reliable prediction of such a flow physics. However, they require a considerable amount of computational resources that overcome the current capabilities of modern clusters and hence they cannot be used for the actual complex geometries and high Reynolds number flows tackled by industry. Even wall-resolved Large Eddy Simulations (wrLES), which aims to resolve at least 80% of the turbulent energy spectrum while modeling the effect on the small unresolved scales on the resolved ones, remains too expensive at high Reynolds numbers.

Since the inner part of the boundary layer is the most demanding in terms of resolution, the LES community came up with the idea of modeling this part rather than resolving it. Such wall-modeled LES (wmLES) require much less computational resources, yet the modeling errors are larger and may become unacceptable. Indeed, most wall models assume that the flow is attached, fully turbulent, aligned, and at equilibrium. Hence, they fail at predicting complex flow features. In the case of flow separation, treated in this work, these assumptions do not hold, and the wall model must be reformulated.

Since DNS and LES perform well on academic configurations and several industrial configurations, coupled with the recent improvement in the Machine Learning community, we have the opportunity to construct databases to train deep neural networks afterwards. Our work is based on the universal approximation capabilities of deep neural networks. A wall model can be seen as a high-dimensional regression problem that takes as inputs (a) instantaneous volume fields (e.g., velocity, pressure gradients) and (b) geometry notions, and that outputs the two components of the wall shear stress, $\boldsymbol{\tau}_w$. Three databases, obtained using a high-order Discontinuous Galerkin (DG) flow solver, are composed of a channel flow at a friction Reynolds number of 950 and the two walls (i.e., the flat upper surface and the curved lower one) of the two dimensional periodic hill at a bulk Reynolds number of 10595.

The next sections present: (i) which stencil is taken as input for the data-driven wall model, (ii) how are the three databases normalized to train the network on a unified and consistent database and (iii) which neural networks are picked.

TEST CASES

Two test cases are considered for the present study. One of them is a channel flow at $Re_\tau = 950$ [1]. The walls are separated by a distance 2δ and the channel is periodic and homogeneous in the streamwise and spanwise direction, respectively of size $L_x/\delta = 2\pi$ and $L_z/\delta = \pi$. A uniform pressure gradient drives the flow. A compressible wrLES using a DG flow solver is performed at Mach number of 0.1 to ensure a fair comparison with the incompressible flow reference. The second test case is the periodic hill flow [8], a geometry used for the development of wall models, and that consists of a channel with a hill (of height h). There is a massive flow separation from the hill top, followed by a reattachment and flow recovery on the flat part. The flow is then strongly re-accelerated on the ascending part of the next hill. The bulk Reynolds number Re_b is $10,959$ and is controlled using a uniform pressure gradient. The control procedure is inspired by the work of Benocci and Pinelli [2], and further modified by Carton de Wiart et al. [3] to take into account compressibility. Note that the flat top wall is subjected to a non-uniform pressure gradient generated by the flow contraction and the separation on the hill top but the flow on that wall does not separate.

INPUTS STENCIL

The input of the wall model is a mix between flow field and geometry data. For the flow fields, the velocity and the pressure gradients are considered. These fields are interpolated from a high-order solution to a probe grid and then projected on the local frame of reference following the wall; the data are therefore expressed in curvilinear coordinates (ξ, η, z). A crucial information for the wall model is the wall normal distance at which the flow fields are extracted, defined as h_{wm}. The curvature K of the wall is also added and has drastically improved the prediction of the $\boldsymbol{\tau}_w$ on the curved wall.

To answer the question (i), the choice of stencil is based on a deep analysis of space-time correlations between instantaneous flow fields and the two components of $\boldsymbol{\tau}_w$ [9]. In Machine Learning, this step is called feature selection. Our work has shown that, near the separation, the high correlation domain is shifted downstream ($\delta\xi/h \simeq 0.5$), indicating that, at a given time, the information should be sought downstream to better characterize the relationship with $\boldsymbol{\tau}_w$. Finally, a stencil going from $-0.5\,\delta\xi/h$ to $0.5\,\delta\xi/h$ relatively to the location where $\boldsymbol{\tau}_w$ is predicted is adopted. As multiple spatial positions are considered, the relative positions are introduced as input.

NORMALIZATION

This section answers the question (ii). The inputs described in the previous section need to be normalized to train the neural network on a unified database. The inputs and outputs of the wall model are summarized in Table 1. Recall that h_{wm} is the wall-normal distance at which the fields are measured and fed to the model. We also define $u_{\|} = \sqrt{(u_\xi^2 + u_z^2)}$, the norm of the wall-parallel velocity. The normalization of h_{wm} is based on the near wall scaling proposed by Duprat et *al.* [4] combined to the work of Zhou et *al.* [5]. The near-wall scaling compatible with separation uses $y_{\nu,p} = \nu/u_{\nu,p}$ with $u_{\nu,p} = \sqrt{(u_\nu^2 + u_p^2)}$ where $u_\nu = \sqrt{(\nu\, u_{\|}/h_{wm})}$ and $u_p = \left|(\nu/\rho)\partial_\xi p\right|^{1/3}$. A natural normalization of the velocity field would be based on the friction velocity u_τ; however, the friction velocity is undefined near separation. An alternative is to use its extended definition $u_{\nu,p}$ defined above. Regarding the pressure gradient, It is non-dimensionalised in an analogous way as the Clauser parameter, using the adapted velocity scale $u_{\nu,p}$, see Table 1. Finally, the outputs are normalized following the definition of the friction coefficient where the friction velocity is replaced by the spatial averaging of $u_{\nu,p}$. No normalization of the curvature is used as it is already dimensionless.

Field		*Normalized*
Velocity	$\boldsymbol{u}$	$\boldsymbol{u}^\star = \boldsymbol{u}/u_{\nu,p}$
Pressure Gradients	∇p	$(\nabla p)^\star = \left(h_{wm}/\left(\rho u_{\nu,p}^2\right)\right)\nabla p$
Length scale	h_{wm}	$h_{wm}^\star = \ln\left(h_{wm}/y_{\nu,p}\right)$
Curvature	K	
Relative pos.	$\delta\xi$	$(\delta\xi)^* = \delta\xi/h$
Wall shear stress	$\boldsymbol{\tau}_w$	$\boldsymbol{\tau}_w^\star = \dfrac{\boldsymbol{\tau}_w}{\frac{1}{2}\rho\langle u_{\nu,p}^2\rangle_{\xi,z}}$

Table 1: Inputs and output of the data-driven wall model.

NEURAL NETWORK ARCHITECTURE

This section aims to answer the question (iii). Since the stencil includes multiple locations, convolutional neural networks (CNNs [7]) are preferred over multi-layer perceptrons. Indeed, the translation-invariance (i.e., convolution) is encapsulated in the obtained model, which is a desirable property. For attached flows, the space-time correlations study has revealed that local and instantaneous data are sufficient to describe the relationship with $\boldsymbol{\tau}_w$. The input stencil for such flows is too big and should be reduced. Such a reduction can be seen as re-weighting of the input data through a self-attention layer [6]. The hyperparameters (e.g., kernel size, padding, stride, dilation, ...) of the model were adjusted to obtain the optimal receptive field. The most successful model (CNN-1D-SAL) contains two consecutive self-attention layers, seven one-dimensional convolutional layers, and one max-pooling layer. The model has been trained through the Mean Square Error (MSE) loss. Such a model performs well on average, but the variance of the outputs is not correctly predicted. One way to retrieve the first and second moment of the output distribution is to use Gaussian Mixture Heads (GMHs). These heads are connected at the end of the CNN (CNN-1D-SAL-GMH) and aim to predict N means, standard deviations, and mixture coefficients (μ_n, σ_n, π_n). The loss function was adapted accordingly. A third model (CNN-2D) composed of two-dimensional convolutional layers was also tested, based on an extended stencil in the spanwise direction.

DISCUSSION

The three models trained on various combinations of databases are validated *a priori*. The obtained results were very promising in the three cases. CNN-1D-SAL behaves well on averaged while CNN-1D-SAL-GMH better predicts the first and second moment of the output distribution. However, it is not able to capture the skewness of the $\tau_{w,\xi}$ distribution. CNN-2D retrieves better two-dimensional structures in the instantaneous wall shear stress field, compared to its two 1D counterparts. The second validation step, the *a posteriori* one, aims to test the model into the flow solver. This validation is first performed on the same test cases as used for the training. Then, the validation will be extended to other Reynolds numbers to evaluate the capabilities of the model to generalize. Those steps are on going work.

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