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Coherent structures in the atmospheric boundary layer using resolvent analysis

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Abstract. *In turbulent flows, large-scale coherent structures play a significant role in the flow dynamics, impacting the production of turbulence and containing the majority of the turbulence kinetic energy. Their identification and characterization, however, require detailed field measurements or refined numerical simulations, which comes at a high cost in particular for highly turbulent and variable flows such as the atmospheric boundary-layer (ABL). In this study, we investigate the ability of the Resolvent Analysis as low-cost tool to model ABL coherent structures, by providing only the mean flow field of the ABL. Resolvent analysis is a theoretical approach that takes the singular value decomposition of the linearized Navier-Stokes operator, treating the nonlinear terms as external forcing. The decomposition provides response modes that can be directly related to the most energetic coherent structures of the flow. Results are compared to the modes obtained from Spectral Proper Orthogonal Decomposition (SPOD) applied to detailed numerical data from Large-Eddy Simulations of a theoretical channel as a first approximation of the ABL to validate the method. It is intended to investigate further more realistic aspects of ABL, such as the Coriolis force and stratification effect. Cases in which the resolvent analysis provides the best agreement with SPOD are discussed. These results indicate that resolvent analysis can be used as a low-cost tool in characterizing ABL coherent structures, which has important practical implications in modeling atmospheric dynamics.*

Keywords: *Turbulent flows, Atmospheric boundary-layer, Large-Eddy Simulations, Resolvent analysis, Proper orthogonal decomposition*

1. INTRODUCTION

The atmospheric boundary layer (ABL) is the region of the atmosphere extending from the surface to a height in the order of one kilometer, where the flow is highly turbulent due to the shear with the surface of the Earth, and highly variable due to changes in surface roughness, solar radiation, air temperature and humidity, among other factors. The ABL has an important role in the exchange of energy, heat, moisture, and momentum between the Earth's surface and the free atmosphere above it (Stull, 1988; Garratt, 1992). Furthermore, many phenomena occurring within the ABL are driven by turbulence, including vertical mixing of gases and particles, formation of low clouds and temperature variation with height. These phenomena have important implications in areas such as meteorology, air quality, pollutant dispersion, wind power generation, among others (Stull, 1988; Wyngaard, 2010), therefore the characterization of ABL turbulence is crucial for many applications.

An important characteristic of turbulent flows is the presence of coherent structures (Brown and Roshko, 1971; Gupta *et al.*, 1971; Kline *et al.*, 1967), which are large, persistent vortices that play a crucial role in energy transfer, mass and momentum transport, as well as in the determination of flow patterns and statistical properties. The study of these structures is done through advanced analysis methods, such as the Spectral Proper Orthogonal Decomposition (SPOD), applied in detailed datasets of turbulent flows, allowing to decompose the velocity fluctuations into different modal components. Due to the high complexity and cost of them, however, techniques such as the Resolvent Analysis have been recently investigated, which are based only on the mean flow conditions and the governing equations of the flow.

The Resolvent Analysis is a method based on the theory of linear stability, which allows the decomposition of the turbulent velocity field into a set of coherent modes, called resolvent modes (Jovanovic and Bamieh, 2005; Bagheri *et al.*, 2009; McKeon and Sharma, 2010). These modes represent optimal solutions of the linearized system and provide valuable information about the dominant coherent structures and the energy associated with each mode. On the other hand, the SPOD is a spectral analysis that is based on the decomposition of velocity fluctuations at different frequencies and wavenumber (Towne *et al.*, 2018). Through the Fourier transform, SPOD identifies the coherent modes that contribute significantly to the energy at different spatial and temporal scales. Here, the database to be analyzed by the SPOD method is generated by a numerical simulation of the ABL.

The simulation of turbulent flows through the numerical solution of the Navier-Stokes equations (known as Direct Numerical Simulation or DNS) comes at a high computational cost due to the increase in the range of scales with Reynolds number (an indicator of turbulence intensity). The alternative is to solve the filtered Navier-Stokes equations, in which only the large scales of the flow are directly resolved, whereas the effect of the smallest scales on the resolved flow is modeled through subgrid-scale models. This technique, known as Large-Eddy Simulation (LES), allows the use of a coarser grid compared to the DNS version of the same flow, significantly reducing the computational cost (Pope, 2000).

By providing detailed information on velocity fluctuations at large spatial and temporal scales, LES is able to capture the main characteristics of coherent structures, including the impact of different forcing terms such as Coriolis and buoyancy forces in their shapes and magnitudes (Freire, 2022). In this work, we perform a comparison between the methods Resolvent analysis and SPOD in capturing the coherent structures present in a theoretical half-channel, as a first approximation of the ABL, with the numerical database given by the LES. Furthermore, we show the importance of eddy-viscosity being treated as part of the linear operator of the Resolvent method. In the future, we intend to extend the study to investigate the influence of Coriolis and buoyancy forces in the simulations.

2. MATHEMATICAL FORMULATION

2.1 Resolvent Analysis

The resolvent analysis aims to identify the optimum modes that describe mechanisms of linear amplification in stable systems. In a flow under some time-periodic forcing, resolvent analysis can be used to obtain information about the relevant structures and the nonlinear terms that excite them (Abreu *et al.*, 2020).

For a turbulent flow, Navier-Stokes equations can be split into linear and non-linear terms that can be treated as forcing terms, the focus of resolvent analysis. Following the formulation presented in Cavalieri *et al.* (2019), the Navier-Stokes equations can be rearranged, leading to the linearized system in the input-output form:

$$\frac{\partial \mathbf{q}'}{\partial t} = \mathbf{L}_{\bar{\mathbf{q}}}\mathbf{q}' + \mathbf{f}, \tag{1}$$

where $\mathbf{q}' = [u', v', w']$ is the time-variant fluctuations ($\mathbf{q} = \bar{\mathbf{q}} + \mathbf{q}'$, with $\mathbf{q}$ being the state vector of flow variables, and $\bar{\mathbf{q}}$ is the time-invariant base flow). $\mathbf{L}_{\bar{\mathbf{q}}}$ is the linearized Navier-Stokes operator about the base state $\bar{\mathbf{q}}$, and $\mathbf{f}$ denotes the remaining non-linear terms, as well as any additional forcing terms added to the equations (Taira *et al.*, 2017; Towne *et al.*, 2018; McKeon and Sharma, 2010; House *et al.*, 2022).

The analysis of the unsteady flow is made in the frequency domain by analyzing the Fourier transform of Eq. (1) into

$$i\omega\widehat{\mathbf{q}}_\omega = \mathbf{L}_{\bar{\mathbf{q}}}\widehat{\mathbf{q}}_\omega + \widehat{\mathbf{f}}_\omega, \tag{2}$$

where

$$\mathbf{q}(\mathbf{x}, t) = \widehat{\mathbf{q}}_\omega e^{i\omega t} \text{ and } \mathbf{f}(\mathbf{x}, t) = \widehat{\mathbf{f}}_\omega e^{i\omega t}, \tag{3}$$

for temporal frequency w. Thus, Eq. (2) can be written as

$$\widehat{\mathbf{q}}_\omega = [i\omega\mathbf{I} - \mathbf{L}_{\bar{q}}]^{-1}\widehat{\mathbf{f}}_\omega, \tag{4}$$

where $\mathbf{A} = [i\omega\mathbf{I} - \mathbf{L}_{\bar{q}}]^{-1}$ is the resolvent operator. $\mathbf{A}$ relates a forcing input to a response of the state vector $\mathbf{q}$.

Given the resolvent operator $\mathbf{A}$, the singular value decomposition (SVD) technique is applied, given by

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^* \tag{5}$$

to obtain the corresponding eigenvalues and eigenvectors. Eigenvectors associated with the largest eigenvalues correspond to the main modes that represent the coherent structures of the flow, more sensitive to external forcing and perturbations.

Equation (5) gives a relationship between inputs and outputs. The superscript $*$ denotes the conjugate transpose of a matrix. $\mathbf{V}$ represents the primary directions in which forcings are most effective, $\mathbf{U}$ represents the responses these forcings will induce, and $\mathbf{\Sigma}$ represents the associated gains mapping between the forcing modes and the associated responses (House *et al.*, 2022).

In the construction of the linear operator $\mathbf{L}_{\bar{q}}$, it is possible to include or not the effect of the turbulent Reynolds stresses by means of an eddy-viscosity ν_t. When it is not included, all turbulent effects are represented by the non-linear forcing term, and the fluid molecular viscosity needs to be used in the resolvent operator. Here, to analyze the effect of eddy-viscosity on the linear operator $\mathbf{L}_{\bar{q}}$, we chose to use the model proposed by Cess (1958)

$$\frac{\nu_T}{\nu} = \frac{1}{2}\left(1 + \frac{\kappa^2 Re_\tau^2}{9}(1-\eta^2)^2(1+2\eta^2)^2[1 - exp((|\eta|-1)Re_\tau/A)]^2\right) + \frac{1}{2}, \quad (6)$$

where ν_T is the total effective viscosity ($\nu_T = \nu_t + \nu$, with ν being the molecular viscosity), η is the non-dimensional wall distance in outer units, and the constants κ and A are given as 0.426 and 25.4, respectively (Pujals *et al.* (2009)).

2.2 Spectral Proper Orthogonal Decomposition

In the study of turbulent flows, statistical methods can be useful to identify coherent structures present in the flow. When working in the frequency domain, the Spectral Proper Orthogonal Decomposition (SPOD) method can be applied to the velocity fluctuation $\mathbf{q}'$ to extract orthogonal modes that optimally represent turbulent kinetic energy. First, we perform a data pre-processing step. We apply a fast Fourier transform (FFT) to the velocity fields in the homogeneous x and z directions. In addition, we also apply the FFT on the velocity versus time fields. This transform allows us to obtain the distribution of energy at different specific frequencies, represented by ω. SPOD method is applied to this transformed field, which is equivalent to solving the integral equation

$$\int \mathbf{C}(\mathbf{x}, \mathbf{x}', \omega)\mathbf{\Psi}(\mathbf{x}', \omega) d\mathbf{x}' = \lambda \mathbf{\Psi}(\mathbf{x}, \omega), \quad (7)$$

where $\mathbf{\Psi}$ are the basis functions, also called SPOD modes, λ is the corresponding eigenvalue and $\mathbf{C}$ is the two-point cross-spectral density. $\mathbf{C}$ is a Hermitian matrix, and thus its eigenvalues are real and the eigenfunctions are orthogonal.

2.3 Large-Eddy Simulation

In this study, the LES code known as LESGO is used, which solves the half-channel flow forced by a constant mean pressure gradient in a fixed Cartesian grid (staggered in the vertical direction). The flow is periodic in both horizontal directions, where a spectral method is used to calculate the spatial derivatives. In the vertical direction, a second-order finite-difference method is used, and a wall model based on the logarithmic law of the wall is imposed as a bottom boundary condition. At the top of the domain, a stress-free condition is imposed, and the Adams-Bashforth method is used for time discretization. The Lagrangian-averaged scale-dependent subgrid-scale model is used (Bou-Zeid *et al.*, 2005), an improved version of the classical dynamic Smagorinsky model. This code has been used in many studies in the past years, in particular in the simulation of the ABL. While in the present study, only the half-channel flow is tested in order to validate the methodology, the next stage of the project will use the same code to simulate the ABL forced by a mean pressure gradient imposed in terms of a geostrophic wind, in the presence of the Coriolis and buoyancy forces that mimic the main drivers of the atmospheric turbulence (Kleissl *et al.*, 2006; Freire, 2022).

One simulation was made, corresponding to $Re_\tau = 5200$. Simulation parameters are detailed in Tab. 1. The results are presented in the next section.

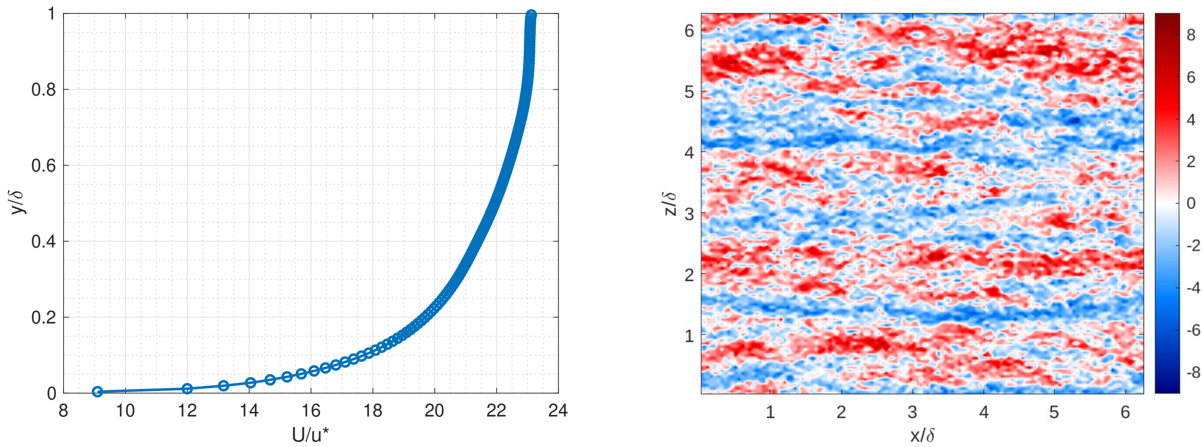
Table 1. Simulation parameters for LES ($\delta = 1$ and $u^* = 1$).

domain size ($X \times Y \times Z$)	$2\pi\delta \times \delta \times 2\pi\delta$
number of grid points ($n_x \times n_y \times n_z$)	$128 \times 128 \times 128$
mean pressure gradient force ($F_i = \langle (1/\rho)(d\bar{p}/dx), 0, 0\rangle$)	$\langle {u^*}^2/\delta, 0, 0\rangle$
simulation time step (Δt)	$0.0001\delta/u^*$
number of simulation time steps (N_t)	200 000

3. NUMERICAL RESULTS AND DISCUSSION

For a forced linear system with white noise, SPOD and Resolvent modes must be identical, which makes the comparison between these modes pertinent. Fig. 1 shows the mean streamwise velocity profile of the flow (used in the Resolvent Analysis) in addition to a snapshot of the instantaneous flow field, which shows the presence of the typical coherent structures of wall-bounded flows (streamwise streaks). Based on the Fig. 1b), their representative wavelengths were chosen as $(\lambda_x, \lambda_z) \approx (3.16, 1.0)$. The temporal wavelength $\lambda_t = 0.2$ was chosen with the objective to obtain a phase velocity $c = \omega/\alpha$ compatible with the mean velocity profile of the flow, in order to capture its coherent structures. α represents the x wavenumber direction. For $\lambda_t = 0.2$, we obtain a phase velocity $c = 16.078$, and frequency $\omega = 31.41$.

Figure 2 shows the comparisons between the first three modes obtained from simulations of SPOD and Resolvent methods. Furthermore, a comparison is conducted between the results obtained from simulations with eddy-viscosity (right column) and without it (left column) on the linear operator of the Resolvent method. It is possible see that



(a) (b)

Figure 1. a) The mean streamwise velocity profile, and b) instantaneous streamwise velocity fluctuation (u') field in the wall-parallel plane at $y/\delta = 0.0352$.

The peaks of the three modes corresponding to the results obtained without considering eddy-viscosity (left column) are significantly higher than those observed when employing the Resolvent method with eddy-viscosity, as well as the results obtained using the SPOD method. Furthermore, these peaks are concentrated close to the first points of y/δ. In contrast, when looking at the results with eddy-viscosity (right column), one can see that the first mode, for all three velocity components, closely resembles the results obtained through the SPOD method. However, in the second mode, deviations in the v and w components become noticeable within the region around $0.2 \leq y/\delta \leq 0.4$. For the third mode, all velocity components do not precisely align with the SPOD modes, but they exhibit a shape and intensity that are similar to the expected behavior. In summary, it can be concluded that the results obtained when accounting for eddy-viscosity closely resemble the outcomes obtained through the SPOD method.

4. CONCLUSION

The present work shows a comparison between the Resolvent analysis and SPOD methods in capturing the coherent structures present in a turbulent half-channel with $Re_\tau = 5200$ with the numerical database given by the LES. The adopted methods are responsible for identifying the coherent modes of the turbulent velocity field, obtaining the optimal solutions of the linearized system, and thus valuable information about the dominant coherent structures.

The presence of eddy-viscosity on the linear operator of the Resolvent Analysis method is analyzed, to verify the proximity of this method with the SPOD method, for a combination of fixed wavelengths (λ_x, λ_z, λ_t), concluding that the eddy-viscosity causes the Resolvent method to approach the SPOD method, indicating the importance of including it in the linear resolvent operator.

As part of an ongoing project, in the future, we intend to investigate further the influence of the Reynolds number in the simulations and add more realistic aspects to the LES code, such as the Coriolis force and other parameters present and used to describe the atmosphere.

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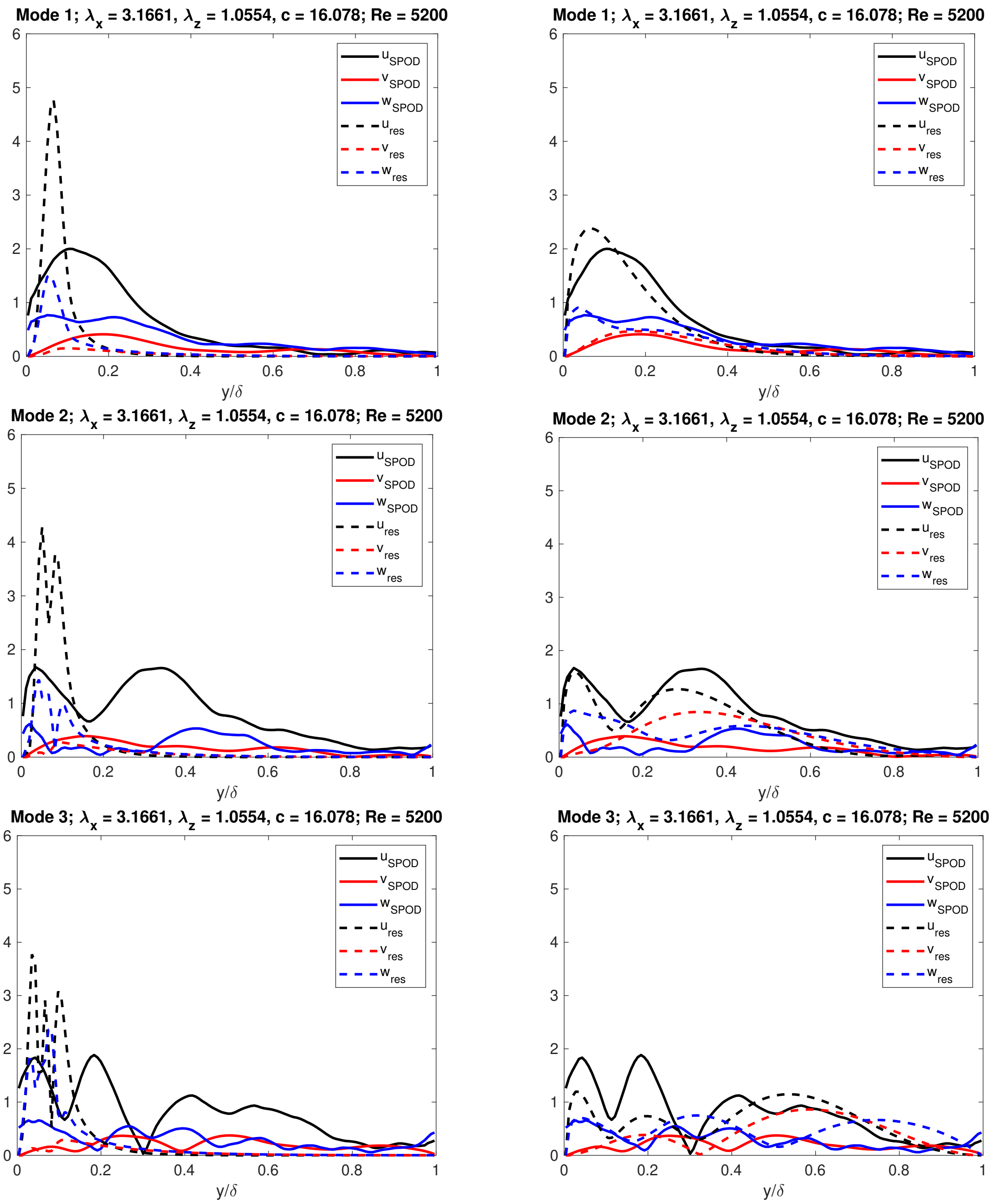

Figure 2. Comparison between the first three modes of SPOD and Resolvent methods of u', v', and w', without eddy-viscosity (left column), and with eddy-viscosity on the linear operator (right column) of the Resolvent method, for $(\lambda_x, \lambda_z, \lambda_t) = (3.1661, 1.0554, 0.2)$, and $Re_\tau = 5200$.

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