

1 Response to Reviewer 2

We thank the reviewer for his/her time and for the constructive comments, which helped improve the quality of the manuscript. We address each comment below.

1.1 Major comments

Reviewer statement 1a: *This paper is about OpenFOAM rather than a generic finite-volume model. This is stated by the authors in line 195 “The results herein proposed are hence representative of the OpenFOAM solver with the standard wall-layer treatment—the set-up that is most commonly adopted when using this code”. This information first comes in line 87. The relevance of the paper would be clarified and improved if this information is clearly stated earlier in the manuscript, in the abstract and maybe the title.*

Response: We thank the reviewer for this comment. We have now pointed out in the abstract, introduction and conclusions that the “class of solvers” considered herein are based on the OpenFOAM “framework” (see quotations below). We refrained from adding the *OpenFOAM* keyword in the title because findings from this study are not limited to solvers built within OpenFOAM but extend to any finite volume software/code/solver relying on these same discretization and physical-modeling procedures.

“(Abstract) The present work assesses the quality and reliability of an important class of general-purpose, second-order accurate finite-volume (FV) solvers in the large-eddy simulation of a neutrally-stratified atmospheric boundary layer (ABL) flow. [...] Simulations are carried out within the OpenFOAM[®] framework, which is based on a colocated grid arrangement.”

“(Introduction) Motivated by the aforementioned needs, the present study aims at characterizing the quality and reliability of an important class of second-order accurate FV solvers for the LES of neutrally-stratified ABL flows. The analysis is conducted in the open-channel flow setup (no Coriolis acceleration) via the OpenFOAM[®] framework (Weller et al., 1998; De Villiers, 2006; Jasak et al., 2007).”

“(Conclusions) [...]This work provides insight on the quality and reliability of an important class of general-purpose, second-order accurate FV-based solvers in wall-modeled LES of neutrally-stratified ABL flow. The FV solvers are part of the OpenFOAM[®] framework, make use of the divergence form of the nonlinear term, and are based on a colocated arrangement for the evaluation of the unknowns.”

We’ve also add a dedicated discussion in the Methodology section on the characteristics of the OpenFOAM framework, that are shared by the considered class of solvers:

“(Methodology) In the OpenFOAM[®] framework, the computational grid is colocated. Although advantageous in complex domains when compared to staggered grids (Ferziger and Peric, 2002), the colocated arrangement is known to cause difficulties with pressure-velocity coupling, hence requiring specific procedures to avoid oscillations in the solution. The standard Rhie-Chow correction (Rhie and Chow, 1983) is here adopted, which is known to negatively affect the energy-conservation properties of central schemes (Ferziger and Peric, 2002). In addition, when approximating the integrals over the surfaces bounding each control volume (as a consequence of the Gauss divergence theorem), the unknowns are evaluated at face-centers and are assumed to be constant at each face, yielding an overall second-order spatial accuracy (Churchfield et al., 2010). Since the divergence form of the convective term is used in combination with a low-order scheme over a non-staggered grid, the solution is inherently unstable (Kravchenko and Moin, 1997). The present work makes use of the linear and the QUICK interpolation schemes (Ferziger and Peric, 2002) to evaluate the unknowns at face-centers. The numerical solver combines the PISO algorithm (Issa, 1985) for the pressure-velocity calculation and an implicit Adams–Moulton scheme for time integration (Ferziger and Peric, 2002). The performances of an alternative solver characterized by a Runge–Kutta time-advancement scheme and a projection method for the pressure-velocity coupling (Vuorinen et al., 2014) are also analyzed in the Appendix.”

Reviewer statement 1b: *The abstract should also indicate that the analysis is restricted to the Smagorinsky subgrid-scale model because this is important to interpret the results.*

Response: This comment was addressed by adding the following sentence to the Abstract:

“A series of open-channel flow simulations are performed using a static Smagorinsky model for sub-grid scale momentum fluxes and an algebraic equilibrium wall-layer model.”

Reviewer statement 2: *The paper considers an “open-channel-flow set-up”, and not an atmospheric boundary layer, and this information only comes in line 150. This information should also be in the abstract and the introduction.*

Response: This point was addressed by adding the following to the Abstract:

“The analysis is carried out within the OpenFOAM[®] framework, which is based on a colocated grid arrangement. The spatially-filtered incompressible Navier–Stokes equations are solved in an open-channel flow setup (no Coriolis acceleration).”

and the following to the Introduction:

“The analysis is conducted in the open-channel flow setup (no Coriolis acceleration) via the OpenFOAM[®] framework (Weller et al., 1998; De Villiers, 2006; Jasak et al., 2007).”

Reviewer statement 3: *The sensitivities that the authors study greatly depend on the resolution, measured in terms of the number of grid points (or an effective Reynolds number [Sullivan and Patton, 2011], or the ratio of the filter size to the integral length scale). Therefore, the grid size that the authors consider in the analysis should also be in the abstract, the introduction, and the conclusions. This information is important to interpret the results. The sensitivity to grid size is particularly large for the resolutions that the authors consider, which are lower than in common ABL studies. In line 165, the authors write “The chosen grid resolutions are in line with those typically used in studies of ABL flows (see, e.g., Salesky et al., 2017).”, but Salesky et al. 2017 uses 160^3 or 256^3 , which is a substantial difference to 64^3 . Resolution studies consider even larger grid sizes [Sullivan and Patton, 2011].*

Response: We agree with the point made by the reviewer. This comment was addressed by extending the analysis to cases up to 160^3 control volumes. The manuscript was edited accordingly throughout. We want to point out that while 160^3 collocation nodes in Cartesian codes run in a matter of hours for ABL flow simulations, FV-solvers supporting unstructured grid approaches are almost two orders of magnitude slower and 160^3 hence represents a state-of-the-art resolution. Overall though we agree that this resolution is relatively modest and hence results are expected to depend on this factor. This aspect of the problem has been pointed out in the Results section of the revised manuscript and in the Conclusions.

Reviewer statement 4: *The statements regarding the dependence of the results on resolution are too general. For instance, the authors write*

in line 5, “It is found that first- and second-order velocity statistics are sensitive to the grid resolution and to the details of the near-wall numerical treatment, and a general improvement is observed with horizontal grid refinement. Higher-order statistics, spectra and autocorrelations of the streamwise

velocity, on the contrary, are consistently mispredicted, regardless of the grid resolution.”

in line 20, “Although mean flow and second-order statistics become acceptable provided sufficient grid resolution, the use of said solvers might prove problematic for studies requiring accurate higher-order statistics, velocity spectra and turbulence topology.”

in line 70, “the excessive damping of resolved-scale energy at high wavenumber is likely to compromise their predictive capabilities for high-Reynolds ABL-flow applications.”

in line 222, “Grid refinement in the horizontal directions leads to an improved matching between the FV and the PSFD solver, both in terms of shape and magnitude.”

in line 233, “Grid refinement in the horizontal directions improves the matching between the FV-based and the PSFD-based [...]”

It might be more useful to say how much this dependence on resolution is, i.e., how much one particular property change when changing resolution around a particular value. In the end, as the grid is refined, we would reproduce better and better more and more properties. The important question is what grid size (or effective Reynolds number, or ratio between the filter size and the integral length scale) we need to obtain certain statistics with a given accuracy, in this case, when using OpenFOAM with a Smagorinsky subgrid-scale model in wall-bounded shear flows. For instance, for direct numerical simulations, we know that second-order methods typically need twice the resolution of spectral methods to similarly represent the variances [Moin and Mahesh, 1998]. What would be the equivalent for OpenFOAM in the model configuration considered in this study? This comment relates to what the authors write in line 83: “Note that the studies conducted with FV-based solvers are mainly focused on first- and second-order flow statistics, which are themselves not sufficient to fully characterize turbulence—and related transport—in the ABL.”. What do the authors mean by “fully characterize”? For some applications, correctly representing the first- and second-order moments might be sufficient, whereas for other applications (atmospheric chemistry, wild fires) representing the spectra and LSMs might be insufficient.

Response:

We thank the reviewer for this critical input. We devoted a significant amount of efforts to this task. Both relative variations of FV profiles as a function of resolution and variations of the FV profiles with respect to reference PSFD and/or experimental ones at different resolutions were evaluated. We concluded that experimental profiles represent a good candidate for the convergence analysis at these relatively low resolutions where convergence is not strictly related to the order of accuracy of the scheme and is often non monotonic. The Results section now features several tables with quantitative measures of convergence of selected flow statistics against corresponding experimental values (streamwise velocity variances, velocity skewness, kurtosis, and integral length

scales). Note that the convergence is non-monotonic in most cases, due to the modest resolution and to the interaction of discretization and physical modeling errors, whose quantification is not trivial for this complex flow system (Meyers et al., 2006; Meyers and B.J. Geurts, 2007; Meyers and Sagaut, 2007; Ghosal, 1996). These tables nevertheless provide useful insight on the performance of FV-based solver and more quantitative information the community will benefit from. It is also apparent that higher grid resolutions are required for FV solvers to match results from the PSFD solver, or to at the least capture the dominant momentum transfer mechanisms in the channel flow system. The latter was identified as the main limitation of the considered class of FV solvers. Given that general-purpose FV solvers supporting unstructured grid setups are typically two orders of magnitude slower than PSFD solvers, going well beyond 160^3 control volumes will be a rather challenging task, and justifies the proposed study.

We have removed the following comment in the revised version of the manuscript: “Note that the studies conducted with FV-based solvers are mainly focused on first- and second-order flow statistics, which are themselves not sufficient to fully characterize turbulence—and related transport—in the ABL.”.

Reviewer statement 5: *The introduction reads too much as a review, the focus on OpenFOAM appearing first and unexpectedly in lines 85-90. It might be useful to focus more the introduction around OpenFOAM, the half-channel configuration, and the kind of grid sizes that are considered in this analysis. This might help setting the right expectations earlier in the paper. In a similar line, the review on LSM between lines 260 to 275 might be shortened.*

Response: We thank the reviewer for this input. We have streamlined the Introduction, which now provides the motivation and objectives of the work. Details regarding the setup of the problem such as the considered grid resolutions, the half channel configuration, etc. are also briefly mentioned, but a detailed discussion of these aspects is postponed to the Methodology section (see revised manuscript).

Reviewer statement 6: *In line 187, the authors indicate that the log-layer mismatch observed in this study is a well-known problem of wall models. In line 218, the authors indicate that rms-deviations observed in this study is a well-known problem in FV-based WMLES. What is then new in this manuscript? The particularization to OpenFOAM at this particular resolution? I guess this comment relates to point 1.*

Response: We thank again the reviewer for this critical input. To the author’s knowledge, this is the first assessment of the performance of this important class of FV-based solvers for the simulation of ABL flows at this level of detail/insight from a flow

physics perspective. For example, no study has previously assessed the capability of second-order accurate FV-based solvers in capturing momentum transfer mechanisms in ABL flows, how this depends on details of the numerical discretization and how it impacts relevant flow statistics. One of the key novel findings is “[...]that this class of FV-based solvers overall predicts a flow field that is less correlated in space when compared that of the PSFD solver and is not able to capture the salient features responsible for momentum transfer in the ABL, at least at the considered grid resolutions. These limitations appear to be the root cause of many of the observed discrepancies between FV flow statistics and the reference PSFD or experimental ones, including the mispredicted streamwise-velocity skewness, the imbalance between sweeps and ejections, and the overall sensitivity of flow statistics to variations in the grid resolution.” With regards to the log-layer mismatch and rms-deviations: Most of the previous findings pertained to relatively low Reynolds numbers. Here we have shown that these problematics are a problem also at ABL Reynolds numbers and that procedures devised to alleviate the log-layer mismatch issue do not seem to work, which motivates further research in the field. We also showed how this mismatch depends on the numerical scheme that is used and how it depends to grid resolution, which is new. Note also that the revised manuscript has been substantially modified and now includes a detailed comparison between the performance of two interpolation schemes for the discretization of nonlinear terms, and how these schemes affect the above quantities has been commented. Further, in an effort to address this comment from the reviewer, the main contributions of this work have now been listed in the Conclusions section of the revised manuscript.

1.2 Minor comments

Reviewer statement 1: *In line 137, I am not sure I understand where $u_\tau = \sqrt{\tau_{\alpha 2,w}|\mathbf{u}|/u_\alpha}$ comes from. I do not understand equations 5 to 6. Related to it "no-slip applies at the lower surface" in line 153 is strange...*

Response: Sub-section 2.1 was expanded to provide a more detailed derivation of the wall-model. Specifically, the following lines were added:

“Employing the no-slip condition for the velocity field, the standard FV approximation of the shear stress at the wall gives (Mukha et al., 2019)

$$\tau_{i2,w} = (\nu + \nu_t) \left. \frac{\partial u_i}{\partial x_2} \right|_w, \quad i = 1, 3,$$

where the subscript f is used to denote the evaluation at the center of the wall face, the subscript c denotes the evaluation at the center of the wall adjacent cell and Δx_2 is the distance from the wall. From the logarithmic law (Eq. 4) evaluated at the first cell-center, one can write $u_\tau = \kappa|\mathbf{u}|_c / \ln(\frac{\Delta x_2}{x_{2,0}})$. Using the definition of friction velocity $u_\tau = \sqrt{\tau_w^2}$, where τ_w is the magnitude of

the wall shear stress vector, along with Eq. 5, and rearranging, the total eddy viscosity at the wall reads...

The sentence "... no-slip applies at the lower surface..." refers to the no-slip condition employed in combination with the wall-model.

Reviewer statement 2: *In line 154, the authors write "The kinematic viscosity is set to 10^{-7} m²/s in the bulk of the flow, resulting in $Re = 10^7$ ". I think the information about Re is meaningless because the effective Reynolds number introduced by the subgrid-scale diffusivity is much smaller. As the authors later say, one can neglect the molecular viscosity against the subgrid-scale viscosity. The value of the viscosity is also a bit strange for an ABL context.*

Response: We agree with the comment. However, the simulations were run by setting the kinematic viscosity at 10^{-7} m²/s. For this reason, the sentence was edited as follows:

"The kinematic viscosity is set to a nominal value of 10^{-7} m²/s, which results in an essentially inviscid flow."

Reviewer statement 3: *Adding colors in the figures might help the reader to distinguish the various cases more easily.*

Response: Colors were added to the figures.

Reviewer statement 4: *In line 227, the authors refer to the results of Del Alamo et al. 2006 regarding skewness, flatness and correlation coefficient. It might be useful to add this data to figure 3.*

Response: Del Alamo et al. 2006 do not refer to quantitative data. In Fig. 3, the measurements from Monty et al. (2009) were added.

Reviewer statement 5: *In table 3, why taking the tangent point to $k^{-5/3}$ to distinguish between inertial and large-scale and not some integral length scale [Pope, 2000]? Moreover, 32 points seem too few to distinguish an inertial subrange.*

Response: We thank the reviewer for this input. We agree that leveraging integral length scales would be a preferable approach to distinguish between the inertial and the

production range. However, depending on the numerical setup, FV-based solvers at the considered resolutions are severely underpredicting integral length scales (see Tab. 4), thus complicating the analysis / interpretation of results. In view of this limitation, and as part of a paper-streamlining effort, we have removed this PSD analysis along with Table 3.

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