Authors response Liqui Lung et al. (2023) - Open Boundary Conditions for Atmospheric Large Eddy Simulations and the Implementation in DALES4.4

Franciscus Liqui Lung
Christian Jakob
Pier Siebesma
Fredrik Jansson

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We want to thank the referees for their in depth review of our submitted manuscript and their comments and suggestions. In this response we aim to address their comments. For readability we have collected the comments from both reviewers and will discuss them per section.

1 Major comments

RC1 Several points in the description of the open boundary conditions are unclear or even not mentioned.

AC We agree with the concerns raised and addressed the comments in the *open boundary implementation* section of this document.

RC1 The reference test case is not sufficiently described, which prevents from really evaluating the performance of the boundary conditions.

AC We have elaborated on the reference case setup and included the initial profiles, a table with all the forcings and for the periodic simulation height profiles at different time intervals for the potential temperature, resolved vertical temperature flux ($\overline{w'\theta'}$), east-west wind velocity (u) and east-west resolved wind variance ($\overline{u'^2}$).

RC1 Many statements seem rather weak, or even quite obvious, in the comments of the simulation results. I think that the conclusions should be strengthened.

AC We clarified the objectives on which we judge the performance of the boundary conditions. The simulations are evaluated statistically and not deterministically. The addition of synthetic turbulence is not to retrieve the same results as the unsmoothed simulation, but rather to mitigate artifacts as a result of the missing turbulence in the input data. To help quantify the influence of the boundary conditions on turbulence, the TKE (which will be renamed as it is strictly speaking not TKE see later comments) is integrated over the boundary layer. This gives an easier to read plot. Details of the adjustments can be found in the *Discussion and Presentation of Results* section of this document.

RC2 The author motivate their study by nesting LES domains into large-scale model domains. It is well known that other LES models which use Dirichlet boundary conditions for time-dependent mesoscale flow inputs sometimes suffer from wave-like structures near the boudaries, so better formulated boundary conditions to overcome this would be highly appreciated. However, as far as I understand, the boundary conditions described herein are only supposed to be used for idealized situations where the inflow and outflow boundary are fixed over the LES simulation period. For example, in a mesoscale-nested simulation, it is likely that the wind speed and direction continuously change in time, meaning that an inflow boundary can become an outflow boundary and so on. While this is still considered in the equations, though not supported by any analysis, the situation where a lateral boundary can become both, inflow and outflow boundary at the same time, is not considered in the equations. For example, this situation can occur if you want to model mesoscale phenomena like sea breezes, local wind systems, convective situations with weak winds, or situations like frontal passages. This is because the radiation boundary condition requires slab averages of the outward-pointing component. If there is a significant inflow at this boundary, the $\langle u_n \rangle$ can become negative. In case this happens, the flow becomes quickly unstable in conjunction with radiation boundary conditions, meaning that the proposed method is only applicable for idealized scenarios. Thus, the use of a slab average actually prohibits that a boundary can be both, inflow and outflow boundary at the same time. I recommend to rephrase the general motivation in this context, in order to avoid the impression that the proposed formulation of the boundary conditions solves the issue in general.

AC Our ultimate goal is to be able to nest DALES in mesoscale models. We agree that mesoscale-nested simulations involve time-varying boundary conditions and this has played an important part in how we defined our boundary conditions. We acknowledge that the presented test setup does not include all the challenges of a mesoscale-nested simulation. However, we believe that the presented setup is a first necessary set of tests that the implementation needs to pass before moving to more complicated test cases in future publications as they may mask basic problems with the open boundary implementation. We are aware of the instabilities that can arise with radiation boundary conditions that use slab averages on time-varying boundaries. This is why we chose not to use slab averages, but instead defined the integration length scales over which we calculate the phase velocity and mass flux correction term. The integration length can conveniently be chosen to be the resolution of the "mother" model. This choice gives maximum freedom to the boundary conditions given the constrains imposed by the mother model (see *boundary implementation* section for more on this). We believe, that the mass correction term plays an important role in preventing any instabilities from building up. From other comments we do realize that the description of this correction term was not clear and we have elaborated on it in the *open boundary implementation* section. We do not believe the presented implementation can only be used in idealized setups and as this is also not our ultimate goal, we do not want to phrase it this way. The goal to be able to do mesoscale-nested simulations has motivated our implementation choices and we therefore do want to mention it. However, we do agree with the reviewer that the presented test case is not sufficient to claim that the setup will work in a mesoscale-nested setup and we will remove any such claims and mention that further testing is required. Since the submission of this manuscript, we have used this implementation to nest DALES in a mesoscale model, we will leave these results however for later publication.

RC2 The description of the boundary conditions lacks important information and is partly misleading. For example, the boundary conditions are formulated as tendencies instead of boundary values. However, the boundary value itself is required for the spatial descretization of the advection term, so I recommend to reformulate the equation towards boundary values. Further, the term slab average is not fully defined. It seems to have a different meaning at the outflow boundary compared to the inflow boundary. Moreover, the formula for the time-scale computation seems to be wrong because the second term in Eq. 13 does not become dimensionless.

AC We have addressed most of the comments that reviewers had on the description of the open boundary implementation in the *open boundary implementation* section. We however do not understand the comment on using tendencies instead of boundary values as we do not see a problem with using current time step values to calculate tendencies for the next time step. We have added the discretisation schemes and believe this will clarify the implementation. The e in the time-scale computation represents a subgrid velocity scale and not the subgrid TKE. In this case we used the square root of the subgrid TKE as the velocity scale and have added this information to the manuscript.

RC2 The setup description of the test case lacks important information. Which surface boundary conditions did the authors use (momentum, heat, SGS-TKE, ...), which numerical schemes were applied (pressure solver, advection and time discretization, ...). Moreover, it is not clear to me how the north and south boundaries were treated (period BC vs. inflow/outflow BC?).

AC We agree with the reviewers that description of the test case lacks information and we have updated the description. We have included the initial profiles, surface boundary conditions, subgrid scheme and a table that includes all forcings. We have also referenced the DALES paper [Heus et al., 2010] for the used discretisation schemes and information on the pressure solver. In the simulations with open boundary conditions the north and south boundaries are treated as open boundaries. Depending on the input velocity, cells on these boundaries will either be inflow or outflow this will change between cells and with time.

RC2 I like the idea of a big-brother simulation to investigate the impact of the open boundary conditions in a systematic manner. However, the performance of the open BC is not sufficiently supported by the test case and the analysis. The authors only used a single setup for a convective boundary layer with a fixed inflow and outflow boundary. However, convection may easily masked systematic effects because instantaneous fluctuations may superimpose weaker systematic biases. For this purpose I think the evaluation of the model need to be extended towards purely neutral flows. Moreover, I think the test scenario should be also extended to a case with changing inflow conditions with respect to the wind speed to i) evaluate the performance of the mass-conservation scheme and ii) to demonstrate that proposed time-dependent relaxation time-scale algorithm works properly. Also a test case with changing wind direction is required to demonstrate that the boundary conditions can also deal with such situations.

AC The goal of this paper is to describe the current implementation of open boundary conditions in DALES and present a first necessary set of tests. We agree with the reviewer that the proposed cases all test and show different aspects and we have conducted some of them in the past (neutral and mesoscale-nested), however for readability we do not want to include them in the current manuscript and we will leave them for future publications. As mentioned before we will remove any claims that can not be supported by the current test case or state that they require further testing. We will also remove any references to simulations not presented in the manuscript.

2 Introduction

RC2 l8: The first part of the sentence sounds strange and should be rephrased.

AC Will rephrase *The results show that when the ration between input and model resolution increases,* to *When smoothing is applied over larger/longer spatial/temporal scales,*

RC2 l12: I wouldn't say LES exists to study small scale weather phenomena but would formulate this in a more general way, e.g. to study turbulent motions.

AC Agree, we will rephrase *study small scale weather phenomena* to *study turbulent motions*

RC2 l25: What do the authors mean by the term "fields"?

AC We mean the variables. We will change *fields at inflow boundaries and propagate fields* to *variables at inflow boundaries and propagate variables.*

RC2 l43-45: It would be useful for the reader if the authors would be more specific, i.e. which model uses which kind of BC. The way the sentence if phrased is too general in my opinion. Also, concerning a description of inflow/outflow BC, the Maronga et al. (2015, https://doi.org/10.5194/gmd-8-2515-2015) paper is more suited reference.

AC We will add a table with information on the different open boundary condition options in the mentioned models. We will also reference Maronga et al. [2015]. Maronga et al. [2015] describes the fixed in and outflow setting present in PALM 4.0, Maronga et al. [2020] however also describes the new possibility of self-and-rans nesting, for which they use prescribed boundary conditions, so we will reference both.

RC2 l48-l49: In addition to the Mazzaro paper it would be nice to add the original literature (Mirocha et al., 2014, https://doi.org/10.1175/MWR-D-13-00064.1, plus the follow-up literature - see also references in Mazzaro et al., 2017) of the cell perturbation method too. Also, to my knowledge, Heinze et al. (2017) used no prescribed boundary conditions as stated in the follow sentence but periodic boundary conditions in combination with a large-scale forcing term inferred from mesoscale model output.

RC2 l54-55: The reference to Heinze et al. (2017) at this point is misleading and not correct. As mentioned before, the study used period BC and the relaxation therein does not refer of a relaxation in space but in time, formulated as a nudging term.

AC We will add Mirocha et al. [2014] as a reference. Heinze et al. [2017] describes the use of ICON-LES nested in COSMO for realistic simulations over Germany. The main simulation uses prescribed boundary conditions as described in the first paragraph of section 2: *Model description, set-up and simulation output*. For reference they do include results of smaller doubly periodic simulations, but they are only included for validation and are not the main simulation of the paper.

RC2 Intro: The manuscript would profit if the authors add some more text to introduce the term "open BC" and distinguish it from period boundary conditions with respect to its advantages and disadvantages. For example, also with periodic boundary conditions you can study larger-scale phenomena, even over heterogeneous land surfaces in particular cases.

AC We will add to the manuscript what type of simulations can be done using periodic boundary conditions and for what type of simulations we need open boundary conditions and why we want to go there to the introduction.

RC2 l53: What do the authors mean with the term "numerical boundary layer"?

AC We mean a thin layer upstream of the boundary where wiggles and perturbations are formed as a result from the very strict Dirichlet boundary condition. We will rephrase *Dirichlet boundary conditions are however known to create reflections and a numerical boundary layer at outflow boundaries* to *Dirichlet boundary conditions are however known to create reflections and perturbations at outflow boundaries.*

RC2 Moreover, a formulation like "often accompanied" is inappropriate here. The authors should be more specific in terms which model uses which strategy to mitigate boundary effects.

AC The references in brackets indicate the models that report that they used a relaxation/nudging technique. For clarity we will rephrase *The prescribed boundary condition is therefore often accompanied with a relaxation zone (...)* to *For this reason Moeng et al., 2007; Zhu et al., 2010 and Heinze et al., 2017 use a relaxation zone in combination with a prescribed boundary condition,* We will also add this information to the table that describes which model uses which boundary conditions.

3 Open boundary implementation

RC1 Eq. (1) does not make sense, since it adds scalar values, like $\partial u_n/\partial t$ or ϵ, and a vector value $\hat{z}$

AC We agree that the notation is wrong. In the revised version we will split the equation for the lateral and top boundaries

$$\frac{\partial u_n}{\partial t} = \begin{cases} -\frac{U}{\rho}\frac{\partial \rho u_n}{\partial n} + \epsilon, & \text{for lateral boundaries} \\ -\frac{U}{\rho}\frac{\partial \rho u_n}{\partial n} + g\frac{\theta - \langle\theta\rangle}{\langle\theta\rangle} + \epsilon, & \text{for top boundary} \end{cases}$$

RC1 Line 139: $x_n - \hat{x} \cdot \hat{n}\Delta x_n$ is a location, not a cell.

AC We will change the wording from *the grid cell directly upstream of the boundary* to *the location one gridsize upstream of the boundary*

RC1 Line 143, *Equation (2) is discretised using a second order forward scheme*: what does it mean exactly? Please provide the expression of the numerical scheme. Idem for the discretisation of (1).

AC Here we made a mistake, this should be a first order upwind scheme and is defined as

$$\left.\frac{\partial u}{\partial n}\right|_i \approx \begin{cases} \frac{u_i - u_{i-1}}{\Delta x_n}, & \text{for } u_B >= 0 \\ \frac{u_{i+1} - u_i}{\Delta x_n}, & \text{for } u_B < 0 \end{cases}$$

For the time derivative discretisation the third order Runga Kutta method used by DALES [Heus et al., 2010] is used. We will add this information to the revised manuscript.

RC1 Line 145, *a Dirichlet boundary condition is used for the boundary-normal velocity components*: I do not agree. A Dirichlet boundary condition for the boundary-normal velocity component would read $u_n = u_n^B$. And a Dirichlet boundary condition for the tendency of the boundary-normal velocity component would read $\frac{\partial u_n}{\partial t} = \frac{\partial u_n^B}{\partial t}$. (3) is actually some kind of nudging of u_n towards u_n^B, with a relaxation time scale equal to Δt. Moreover the time discretisation of (3) should also be indicated.

RC2 2.1.2 Inflow: What does it exactly mean that the Dirichlet condition is implemented as a tendency term? Suppose there is a mesoscale model input which changes over time and the LES model is in between 2 mesoscale model timesteps. How exactly are the BCs for the velocity vector and other quantities computed? I guess at the end DALES requires some kind of boundary values for each prognostic quantity for the spatial discretization rather than a tendency term? Moreover, as the authors mentioned that a tendency term work well with the pressure solver, at what stage are the boundary values imposed, before or after invoking the pressure solver?

AC We agree that the description given by RC1 is more accurate than the current one and we will change *a Dirichlet boundary condition is used for the boundary-normal velocity components* to *the boundary-normal velocity at the boundary u_n is nudged towards the input value u_n^B with a relaxation time scale equal to the integration time scale used by DALES. The discretisation of the time derivative is given by a third-order Runga Kutta scheme used by DALES and is described in Heus et al. [2010].* In the given setup the input was given at the same spatial and temporal resolution as the simulation, so the case described by RC2 where DALES would be in between two input time steps does not occur. However, the current implementation has been used to simulate more realistic cases in which DALES was coupled to a mesoscale model. In this case, the boundary input data is linearly interpolated in time if DALES is in between two mesoscale time steps. This information will be added to the manuscript. Boundary input is required for all the prognostic variables of DALES. In the implementation the tendencies are applied before the pressure solver. The order does however not matter as the pressure solver uses homogeneous Neumann boundary conditions $\frac{\partial p}{\partial n} = 0$ and has therefore no influence on the tendencies of the boundary-normal velocity components at the boundaries.

RC1 Eq. (4): S(B) is not defined.

RC1 Eq. (5): S^{int} is not defined. I understand that it is a patch around the boundary, but it should be defined exactly.

RC1 Eq. (6) is definitely unclear to me. Is ϵ a constant or does it depend on space and time? Is the $\epsilon(S^{\text{int}})$ the same as ϵ? If ϵ is a constant, (6) is indeed only the time derivative of (5), which does not involve any ϵ. The way ϵ is actually estimated should be rewritten clearly.

RC2 l170: I disagree with this interpretation. The boundary values enter the equations via the resolved- and subgrid-scale advection terms and not via the pressure term.

AC We agree that the section on the mass correction term ϵ needs clarity, especially since it's to our best knowledge a new approach. The following adjustments will be made:

- l156 rephrase to *The input boundary-normal velocity components integrated over the lateral and top boundaries $S(B)$ satisfy the continuity equation conform the reference density profile used by DALES.*
- l159 rephrase to *The lateral and top boundaries are subdivided into patches S^{int} defined by Δy^{int} and Δz for the west and east boundaries, Δx^{int} and Δz for the north and south boundaries and Δx^{int}*

and Δy^{int} for the top boundary. We enforce that the mass flux integrated over each patch equals the mass flux given by the input velocities integrated over the same patch.

- l162 rephrase to *To obtain the correction factor ϵ, we define ϵ to be constant (in space) within a single integration patch S^{int}, but can differ between patches. To obtain an expression for the correction term on a particular integration patch $\epsilon\left(S^{int}\right)$, we take the time derivative of eq. (5). Further, we define $\frac{\partial \tilde{u}_n}{\partial t} = \frac{\partial \tilde{u}_n}{\partial t} - \epsilon$ as the tendency from either eq. (1) or (3) minus the correction term. Within DALES the tendencies for the boundary normal velocities are first calculated without the correction term. These tendencies are then used to calculate the correction term e using eq. (6) for each integration patch. The correction factor is then added to the tendencies before applying them to make sure mass is conserved.*
- l165-169 rephrase to *The correction factor ϵ can be physically interpreted as the correction required to force the mass flux through the integration patch S^{int} to the mass flux given by the input. Since the constrain is set on the integrated quantity, fluctuations smaller than the set integration patch are conserved. Smaller values for Δx^{int} and Δy^{int} impose more strict boundary conditions, with Dirichlet conditions in the limit where $\Delta x^{int} = \Delta x$ and $\Delta y^{int} = \Delta y$. When used in a nested simulation, Δx^{int} and Δy^{int} could be set to the gridsize used by the mother model. In this setup the total mass flux through a mother cell at the boundary of the child model is conserved, while the child model is free to generate turbulence on smaller scales. This is illustrated in 2D in fig 1 in which the blue cells correspond to the mother model and have a resolution of Δx^{mother} and the brown cells to the child mother (DALES).*
- l170-174 rephrase to *The role of the correction term is to conserve mass integrated over the domain, such that the pressure solver, which needs to find a solution that conserves mass locally, can find a solution. It is possible to implement the tendency from the correction factor as a non-homogeneous Neumann boundary condition for the pressure solver, such that all the tendencies as a result of the continuity requirement are together. We chose however, to add the term in the equations for the boundary-normal velocity components and use homogeneous Neumann boundary conditions for the pressure field, because this allows us to keep using the Fourier pressure solver present in DALES [Heus et al., 2010], by using cosine basis functions only.*

RC2 Headings of 2.1 and 2.2: The logical structure is misleading or the heading is poorly phrased. When 2.1 is about boundary-normal velocity components, I would expect that 2.2 is about boundary-parallel components and not about cell centered variables.

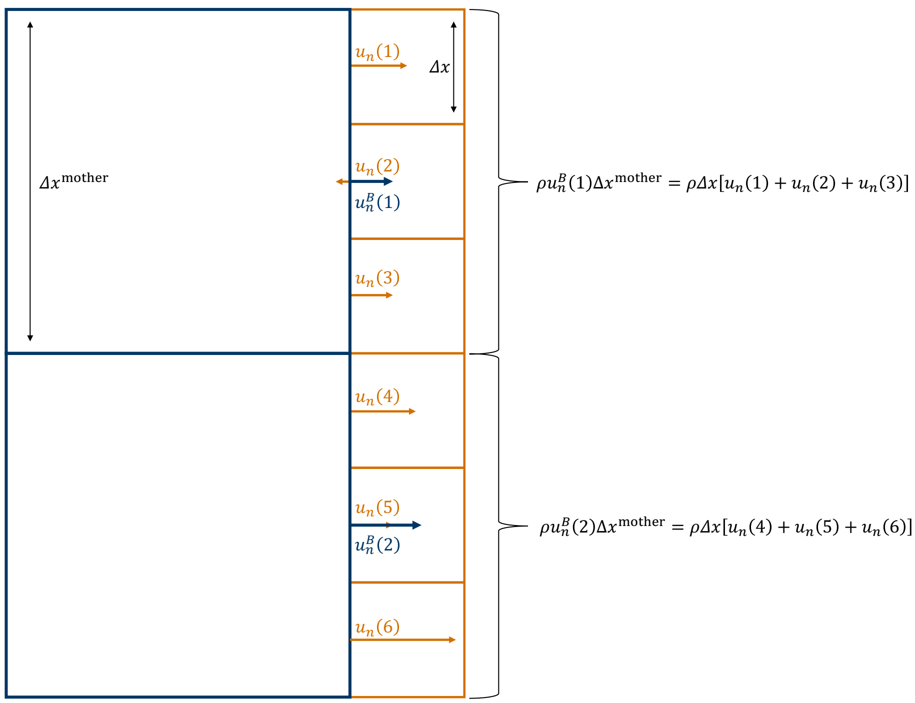

Figure 1: 2D illustration of a nested setup in which the integration length scales are set to the gridsize of the mother model. In this setup the mass flux through a mother cell (blue) at the boundary of the child model (brown) is conserved, while the child model is free to generate turbulence on smaller scales.

AC The sections are divided between variables located at the boundary, the boundary-normal velocity components, and variables that are located offset from the boundary, since they differ in the implementation of their boundary conditions. We agree that the tangential velocity components are strictly speaking not cell-centred variables and we will change the heading of 2.2 to *Boundary-tangential velocity components and cell-centered variables.*

RC2 l190: What does the term "homogeneous Neumann condition" exactly mean? I see it is defined later in Eq. 11, but should be mentioned already when first used.

RC1 Eq. (7): why do you choose a zero normal flux condition at outflow for all variables but u_n? You could have made other choices: please elaborate a little bit.

AC The term homogeneous Neumann condition means a zero normal flux condition $\frac{\partial \psi}{\partial n} = 0$, we will include this in the revised manuscript. The choice to use this condition for all variables except for the boundary-normal velocity component is based on the results of Sani and Gresho [1994]. The homogeneous Neumann conditions for the non boundary-normal velocity components at outflow boundaries are chosen, because they are less strict then a condition on the variable itself [Sani and Gresho, 1994]. Therefore, they tend to produce less disturbances. According to Sani and Gresho [1994] and Craske and Van Reeuwijk [2013] setting homogeneous Neumann conditions for the boundary-normal velocity components results in a ill-posed system with fluctuations in the pressure field and is not suited for turbulent flows. Craske and Van Reeuwijk [2013] conclude in their literature review in their introduction that radiation boundary conditions give the least amount of disturbances at outflow boundaries. Sani and Gresho [1994] also find that radiation boundary condition perform the best out of three boundary conditions tested. We will include this in the revised manuscript.

RC2 l200-201: To my knowledge this is exactly what is done in PALM (see Hellsten et al., 2021; Kadasch et al., 2021) and in WRF (Moeng et al., 2007; Mirocha et al., 2014), which does not seem to cause significant problems in both models. At least the authors should mention this. Furthermore, this raises the need to improve the argumentation why special Robin boundary conditions are required in conjunction to what happens in DALES when large gradients occur at the boundaries.

AC The potential issue of large gradients and tendencies is a result of less strict or "free" outflow boundary conditions. At outflow boundaries the LES can diverge from the mother model due to the radiative and homogeneous

Neumann boundary conditions. When an outflow boundary changes to an inflow boundary, Dirichlet boundary conditions instantly force the solution to be equal to the input. This can result in large tendencies. Palm uses prescribed boundary conditions in their nested setup, which means that at outflow boundaries the solution is also restricted by the prescribed values from the mother model. So the LES is not free to diverge, which means that the issue of large gradients/tendencies is not present. We however want the LES to be free and force it minimally at outflow boundaries. We will include this information in the revised manuscript to clarify the source of this potential problem.

RC1 Line 206 and Eq. (9), *advection over an inflow boundary nudges the boundary value to a given input value*: this sentence corresponds to the equation

$$\frac{\partial \psi}{\partial t} + u_n \frac{\partial \psi}{\partial n} + \frac{\psi - \psi^B}{\tau} = 0 \tag{1}$$

which is different from what is implemented. Actually (9) corresponds to the nudging inflow condition for u_n (3) (without ϵ, and with a more general relaxation time scale). But since ψ is discretised one half-cell into the domain and not on the boundary, you have to decide what the value of ψ is on the boundary. For this, you assume that ψ is locally transported at speed u_n, i.e. $\frac{\partial \psi}{\partial t} = -u_n \frac{\partial \psi}{\partial n}$

RC2 l227: Isn't e usually being defined as the SGS-TKE? If yes, the units do not match (term in brackets needs to be dimensionless). If not, how is a subgrid-velocity being defined? SGS-models usually give estimations for the SGS-TKE but not for the velocities. There are formulations for SGS-velocites (see e.g. Weil et al., 2004; Weil, J.C.; Sullivan, P.P.; Moeng, C.H. The Use of Large-Eddy Simulations in Lagrangian Particle Dispersion Models. J. Atmos. Sci. 2004, 61, 2877–2887), but I have the impression that the authors mean something different.(?)

AC We get the confusion around the description of the origin of the Robin boundary condition. We will change line 206-208 to *To derive the inflow boundary condition, we assume that advection is the only process taking place at the boundary,*

$$\frac{\partial \psi}{\partial t} + u_n \frac{\partial \psi}{\partial n} = 0 \tag{2}$$

We also impose that the boundary value is nudged towards a given input value ψ^B over a timescale τ,

$$\frac{\partial \psi}{\partial t} = \frac{\psi - \psi^B}{\tau} \tag{3}$$

Combining these two constrains gives

$$-u_n \frac{\partial \psi}{\partial n} = \frac{\psi - \psi^B}{\tau} \tag{4}$$

In the definition for the variable timescale, e is a subgrid velocity scale and not necessarily the TKE. We have used the square root of subgrid TKE as the velocity scale. We will make this clear in the manuscript and to avoid confusion, we will use a different symbol.

RC2 l244-245: Can the authors please specify if this is their personal experience, or if it is experience deduced from previous studies? To my knowledge, the current state of literature does not support to make such a statement - there exists no extensive quantitative comparison between different methods so far. Also, I strongly doubt that temperature fluctuations give perse a better solution than just adding perturbations onto the velocity components because the physical mechanisms of turbulence development differ and might not fit to the physical setup. For instance, in purely-shear driven flows this can lead to long persisting streak-like structures.

AC This is from personal experience. In our opinion the problem of starting turbulence at the inflow boundary is similar to spinup of turbulence in a periodic simulation. However, since there is no recycling due to the lack of periodicity, spinup time now equates distance from the inflow boundary. In our personal experience of getting turbulence started in neutral periodic cases, small random temperature fluctuations were more efficient. We will clarify that this is our personal experience.

RC2 Equations - general: punctuation is missing

AC We will address this.

4 Test case setup description

RC1 The reference test case is not really described. It is only said that it is a simulation of the development of a dry convective boundary layer, along with a three-line description of the vales of parameters.

RC1 line 271 with periodic boundary conditions: I suppose that periodicity is achieved in the x and y directions, but not in the z direction?

RC2 l265: Can the authors please be more specific? A w* = 1.5m/s can be achieved in different ways, e.g. by altering the surface flux or the boundary-layer depth. What was the prescribed heat flux in the simulations and how was the initial profile of potential temperature being defined?

RC2 l270 and following: If I understand right, you did perform a forcing where the open BC LES is driven by a period LES. In this regard, it is not clear to me how the coupling was realized. Did you take spatially resolved data, or did you only took horizontal mean profiles? Did you prescribed boundary values at all lateral boundary, i.e. the east, west, north, south and top boundary, or only that the west boundary? I might be wrong, but according to Fig. 3 it looks like you used periodic BC along y. So my question: Does the north/south boundary act as inflow/outflow boundary at the same time? Does the left inflow boundary could be also an outflow boundary (in a CBL with 3m/s mean wind this can happen)? Same with the right "outflow" boundary.

RC2 I strongly recommend the authors revise the setup description and add more details to allow for a better understanding what was done. Furthermore, I am interested how the authors realized the coupling technically (some note in the text might be nice). Was is realized by an offline approach where the data is stored in a separate file or via an MPI coupling strategy between the big-brother and the open-BC simulation?

AC We agree with the referees that information is missing in the description of the reference case. We will include the initial profiles, a table with all the forcings (including the surface heat flux) and height profiles of the potential temperature at different time intervals to show the development over time of the boundary layer. For the simulation with periodic boundary condition periodicity is applied at all lateral boundaries and a no stress boundary condition at the top. For the simulation with open boundary condition, open boundary conditions are used at all lateral boundaries and the top boundary. So there's no periodicity at the north and south boundaries. Instantaneous cross-section output at every time step from the periodic simulation at the boundaries is used as input for the open boundary conditions. For the current setup this means that the west boundary will be mainly inflow and the east boundary outflow. The north and south boundary will be both in-and outflow at different sections of the boundary with cells changing from in-to output with time. The coupling is done offline, with the periodic output being stored and then used for the simulation with open boundary conditions. This information will be added to the manuscript.

RC2 l263-264: For demonstrating the benefit of a newly developed method it is inappropriate to say that other test cases are not shown because they yield similar good results. Either you have conducted these tests and show some results of them, or you don't. In my opinion, purely neutral tests give different insights in the performance of a method as just a convective case. Same with cloudy boundary layers, where it is not straightforward how cloud prognostic quantities provided by mesoscale scales are treated in the LES at the boundaries.

AC We agree that every test case will show different features of the implementation. However, the goal of this paper is not to test the boundary conditions in every scenario, but to give a description of the implementation and a first necessary test case that we believe the implementation should pass. The implementation is currently being used in more advanced test cases (such as mesoscale-nested simulations), but we will leave those for future publications. We will adjust any statements or remarks that can not be backed up by the presented test case or state that further testing is required. We will also remove references to cases not presented in the current manuscript.

RC2 l267: Do the authors have arguments why they used such an anisotropic grid?

AC The anisotropic grid is chosen for computational reasons. More resolution is required in the vertical, since the vertical gradients of the mean temperature, moisture and wind as well as the corresponding turbulent fluxes are much stronger in the vertical than in the horizontal direction. Limiting the horizontal resolution to the same resolution as the vertical would significantly increase the computational costs.

RC2 l268: Was the dt really fixed to 5s? In a CBL the vertical component can become about 10 m/s. In conjunction with a dz = 20, time steps of 2s would be required to maintain numerical stability of the advection equation.

AC Yes, the time step was fixed at 5s. In these simulations the vertical velocity stays below 5 m/s. For the chosen time integration method (third order Runga Kutta) and the second order central discretisation scheme used, the critical Courant number for one-dimensional advection is $\sqrt{3}$ [Baldauf, 2008] (and not 1). This means that the upper limit for the time step is around $\frac{20}{5}\sqrt{(3)} \approx 7s$, which makes the chosen time step of 5s stable. We however agree that it is close to the critical value and have repeated the simulations for a 2s timestep. The results and figures have been changed with no influence on the conclusions.

RC1 lines 280 and 306: *boundary conditions* should be *boundary data*.

AC We will change this.

5 Discussion and presentation of results

RC1 A better overview of the solution should be given (e.g. some snapshots), and aspects which could have an impact on the performance of the OBCs should be emphasized (e.g. fluctuations in time of the direction - incoming or outgoing - of the flow near the open boundaries).

AC We will add profiles of the potential temperature field at different time intervals to show the evolution of the boundary layer. We will list the expected challenges for the open boundary conditions. These include reflections at outflow boundaries, changing from in to outflow conditions at the north and south boundaries and for the smoothed simulations the generation of turbulence downstream of the inflow boundary.

RC1 In my opinion, the critical presentation of the numerical results (Section 4) should be improved, and the conclusions should be strengthened.

RC1 All figures visually compare reference fields with other ones obtained in simulations with OBCs, but no difference is never quantified. For instance: *The TKE field near the outflow boundary is not affected by the smoothing* (line 387) , or *the wavelet cross-section remains close to the periodic cross-section* (line 390). Please quantify.

RC1 The objectives should be explained: what do the authors want from the OBCs ? What are the key properties and diagnostics that should not be impacted by open boundaries? In particular, do you expect to reproduce the behavior of the reference solution from a statistical point of view or from a deterministic point of view? What are then the quantitative criteria that will be used to assess the performance of the OBCs?

AC Ideally the boundary conditions have minimal influence on the solution from a statistical viewpoint. We would like the mean field and the turbulence properties such as the length scales and energy distribution to be unaffected by the numerics of the boundary condition implementation. We will highlight this in the description. To condense the information in the 2d panels into more directly quantifiable information, we will integrate the TKE cross-sections over the boundary layer and present them as well. For the panels we will only show the results for the corners and for $\sigma_t = 6\Delta t$ and $\sigma_x = 4\Delta x$. This would give a line for the simulation with open boundary conditions and for the simulation with periodic boundary conditions. Ideally we would like the mean of these lines to be comparable and the variation around the mean to be within the variance of the reference simulation.

RC2 Fig. 2: It would be easier to understand if you show absolute values rather than differences. Further, did you compute the profiles from the entire xy-domain or did you exclude some areas near the boundaries? In my opinion it does not make much sense to include areas where the flow is potentially affected by the boundaries because this can bias the result, even if the flow features in the interior of the model domain perfectly match.

AC Changing the panels to show absolute values will make it very difficult/impossible to see any differences as they are small compared to the absolute values.

Instead, we will include the absolute profiles separately when we show the development of the periodic simulation in time. The profiles are calculated from the entire xy-domain. We do agree that this can be very strict for the reason you mention. However, since we are looking for differences we wanted to include the boundaries as well.

RC1 Figures 3 to 6: Those figures could be complemented with the difference between the two panels. And the conclusions fully depend on the criteria: do you want a statistical matching or a deterministic matching between the two panels? How could you quantify it?

AC The solutions only need to agree in a statistical point of view. Due to the chaotic nature of the system they differ in the locations of their turbulent structures. We therefore think that showing differences does not show any relevant information. The fact that they are so similar in a deterministic point of view only goes to show how small the influence of the boundary conditions is, but it is not a requirement. We will clarify this in the manuscript.

RC2 l338-339: To thoroughly evaluate this, xz cross-sections are required. It could well be the case the authors just randomly picked a height which is only weakly affected, while other heights show significant up- or down-drafts near the boundaries.

AC We will include xz-cross sections to convince the reader we did not cherry pick a height level.

RC2 l339-340 and Fig. 4: Resolved or subgrid TKE? In the first case, how did you calculate the TKE (formula, time-averaging of the total fluxes, etc.)? In the next sentence you mention that the TKE is averaged over half an hour, which partly answers my question, but I have the impression that the calculation of TKE is not completely correct in this case. According to what you wrote, you computed instantaneous values of TKE from $\sum_i \left\langle (u_i'(t))^2 \right\rangle$ and average these over time. This only works when u' refers to a phase average where homogeneous conditions along y apply. However, if the north/south boundaries are also in/outflow boundaries, this is strictly speaking not the case. Alternatively, $u_i'^2$ can be computed via a time average.

AC That is indeed how we compute what we call the TKE. To be completely correct, we will include the formula how we compute it and not call it the TKE.

RC2 caption Fig. 4: How can a black line indicate a ”fixed” ratio? I guess you mean something like ratio between horizontal and vertical advection?

AC We agree that the description is not clear. We will change it to *The slope of the black line is given by the ratio between the horizontal velocity scale and the vertical velocity scale,* $\frac{U}{w^*}$.

RC2 l352-354: Which data was exactly used for the wavelet analysis? Did you use a spatial or a temporal data series for the wavelet analysis. In the latter case, at which distance from the inflow boundary? Did you use timeseries at at single point of time dependent yz cross section data. Which mother wavelet was employed? More specific information is required.

AC An instantaneous xy-slab has been used to calculate the wavelet analysis. For each x line a (spatial) wavelet analysis is performed. The average of these power spectra is shown. A morlet wavelet is used as the mother wavelet. We will add these specifications to the revised manuscript.

RC2 355: I do not understand why the analysis window is outside the domain. Actually the hatched area is defined by the cone-of-influence in the wavelet literature, describing the area in the scalogramm which is not affected by boundary effects. The sentence should be rephrased accordingly.

AC The reviewer is right that the hatched area is the cone-of-influence. The cone-of-influence describes the area that is potentially affected by boundary effects. These boundary effects result from the stretched wavelet extending beyond the edges of the domain. That's what we meant with ”the analysis window is outside the domain”. We will add the above information to the manuscript.

RC1 Lines 358-360, ... *shows similar results for both simulations... no clear differences visible...*: in my opinion, this is exaggerated. One should better explain why we can consider that the differences are not significant, which again depends on the criteria that have been chosen.

AC We tried to quantify this by using 2.5 upper and lower percentiles. We will use this information more in the text to support our claims. We will also state the criteria more clearly. Which is that they should match statistically. For any wavelength, the power present should be around the mean of the periodic simulation and with similar variation. They don't have to agree deterministically as turbulent structures can be located at different locations.

RC1 Section 4.1: boundary data are perfect in this experiment, with the same spatial and temporal resolution as the reference simulation. Dirichlet boundary conditions everywhere would therefore give a perfect result. So it is not surprising that the results are good in the vicinity of the inflow boundary. It is what happens near the output that is a priori the most interesting.

RC2 l363 and following: I agree, but this is not surprising as you simply forced an LES with output from another LES under idealized conditions (no changing wind direction, not much change in mass flux, etc.). The authors should put their statements into the context what their test case really shows.

AC It is true that perfect boundary information is given. Dirichlet conditions are however not employed everywhere so the solution is not predetermined and therefore not necessarily the same as the reference simulation. The inflow boundary in this case is indeed the least interesting and we would expect good results there. It is a sanity check that needs to be passed so that we have a good benchmark from which we can degrade by coarsening the temporal and spatial resolution of the input. Also, disturbances from the eastern, north and south boundaries could still propagate upstream and disturb the solution in the interior of the domain. We think this "best-case" scenario is a test that the implementations has to pass, even though it might not look too interesting. We will emphasise that this scenario is designed to test the implementation on the most basic level, as due to the ideal boundary information, any disturbances can only be blamed on the implementation.

RC1 Several statements are quite obvious: smoothing the input data results in a reduced TKE downwind of the inflow boundary, and deteriorates the solution; adding synthetic turbulence helps to generate developed turbulence faster... Again defining, from the beginning, clear desirable quantitative criteria would help.

AC We agree that a reduced TKE downwind of the inflow boundary is to be expected when smoothing the input fields. The goal of adding synthetic turbulence is to generate turbulence faster, however this does not mean that it would necessarily work. Since it is impossible to add "real" turbulence that the LES agrees with, it would be a realisitic possibility that the perturbations are dampened and wouldn't help. To make this clearer, we have added the following sentence to the text: *The better performance when using synthetic turbulence may appear trivial. However, as we cannot add turbulence that is directly compatible with the LES solution, the synthetic turbulence could be dampened or generate artefacts near the inflow boundary. The fact that it does not, shows the value of using it in our implementation.*

RC1 Lines 385 and 421: it is mentioned that a burst of TKE is observed, but is there an explanation for it?

RC2 l392-397: This is an interesting point because it systematically investigates the overshooting of turbulence also seen in previous studies (Munosz-Esparza and Kosovic, 2018 - https://doi.org/10.1175/MWR-D-18-0077.1 ; Kadasch et al., 2021). I would encourage the authors to also discuss their findings in the context of previous studies.

AC Will have a look at these studies and compare their results to ours. We notice that the TKE burst roughly happens on the line with a the gradient given by the ratio between the convective (vertical) and horizontal velocity scales. Our hypothesis is therefore that it is a clash between fields that are mainly governed by information supplied at the lateral inflow boundary, which lack developed turbulence and the fields originating from surface convection that do have developed turbulence. We believe that the sudden transition from non turbulent flow to turbulent flow causes an overshoot in TKE. This phenomena is common during the spinup time of (periodic) turbulent simulations. During the first hour the turbulence in the boundary layer needs to build up. Only after this is developed it is capable of transporting the accumulated surface moisture and heat flux through the boundary layer causing a peak in TKE but also in cloud fraction if clouds are formed on the top of the boundary layer [i.e. Siebesma and Cuijpers, 1995]. We will add this explanation to the manuscript.

RC1 Section 4.3: the goal of this section is not clear to me. Do you expect for the solution to reproduce the reference solution from a deterministic point of view, or to have a correct level of turbulence? The key question is perhaps the following: which scales are closer (in some sense to be defined) to the reference ones when this artificial turbulence is added?

AC The goal is not to reproduce the reference simulation, as it is not possible to recreate the full turbulence field from the few parameters that the synthetic turbulence routine uses. The goal is to speed up the turbulence generation and therefore shorten the turbulence build up length. Since it was found that the lack of developed turbulence resulted in the distortions found in the previous section we also wanted to see if adding synthetic turbulence is enough to mitigate these. We will describe these goals more clearly.

RC1 A suggestion: To the best of my knowledge, the introduction of a variable timescale τ for the inflow condition (Eq. (13)) is something new. In my opinion, this is a possible contribution, that is worth being discussed and emphasized. In other words, you could discuss more in depth this aspect, by comparing results with a Dirichlet inflow condition on u^B ($\tau_0 = 0$), a Dirichlet condition for the tendency $\frac{\partial \psi}{\partial t} = \frac{\partial \psi^B}{\partial t}$, and intermediate conditions with several values of τ_0 and p, including $p = 0$ (fixed timescale $\tau = 2\tau_0$). Relevant diagnostics should make it possible to decide if the time and space variability of the timescale has a significant effect.

AC We agree that these test would be interesting. However, we are afraid that extensive testing of all these different inflow conditions would distract from the main story. Furthermore, since the condition is developed with time-varying boundaries in mind, a different test case might be more suited for testing the different conditions. The Dirichlet limit is present in the sensitivity profiles.

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