

Interactive comment on “Adjoint-based Calibration of Inlet Boundary Condition for Atmospheric CFD Solvers” by Siamak Akbarzadeh et al.

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The authors would like to thank the referees for carefully reading our manuscript and for giving such detailed comments which substantially helped to improve the quality of the paper. In the revised version of the manuscript, we have tried to address all the points that were raised. The points that relate to the text's language and grammar are not discussed here. In the following, the comments will be discussed one by one.

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- **Anonymous Referee #1**

- a) Page 2 states "Mainly two different methods are used to set the inflow boundary conditions for ABL flow simulations". There are various other methods that are used within the community such as using white noise, Mann spectrum, (concurrent) precursor methods, etc. For a detailed discussion of turbulence inflow generation methods see Wu, Annu. Rev. Fluid Mech. 2017. 49:23–49 and Stevens and Meneveau, Annu. Rev. Fluid Mech. 2017. 49:311–39 for applications of such methods to wind farm applications.

It was not the intention of the authors to say that the mentioned methods are the only available solutions to generate an inflow boundary condition for CFD solvers. However, it was not probably clear in the text that we are discussing in the context of the RANS steady simulations. The inflow boundary generation, which is now in 3.1.1, refers to the suggested scientific works and does not include the explanation of the analytical function approaches.

- b) Figure 1: The description of figure 1, and in particular the description of the strangely oriented circle, took me quite some time to understand. The description of this figure should be improved.

Both the description in the text and the figure itself are improved.

- c) Can the method only be applied when the actual computational domain is cylindrical?

The method can be applied to other computational domain which does not have cylindrical shapes. It is now mentioned in the text. Moreover, the added Ishihara test case proves this too.

- d) Figure 3: It is unclear what the green grid cell is. Please clarify.

The figure is changed (see figure 2), and the forest part is clear now.

- e) Figure 5: The caption states the velocity field at 40 meters is given. What is meant? The velocity field at 40 meters from the ground level indicated in

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panel 5a?

It is now the figure 9. It shows the velocity field on a plane which has a 40 [m] perpendicular distance from the terrain's surface points (basically a slice of the domain that follows the terrain).

- f) Figure 6: Can it be indicated in the figure which calculations are performed simultaneously (primal and adjoint solver?) or are the different blocks in the figure performed sequentially? If so, in what order.

The flow chart is updated, and it is now mentioned that all steps are performed sequentially. The optimizer decides if the gradient or the cost function value is needed. Then the corresponding path and steps will be followed.

- g) 1. The section starting with "As it was explained in" on page 13 is rather vague. It is unclear to me what the smoothing function does exactly. I think the authors should explain this in more detail, so readers would be able to implement this part of the solution method by themselves.

2. The fitted profile in figure 3b is neither a logarithmic nor a power law. How exactly is the 1D inflow generating domain adjusted to achieve this? How strong can the deviation from the logarithmic/power law be before the code becomes unstable? How would one run the simulation in such a case (one may end up in an infinite loop in the diagram outlined in figure 6).

The profile in figure 3b is the profile in the middle of the forest and above it. The velocity for the heights above the forest is used for gradient validation, not the inflow calibration. The logarithmic or power-law function discussion is about the inflow boundary, not the profile inside of the domain.

The smoothing is now explained in Section 4.2. The output of the optimizer is first filtered to avoid sharp spikes. Then it is checked if it is close enough to a logarithmic or power-law function. If either of these functions is fitted and its coefficient of determination is above 0.96 the smoothed inflow from

C3

optimizer (not the fitted profile!), is accepted for the CFD solver. Otherwise, the optimization takes the last fitted profile and asks for a new gradient evaluation. In this way, the inflow boundary is not necessarily a logarithmic or power-law profile, and, moreover, it is not so unrealistic to be problematic for the solver. As mentioned in the reviewer's comments and in the new manuscript, alternatively, constraints or penalization term can be added to the objective function. This will be explored in future works when for instance the inflow turbulence properties are also considered as design parameters.

- h) Does the computational time required by the adjoint solved depend on the initial wind direction and speed that is selected?

Of course, the adjoint solver inherits some of the properties of the original solver. The inflow wind speed and direction affect the computational time of the primal solver. Subsequently, the run time of the adjoint would be some how dependent on these parameters. In other word, it is case dependent.

- i) 1. Figure 8: It is not entirely clear to me what exactly is meant by the reference profile in figure 8a.

It is the target inflow boundary. The legend of the plot is updated (see figure 11).

2. Page 14 just below figure 8 states: "Indeed, the output of the optimizer could be the exact reference profile if the convergence criterion was stricter." I am not sure what is meant here. When I look at figure 8b it seems that the calibration is performed on the velocity profile over the hill and this seems to match quite closely. When the velocity profile is calibrated at a specific location it could mean that any deviations with respect to measurements, caused by the used simulation method, would accumulate at another location in the domain (for example at the inflow). Is something like this happening? It would be good to discuss how the solution reacts to this.

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Although a tighter error criterion would improve the accuracy of the optimized profile, it also increases the calibration iterations and subsequently the number of CFD solver calls. The sensitivity of wind speed at a certain point in the domain to a very small change in the inflow boundary is dependent on many parameters such as terrain complexity, wind direction, CFD model, etc., and cannot be easily generalized.

- j) At the end of the manuscript the authors mention various extensions of the method. I am unsure whether various of these effects could be represented using this methods. Due to the use of the 1D domain to generate the vertical profile means that there is no information on the three-dimensional structure of the flow. It is known that for various properties of the atmospheric boundary layer capturing this three dimensional structure is crucial. I do not see how that can easily be incorporated in this method. Can the authors discuss in more detail what the effect of missing some of the three dimensional flow statistics, spatial flow correlations in the inflow are lost, is?

In general, adding the differentiation of the turbulence model with thermal stratification and Coriolis force to the current adjoint model would definitely improve the accuracy of the calibration. Moreover, the usage of the 1D inflow does not reflect the 3D structure of the flow. In order to overcome this limitation, this method could be extended to optimize the inlet BC as a spatially 2D field with three velocity components. However, a more sophisticated smoothing or penalization is needed to avoid having an unrealistic inlet field.

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• **Anonymous Referee #2**

1. In general, I found the notation confusing and difficult to understand. In some cases I was unable to follow the derivations because of the confusing notation. Below are a few specific suggestions to clarify or reword the notation:
 - a) It would be clearer if vectors and tensors were clearly identified in the text. Using Gibbs notation, either denote vectors as boldface italic and tensors in boldface or use vector symbols above. Alternatively, use index notation. For example, it's confusing to differentiate between the vector V and (scalar?) $V(z)$.
 - b) What is meant by the subscripts x, y, z in equation 6?
 - c) $V(z)$ is never defined. I assume it is the magnitude of the planar-averaged velocity vector.
 - d) Equation 12: I'm not sure what is meant by $(U, q)R$. I would guess that U and R are vectors and that term can be expanded as $U_x R_1 + U_y R_2 + U_z R_3 + q R_4$.
 - e) In equations (14)-(16) What do δV and δp mean? What are J_T and J_Ω ? Without knowing what this means, I was unable to follow the adjoint equation derivation.
 - f) Equation 8: Why not use an equality instead of the right arrow? (equality is now used in Eq. (1))

The suggestions are considered in the new manuscript:

- The italic bold letter is a vector (e.g. \mathbf{U} , $\overline{\mathbf{U}}$) and the normal bold letter stands for a tensor (\mathbf{D}).
- The terms with δ removed and all the equations are represented and explained by derivative symbol, ∂ .
- $V(z)$ is not anymore in the text.

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- Γ and Ω represent the boundary and the volume of the computational domain respectively. As a result, J_Γ and J_Ω are the part cost function which is dependent on flow state values on the boundary and the interior of the domain. This has been clarified in the manuscript.

2. I would significantly rework the structure of the paper to better integrate related ideas. As written, I'm not sure that someone could replicate this algorithm from the details of the paper.
 - a) I would combine Section 3-5. Section 3 and 4 are closely related since the adjoint equations are needed to calculate the gradient. Section 5 is part of the adjoint equation derivation and should be included in Section 4. As it stands, it's hard to follow which sections are part of the adjoint-based optimization method description.
 - b) Pg. 12 line 16 through pg. 13, Figure 6, and parts of pg. 9 lines 14-19 are related to the flow solver. I would put these details at the top of Section 2: "Flow Model" or with the details of the adjoint equations and gradient-based solver. It would be particularly helpful to have the $k-\epsilon$ turbulence model mentioned in Section 2.

The suggestion that the structure of the paper could be improved was common among the reviewers. The new manuscript is restructured as follows: The gradient-based optimization and the theory of adjoint method are briefly presented in Section 2. The derivation of the adjoint equations and its BCs from the primal flow model is explained in Section 3. Finally, the numerical results and the conclusions are presented in Sections 4 and 5.

3. This method appears to be related to existing methods in meteorological applications (3DVar) or in existing wind energy papers (see the 4DVar implementation in Bauweraerts and Meyers, BLM, 2019). This is touched on in the introduction, but a more explicit discussion of how your method is related to existing approaches would be helpful.

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The existing 4DVar implementation by ? is one of the recent studies related to this subject. Instead of calibration of the inflow boundary, they optimize the whole initial field of the domain. They have developed an adjoint solver for a LES-based primal flow model and calibrate the initial flow field with the LIDAR measurements data from the whole of the domain. This is now mentioned in the introduction.

4. Is Section 2.1 used directly in the paper? My understanding is that these inflow conditions are calculated from your algorithm. This section may not really be necessary if that is the case. Also, how are equations (3) and (4) used simultaneously? What is z_{ref} ? How do you get n ?

This has been clarified in Section 4.2.

5. pg. 4, line 27: What do you mean by "error-prone"? Finite difference is simply too expensive to really be used in a gradient-based algorithm. I think that is sufficient justification for using an adjoint-based derivation.

To avoid confusion, and based on some other comments, this has been deleted. The intention was to mention some of the disadvantages of the FD method. As said, the FD is too expensive for CFD gradient-based optimization. However, its usage should not completely be ruled out. For instance, there have been some studies on the application of FD to some selective terms in the discrete adjoint differentiation of CFD solvers (see for example *An aerodynamic design optimization framework using a discrete adjoint approach with OpenFOAM* by He et al., 2018).

6. Top of p. 5: It's not really multiplication, but the inner product of the state equations and the adjoint variables.

Corrected.

7. p. 5, line 22: What is the effect of neglecting changes in eddy viscosity? Shouldn't changing the inflow conditions change the eddy viscosity of

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the simulation. How is assuming "frozen-turbulence" relevant to the RANS model?

There is no doubt that the turbulence contribution to the adjoint equations cannot simply be ignored. In some applications, frozen-turbulence can produce the wrong sign for the local sensitivity (Zymaris et al., 2009; Papoutsis-Kiachagias et al., 2015)). In the context of inflow calibration, the authors believe that the differentiation of the turbulence model is better to be included when the inflow turbulence properties are also design parameters, which can be explored in future works.

8. Beginning of Section 4: Adjoint methods are generic and applicable to many problems. I don't think it's necessary to point out the specific differences between your application and the Othmer's application.

This paragraph is removed.

9. I'm not sure that Section 6 is really necessary. Showing that the gradient-based solver can find a solution is sufficient to demonstrate that the method works.

As one of the reviewers has pointed out, the accuracy of the gradient computation is an important element of any gradient-based optimization. As a common practice in scientific studies, the validation of a newly implemented adjoint solver is presented.

10. It would be nice to show the application of the optimized inflow boundary condition for evaluating a specific site's wind resources or designing a wind farm. This is the real application and importance of this work, so I would make this a bigger point with an example.

This point has been raised by other reviewers. Due to time limits and available sites in the project, this was not considered for this study. For sure this will be tried in the future.

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• **Anonymous Referee #3**

1. I believe the paper would benefit from the addition of some more references in selected places, i.e.:

- a) Section 1 - lines 20-25, where the authors mention that their adjoint approach has not been applied before in the framework of wind resource assessment. It would be nice to add some references to recent works where adjoint optimization is used in the context of wind energy. e.g. blade shape optimization: Dhert, Ashuri, Martins, Wind Energy 2017
wind-farm control: Goit & Meyers, J Fluid Mech 2016; Munters & Meyers, Phil Trans Roy Soc A, 2017; Vali et al., Control Engineering Practice 2019
wind-farm layout optimization: King et al., Wind Energy Science 2017

- b) Section 3 - 3.1.1, where the adjoint method is introduced through the formal Lagrange method. A reference to e.g. Hinze, Michael, et al. Optimization with PDE constraints. Vol. 23. Springer Science & Business Media, 2008 seems appropriate. Also, the explanation of the necessity and philosophy of the adjoint method is quite poor. The authors could improve this by explicitly mentioning that eq. 11 is expensive since the term $d\psi/d\alpha$ requires a PDE simulation for every dimension in alpha, and showing explicitly that this term drops out in the adjoint method. I advise the authors to either expand on their explanation of the adjoint methodology, or to refer in to references where it is explained in detail.

The recommended references are added to the corresponding sections. The adjoint method explanation is improved.

2. page 2, lines 3 - 4: The authors first mention the disadvantage of the FD method as being error-prone. In context of the current manuscript, this is misleading in my opinion. The loss of accuracy due to finite-precision arithmetic can be circumvented by using a complex-step finite differentiation.

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Also, since the authors use the continuous adjoint method without a grid convergence study, the computed adjoint gradients could certainly be less accurate than a finite-difference approximation. I feel the authors should remove this claim, or at least put more emphasis on the fact that FD computational cost scales with the input dimensionality, whereas this is not the case for the adjoint method.

It has been mentioned in the manuscript that the complex-step method would circumvent the difficulties of FD. However, it should also be noted that the implementation of a complex-step method on a large code which is not written with complex variables (e.g. OpenFOAM) is not straight forward too.

In the manuscript, the emphasis is put now on the advantages of the adjoint method in terms of the computational cost for a large number of design parameters.

3. page 3, line 10: ABL flow simulations → ABL RANS simulations. Please add the term RANS here, to avoid confusion with the generation of inflow conditions for turbulence-resolving simulations (DNS/LES), which is a whole research field on its own.

Corrected. It is now in Section 3.1.1.

4. page 11, line 1: "For gradient evaluation, the 1D velocity profile inflow is rotated by 30". This seems like a very large step for a finite-difference gradient approximation. Why did the authors not take a much smaller rotation, e.g. of 1? Intuitively, 1 still seems large enough to avoid influence of round-off errors.

Please be aware that, the 30 is not the step-size. First, a simulation is carried out with $WD=270$. The velocities, above the forest, are taken as pseudo measurements. Then, using these measurements, the adjoint gradient is

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computed for the simulation with $WD=240$. The finite difference gradient is also carried out for $WD=240$ in which the step-size is 0.2.

5. page 11, around line 10: The statement: "most importantly, their signs show that they can be used for the purpose of gradient-based calibration" is misleading. The authors seem to state that, in laymans terms, having a gradient that point approximately in the right direction is sufficient for optimization. However, this claim should be nuanced. Gradient inaccuracies can severely impact the performance, stability and convergence of a given optimization algorithm. For instance, in quasi-Newton methods this could lead to instabilities because of poor Hessian approximations, and in CG methods this could lead to non-conjugate search directions in successive iterations. Furthermore, related to comment nr. 2 and comment nr. 4, I feel the authors should be careful in attributing discrepancies between adjoint and FD gradients to inaccuracies of the FD gradient. Intuitively, I would expect the frozen turbulence assumption and the grid resolution (combined with continuous adjoint approach) to be the main reasons for discrepancies.

No doubt the accuracy of the gradient is as important as its sign due to the reasons which are mentioned above. Otherwise, we would not put such a section in the manuscript. However, the words should have been chosen more carefully.

The point regarding the FD error is considered in the manuscript.

6. page 12, line 18: The authors mention some facts about computational cost of their simulations. These facts can be made more illustrative by also explicitly mentioning the wall-time of a primal flow run, and explaining why the run-time of the adjoint solver is 60% of the primal (e.g. because the adjoint equations are linear)?

The wall-time of the primal run is given in the new manuscript. Please also refer to the following response:

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- Anonymous Referee #4, question: 10

7. (suggestion) page 13, line 5: "The optimizer may ask for a cost function evaluation with a new inflow boundary which is highly unrealistic for an ABL domain. ... the curve fit capability is used to smooth and fit the new inflow to a boundary which has a log/power law characteristic." The authors manually post-process the new iterate of inflow conditions during the optimization process. Although I agree that it is undesirable to run RANS with unrealistic inflows during optimization, this manual post-processing will can have a significant detrimental impact on the convergence of the optimization. Since this post-processing imposes a log/power law profile, it seems more natural to directly use the parameters for such log/power profiles as decision variables, in contrast to optimizing the individual inflow velocities at every height. This would directly inform the optimizer of the desired log/power law profile, and could improve convergence a lot.

As it is explained in the manuscript and before in this document, the point of smoothing is to avoid enforcing the boundary to have either a logarithmic or power-law function shape. Otherwise, optimizing the function parameters would be straightforward. As in the Ishihara case, the inflow boundary can be neither a logarithmic nor a power-law, but still being able to reproduce the measurements with acceptable tolerance. Of course, the approach can be improved by for example adding corresponding constraints to the objective function.

8. (suggestion) page 13, line 18: "This can be explained by the fact that in early iterations the derivative of cost function wrt WD is much bigger than wrt inflow". This spike might be avoided and convergence could possibly be improved by using quasi-Newton optimization methods (e.g. BFGS), this is a suggestion for future applications of the methodology.

Thank you for the helpful suggestion. We think also this will help.

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• **Anonymous Referee #4**

Specific comments:

1. The purpose of section 2 is not clear. Do you want to give general description of inflow boundary condition and forest effect, or are these the techniques you will use in your study? If it is the former then they should go to Introduction, if it is the later, then you should explain them together with the discussions in Section 3 and Section 4.

This part is now moved to Section 4.2 where the optimization steps are discussed.

2. You have Section 3, subsection 3.1 and sub subsection 3.1.1, but no following subsection (e.g. 3.2 etc) or following sub subsection (e.g. 3.1.2 etc). So, I suggest that you put all the contents in this section under a single section heading without any subsection. But my main concern for this section is once again, it is not clear whether you are trying to explain a general method for gradient evaluation in optimization or is it for your specific problem? The section lacks explanation that may be necessary for some one not familiar with Gradient-based optimization. Therefore, some more discussion will be required. For example, what is the role of design variable α , what will your algorithm do to optimize it and why can you write Eq. (11). Furthermore, last sentence in section 3.1 (line 28 and 29) will not come as obvious to many readers.

The new restructured manuscript should not have this problem. Moreover, both the gradient-based (Section 2) and the CG optimizer (Section 4.2) are explained in the paper.

3. Section 4, 1st Paragraph: The purpose of this paragraph is not clear. Summarizing the differences between your work and that of earlier work is not

C14

really necessary. Because the two works deal with different optimization problem, all three differences stated in the manuscript are obvious.

The paragraph is removed.

4. The forest model, Eq. (18) should be a part of original Lagrangian and should also appear in Eq. (15) and (16).

Corrected.

5. Why do you not have convective (and cross-convective) terms in Eq. (19)? I still see them in Eq. (16). If it is an error, then please correct it. If you have a proper reason why they can be neglected, you must explain that.

It is not used anymore in the new manuscript (see Eq. (21)) but $-2\mathbf{D}(\overline{\mathbf{U}})\mathbf{U} = -\nabla\overline{\mathbf{U}}\cdot\mathbf{U} - (\mathbf{U}\cdot\nabla)\overline{\mathbf{U}}$

6. It is not clear what ω_j is.

It is the volume of the cell in which the measurement is located.

7. It has become more common (at least in academic researches) to use large-eddy simulations (LES) for ABL and wind farm simulations. But authors preferred to use RANS in their work. Can you please discuss why you chose RANS? Was it because RANS is cheaper or was it because it is easy to implement adjoint equations for RANS problem? In reality both inflow profiles and measured velocity at the measurement points VM will vary with time. Furthermore, dynamic behavior of flow field as well and wind farm are receiving more interest in wind energy community (e.g. farm level controller). So, it seems LES would have been preferred simulation method.

As it is mentioned in the new manuscript, there are some studies that use measurements to calibrate the LES-based models (Bauweraerts and Meyers, 2018). However, due to the computational cost, the most common CFD solvers in the wind energy industry is still steady-state RANS-based models. Also, RANS is the model of choice here because of the scope of the

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current project. We completely agree the LES is gaining momentum due to its superior predictions in many cases compared to RANS.

8. Pg. 12, Line 14–15: It is not clear why you used velocity profile from a reference simulation instead of the velocity measured by the met-mast. Also, if your reference simulation and actual simulation were performed in the similar condition, then you will obviously get good optimization result. Please provide further information regarding this issue.

Indeed, the main idea of this work is using measurements to calibrate the inflow boundary of the solver. For the Ishihara case, the measured wind speed U_x was used for the optimization process. Since it is a wind tunnel experiment, it is fair to assume the wind direction to be the x axis. Although the wind speed at six different heights was available for the Kassel case, the wind direction data was present at only two heights. Therefore, we used the pseudo measurement to prove the validity of the methodology. However, the profile from which the pseudo measurements are selected essentially follows the trend of the real measurements of the domain. Please see the comparison in the attached figure, which has not been included in the paper because it may confuse the reader.

Fig. 1. Comparison of the velocity profile over the hill from which the pseudo measurements are chosen and the velocity speeds measured by the met-mast.

9. Pg. 12, Line 16–18: You need to provide more information about conjugate-gradient algorithm.

An elaborate explanation has been added to Section 4.2.

10. Pg. 12, Line 19: Are you sure that the run-time of adjoint equations is 60% of the primal equations? For most work that I am aware of and from my personal experience, adjoint equations always took longer time to simulate.

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Yes, in most of the adjoint simulations that we have carried out with this adjoint solver the run-time is 60-75% of the original flow run-time. A couple of points should be considered: a) The main driver of this adjoint solver is the source term which is the difference between the measurement and simulated results. This source term appears only for a few cells in which the measurements are located. Though, comparing to other adjoint solvers for shape and topology optimization this can be seen as a simpler solver. b) The turbulence is not differentiated; meaning there are no adjoint turbulence equations to be solved.

In the new manuscript, instead of a certain percentage, a range is given.

11. Pg. 13, Line 4–10: You are fitting the inlet boundary condition from the optimization to a logarithmic or a power law. This may not be a good idea, if you want to exploit the full potential of your optimization scheme. Therefore, instead why do not you add some sort of constrain to your system or add appropriate penalty term to the cost functional?

This point is discussed before in this document. Please refer to the following responses:

- Anonymous Referee #1, question: g
- Anonymous Referee #3, question: 7

12. I do not think you have presented sufficient result to consider this manuscript as a technical paper. You only have figure 8 as the results for one simulation case. Please define and perform optimization for more simulation cases. Also, you need to provide further discussion of your result.

The results for the Ishihara et al. test case is also added in the new manuscript. We hope this is sufficient for the scope of the paper. In future work, we will investigate more cases with different complexity. Our main aim here is to provide the general framework and initial case studies.