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

Anonymous Referee #3

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The authors present their research on calibration of inlet boundary conditions for atmospheric CFD using adjoint gradient-based optimization techniques. The methodology is certainly useful and of interest to the general community. However, I believe the quality of the paper can be increased significantly if the authors address the comments below:

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 necesseity and philosphy 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.

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. 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.

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.

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.

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.

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 walltime 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)?

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 postprocessing 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.

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.

9. Figure 2 - avoid rainbow colormaps, which can be misleading and are unintelligible in black & white. Use a standard perceptually uniform colormap such as parula (Matlab) or viridis (matplotlib). Same for Figure 5

10. Typographically & gramatically the paper needs to be proofread in detail. For instance,

- eq. 7: is missing a parenthesis (before V_M_i

- eq. 15: is missing a parenthesis (before \delta V

- page 5, line 15: as followings -> as following

- page 11, line 9: higher that -> higher than

- page 11, line 11: because at it was shown in -> because it was shown in

... and quite some more.

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