Adjoint-based Calibration of Inlet Boundary Condition for Atmospheric CFD Solvers

S. Akbarzadeh[1], **H. Kassem**[2], **R. Buhr**[3], and **G. Steinfeld**[4]

[1,3,4]ForWind, Center for Wind Energy Research, Carl von Ossietzky University Oldenburg
[2]Fraunhofer Institute for Wind Energy Systems - Fraunhofer IWES
[1]*contact: siamak.akbarzadeh@forwind.de*

Abstract. An adjoint solver is developed for optimization of inlet velocity boundary condition for incompressible atmospheric boundary layer (ABL) CFD simulations. Using the wind speed observations in the interior domain, the solver computes the gradient of the calibration objective function with respect to inlet velocity components as design variables. The algorithm is implemented in the open source CFD package OpenFOAM. Further, the DAKOTA optimization package is coupled with OpenFOAM and numerical studies are carried out to determine the inlet velocity profile of a 3D domain with a cosine shaped hill. The CFD simulation with optimized inlet velocty profile shows good agreement with experimental study.

1. Introduction

CFD solvers are being extensively used for site assessment in the wind energy industry. However, developing algorithms that capture all the physics of such complex flow regimes is an ongoing research. Often measurement data (e.g wind speed, wind direction and roughness) within the area of interest are used to calibrate the available atmospheric boundary layer (ABL) CFD solvers. In CFD applications, due to computational cost, gradient-based optimizers are more favourable than others such as genetic algorithm and evolutionary strategies. To compute the gradients, the finite-difference method is relatively simple but prone to error due to step-size and round-off error. Moreover, for a high number of design parameters the method becomes prohibitively expensive. In the adjoint method [5] the sensitivity of the objective function can be calculated independently from the number of parameters and this considerably reduces the cost of computation. The inlet velocity is one of the most important boundary conditions and its effect on the simulated flow field is crucial. The available continuous adjoint solver of OpenFOAM is based on the topology optimization of duct flows. In this study the available adjoint solver is further developed for ABL CFD solver calibration via inlet velocity profile optimization.

The structure of the paper is as follows. In Section 2 first the theory of adjoint method is briefly explained then the adjoint equations and its boundary conditions (BCs) are derived for computing the gradient of a calibration cost function with respect to (w.r.t.) inlet velocity. Numerical results for optimization of the inlet velocity for a neutral ABL over a 3D hill are discussed in Section 3. Finally, the conclusions are presented in Section 4.

2. Adjoint Model

2.1. Background

The ABL flow model in the neutral condition consists of steady-state Reynolds Averaged Navier-Stokes (RANS) equations for incompressible fluid flows:

$$(R_1, R_2, R_3)^T = (\mathbf{v}\cdot\nabla)\cdot\mathbf{v} + \nabla p - \nabla\cdot(2\nu_{eff} D(\mathbf{v})) \tag{1}$$

$$R_4 = -\nabla\cdot\mathbf{v} \tag{2}$$

where R is the spatial residual of the equations that is driven to zero. The variables $\mathbf{v}$ and p are the state variables velocity and pressure, ν_{eff} stands for the sum of kinematic and turbulent viscosity and D is the rate of strain tensor, $D = \frac{1}{2}(\nabla\mathbf{v} + (\nabla\mathbf{v})^T)$. A modified $k-\varepsilon$ model [1] is used for turbulence modelling, which is consistent with Monin-Obukhov similarity theory.

Calibration algorithms seek to maximize agreement between simulation outputs and measurements. In the context of ABL based model calibration the data are often wind speed and direction at one or more locations of a potential wind farm site. The calibration can be formulated as a constrained optimization problem with a scalar objective function as follows:

$$\text{minimize}\;\; J(\mathbf{v}_M, \mathbf{v}_S, \alpha) = \sum[\mathbf{v}_{M_i} - \mathbf{v}_{S_i})]^2 \quad i = 1,\ldots,n \quad ; \quad \text{subject to}\;\; R_{1,2,3,4}(\mathbf{v}, p, \alpha) = 0 \tag{3}$$

where $\mathbf{v}_{M_i}$ and $\mathbf{v}_{S_i}$ are the measured and simulated wind velocities at the same location. The α represents the design variables which are considered to be the velocity at inlet faces of the CFD mesh through this work. By introducing the adjoint variables $\mathbf{u}$ and q, the cost function can be reformulated to a Lagrange function as

$$L := J + \int_\Omega (\mathbf{u}, q) R \, d\Omega \tag{4}$$

where Ω is the flow domain. Every change in the design variables, α, influences the flow fields $\mathbf{v}$ and p. However, the adjoint variables can be chosen such that the variations of state variables vanish. Then the sensitivity of the cost function can be given by

$$\frac{\partial L}{\partial\alpha} = \frac{\partial J}{\partial\alpha} + \int_\Omega (\mathbf{u}, q)\frac{\partial R}{\partial\alpha}\, d\Omega \tag{5}$$

which excludes the state variables sensitivities and its computation is relatively cheap.

Although the theory presented here is mostly based on the work of C. Othmer [4], there are some differences that can be summarized as following: a) in the duct flow optimization, which cost function is pressure loss, the term $\frac{\partial R}{\partial\alpha_i}$ is equal to the velocity at each volume cell; here the design variables are inflow boundary velocities instead of the volume porosity distribution and the term $\frac{\partial R}{\partial\alpha} = \frac{\partial R}{\partial\mathbf{v}_{inlet}}$ is computed with reverse hand differentiation of the solver implementation; b) the cost function is defined for calibration and uses the interior velocity observations; c) the new adjoint equations and boundary conditions are derived based on the definition of the cost function and the characteristics of the ABL domain.

2.2. Adjoint Equations

To zero out the variation of state variables w.r.t. design parameters and by neglecting the turbulent viscosity variation, assuming the "frozen-turbulent" hypothesis, the following expression should hold:

$$\delta_{\mathbf{v}}J + \delta_p J + \int_\Omega \mathbf{u}\cdot\left[\delta\mathbf{v}\cdot\nabla)\mathbf{v} + (\mathbf{v}\cdot\nabla)\delta\mathbf{v} - \nabla\cdot(2\nu_{eff}D(\delta\mathbf{v}))\right] d\Omega - \int_\Omega q\nabla\cdot\delta\mathbf{v}\, d\Omega + \int_\Omega \mathbf{u}\cdot\nabla\delta p\, d\Omega = 0 \tag{6}$$

Decomposition of parts into interior domain, Ω, and its boundaries, Γ, leads to reformulation of Eqn. (6) as follows

$$\int_\Gamma \big[\mathbf{u}\cdot\mathbf{n} + \cancelto{0}{\frac{\partial J_\Gamma}{\partial p}}\big]\delta p\, d\Gamma + \int_\Gamma \big[\mathbf{n}(\mathbf{u}\cdot\mathbf{v}) + \mathbf{u}(\mathbf{v}\cdot\mathbf{n}) + 2\nu_{eff}\mathbf{n}\cdot D(\mathbf{u}) - q\mathbf{n} + \cancelto{0}{\frac{\partial J_\Gamma}{\partial \mathbf{v}}}\big]\delta\mathbf{v}\, d\Gamma$$
$$+ \int_\Gamma \big[-2\nu_{eff}\mathbf{n}\cdot D(\delta\mathbf{v})\cdot\mathbf{u}\big]\, d\Gamma + \int_\Omega \big[-\nabla\cdot\mathbf{u} + \cancelto{0}{\frac{\partial J_\Omega}{\partial p}}\big]\delta p\, d\Omega$$
$$+ \int_\Omega \big[-\nabla\mathbf{u}\cdot\mathbf{v} - (\mathbf{v}\cdot\nabla)\mathbf{u} - \nabla\cdot(2\nu_{eff}D(\mathbf{u})) + \nabla q + \frac{\partial J_\Omega}{\partial \mathbf{v}}\big]\,\delta\mathbf{v} d\Omega = 0 \tag{7}$$

Due to the definition of the cost function Eqn. (3), its direct variation comes only from the interior domain. Moreover, it does not have any derivative w.r.t. pressure field. The corresponding terms are zeroed out in Eqn. (7). The only cost function derivative that remains is w.r.t. velocity in the interior domain and at the locations where the measurements are available:

$$\frac{\partial J_\Omega}{\partial \mathbf{v}} = -2(\mathbf{v}_{M_i} - \mathbf{v}_{S_i}) \quad i = 1,\ldots,n \tag{8}$$

and the adjoint equations can be derived as

$$-2D(\mathbf{u})\mathbf{v} = -\nabla q + \nabla\cdot(2\nu_{eff}D(\mathbf{u})) + \big(\frac{2}{V_i}\big)(\mathbf{v}_{M_i} - \mathbf{v}_{S_i}) \tag{9}$$
$$\nabla\cdot\mathbf{u} = 0 \tag{10}$$

where V_i is the cell volume. In comparison to derived equations in [4], the design variables, α, are not anymore in the adjoint momentum equation. Instead, the difference between measurement and simulation at observation locations is present as a source term.

2.2.1. Boundary Conditions

The boundary integrals of Eqn. (7) can be mathematically re-formulated [4] and reduced to

$$\int_\Gamma \big[\mathbf{u}\cdot\mathbf{n}\big]\delta p\, d\Gamma = 0 \tag{11}$$
$$\int_\Gamma \big[\mathbf{n}(\mathbf{u}\cdot\mathbf{v}) + \nu_{eff}(\mathbf{n}\cdot\nabla)\mathbf{u} - q\mathbf{n}\big]\cdot\delta\mathbf{v}\, d\Gamma - \int_\Gamma \big[\nu_{eff}(\mathbf{n}\cdot\nabla)\delta\mathbf{v}\cdot\mathbf{u}\big]\, d\Gamma = 0 \tag{12}$$

where $\mathbf{n}$ is the unit normal vector from the boundary faces. The adjoint BCs should be chosen such that the above equations are held meaning that after any small perturbations of flow fields, $\mathbf{v}+\delta\mathbf{v}$ and $p+\delta p$, the primal equations are still satisfied. Except for the inlet, which is part of $\frac{\partial R}{\partial \alpha}$ in Eqn. (5).

Generally, for an ABL CFD domain no-slip wall and zero pressure gradient conditions are imposed on the ground. Moreover, zero gradient velocity and fixed zero pressure are applied at the outlet and top of the domain. Based on the derivations shown in [4] and after some modifications due to the calibration objective function the adjoint BCs can be given by

$$\text{ground (wall):} \qquad \mathbf{u} = 0 \qquad \mathbf{n}\cdot\nabla q = 0 \tag{13}$$
$$\text{top/outlet:} \qquad q = \mathbf{u}\cdot\mathbf{v} + |\mathbf{u}|_n|\mathbf{v}|_n \qquad |\mathbf{u}|_t = 0 \tag{14}$$

where underscripts n and t represent the normal and in-plane components respectively. The design variables are the inlet velocities, $\delta\mathbf{v}_{inlet} = \delta\alpha$. Though, the adjoint variables at inlet should not be chosen to zero out the inlet velocity perturbations. As a result, the zero gradient condition is imposed on the inlet for both adjoint velocity and adjoint pressure to have a well-posed system. Then to compute the sensitivity, based on the implementation of the solver in OpenFOAM, the term $\frac{\partial R}{\partial \alpha}$ in Eqn. (5) is hand reverse-differentiated.

3. Numerical Results

As a case study, an ABL domain with a 3D hill at the center is considered (see figure 1). The hill has the shape $z = h\cos^2(\sqrt{x^2+y^2}/2L)$ with $h = 40$ m and $L = 100$ m. The scaled wind tunnel study of the case has been presented by Ishihara et al. [2] and several authors have published the CFD simulation results of similar cases [3]. The domain is meshed with the in-house *terrainMesher* of the Fraunhofer IWES. A mesh independence study is conducted to verify the suitability of a mesh of two millions hexahedral elements. The primal flow field of the test case is simulated with the in-house CFD solver [1] which is a customized ABL-based version of the *simpleFoam* solver in the OpenFOAM package with a modified $k-\varepsilon$ turbulence model which behaves like standard model for the neutral condition. The roughness value of the domain is set to be $z_0 = 0.04$ m. The operational Reynolds number based on the free-stream velocity, hill height and air kinematic viscosity is $Re_h = 1.5\times10^4$.

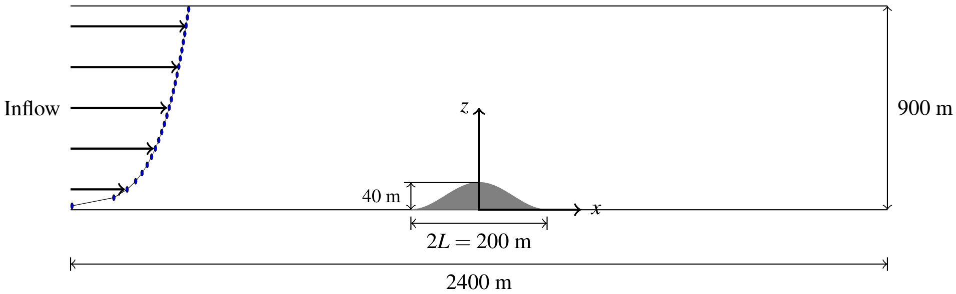
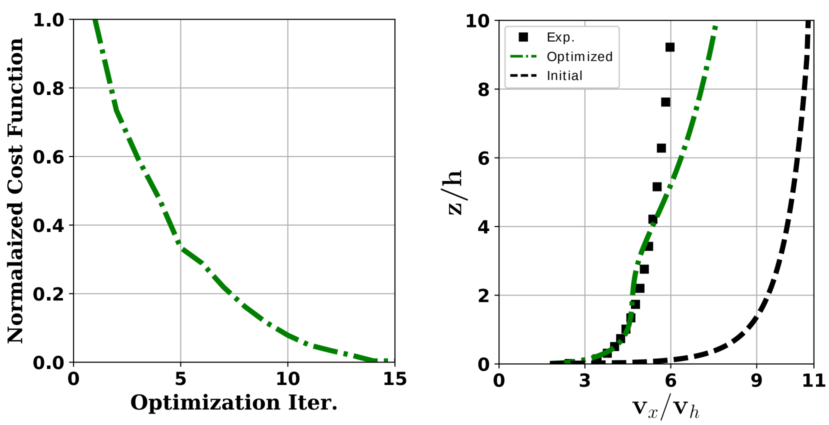


Figure 1: Main dimensions of the test case with 1000 m length in y direction.

To optimize the inlet velocity profile, the primal and adjoint solvers are coupled with the DAKOTA optimization package . The local gradient-based “CONMIN-frcg” solver of DAKOTA is used which is based on the conjugate-gradient algorithm of Fletcher-Reeves. Using Ishihara et. al wind tunnel measurements, the normalized x component of velocity over the hill ($\mathbf{v}_x/\mathbf{v}_h$) is used to define the solver calibration objective function Eqn. (3). To avoid having unrealistic inlet profiles during optimization, the curve_fit capability from the Scipy library of python is used as a simple parametrization. The average run-time of the adjoint solver is 60% of the primal flow run. Figure 2 shows the history of optimization

Figure 2: Optimzation history (left) and inlet velocity profiles comparison (right).



and the comparison of inlet velocity profiles. The optimization has converged after 15 iterations with total number of 42 solver calls including 25 primal (cost function evaluation) and 17 adjoint (gradient evaluation). The optimal velocity profile is in good agreement with the experiment for heights $\frac{z}{h} < 4$. The explanation can be that the hill does not affect the wind flow at higher heights. Consequently, the sensitivity of objective function at those heights of the inflow is not considerable. The comparison of velocity profiles over the hill, shown in figure 3, confirms that the optimized inlet boundary is able to re-produce the experiment velocity profiles.

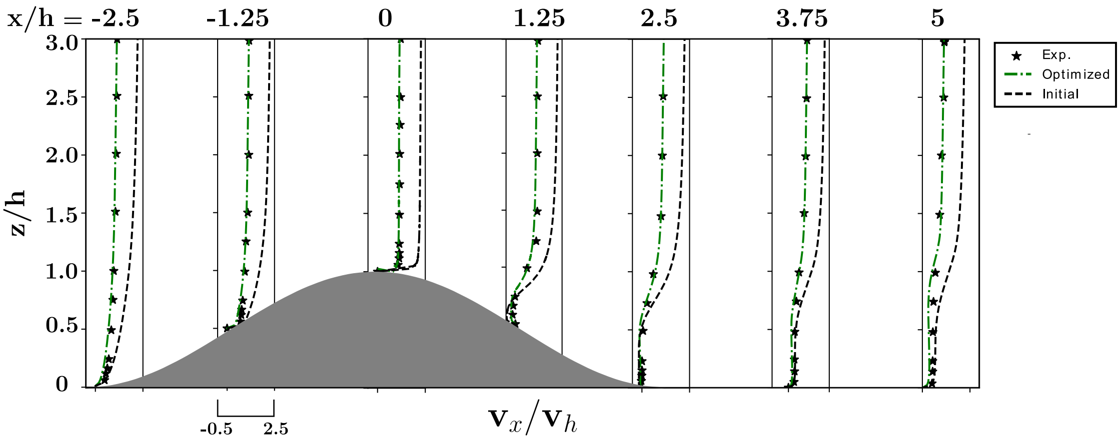


Figure 3: Normalized vertical profiles of longitudinal velocity component on the central plane of the hill. $\mathbf{v}_h$ is the velocity at the hill height in undisturbed region of the domain between inlet and hill.

4. Summary

In this paper, it has been shown that the ABL CFD solvers can be calibrated via adjoint-based inlet boundary optimization. Based on the frozen-turbulence hypothesis, the adjoint equations and its boundary conditions for such problem are derived. The developed solver has been coupled with the DAKOTA optimization package and applied to a 3D ABL domain with a cosine shaped hill. Using the wind tunnel observations over the hill, the optimal inlet velocities have been found which is in good agreement with the experimental study. The presented adjoint solver has the potential to be further developed by including forest and turbulence model. The thermal stratification can also be considered by differentiation of the temperature equation. A more sophisticated parameterization scheme may improve the run-time of the optimisation by reducing the number of solver calls.

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