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Multiple shooting for turbulent flow reconstruction in the atmospheric boundary layer using large-eddy simulation

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Turbulent flow reconstruction in the atmospheric boundary layer (ABL) is important as a data assimilation technique in the context of weather forecasting, or as a form of state estimation to close the feedback loop in practical model-predictive control (MPC). Following Alreweny et al. (2024) [1], in this work, flow reconstruction is approached as a four-dimensional variational data assimilation (4D-VAR) problem in the strong formulation, subject to a state model based on large-eddy simulations (LES), based on LiDAR measurements of the neutral ABL. In particular, building further on Janssens and Meyers (2024)[2], this study proposes a parallel-in-time multiple shooting algorithm to accelerate the PDE-constrained optimization.

Following a Bayesian maximum a posteriori approach, the assimilation problem balances a likelihood term (the reconstruction error compared to measurements) against a regularizing background distribution (the prior information on the spatiotemporal correlations in the flow). In the strong formulation, the initial state is optimized with the state equations – here LES of the turbulent ABL in neutral conditions – arising as a strong constraint, i.e. a deterministic model, resulting in a large-scale PDE-constrained optimization problem. As a background model, the initial state is regularized (in space) using the HGW model[3].
As opposed to previous single shooting approaches, this study leverages the multiple shooting paradigm to accelerate the computations. The augmented Lagrangian method is used to solve the equality constrained optimization problem originating from the multiple shooting approach, in combination with a classical limited-memory BFGS method for the unconstrained inner problems. To impose divergence-free initial conditions for the shooting windows, the optimization is performed in a three-dimensional solenoidal basis. Finally, aiming towards real-time applicability, the multiple shooting paradigm is exploited in full by processing the windows parallel-in-time, which allows for significant parallel speed-ups compared to state-of-the-art single shooting formulations. This is the first time multiple shooting is applied in the context of the three-dimensional Navier–Stokes equations in the turbulent regime.

As a test case, we consider a series of virtual LiDAR measurements from a fine-grid reference LES, whereas the turbulent flow field is reconstructed on a coarser resolution. Figure 1 shows a snapshot of the reference field and the coarse reconstruction over the LiDAR scanning range. The results demonstrate that multiple shooting is able to achieve the same level of accuracy as single shooting in terms of the reconstruction error. However, the parallel-in-time implementation enabled by the multiple shooting paradigm allows for significant parallel speed-ups, thereby accelerating the optimization up to 50% (depending on the number of shooting windows and HPC infrastructure). This demonstrates the potential of multiple shooting for large-scale PDE-constrained optimization problems and its applicability for turbulent flow reconstruction.

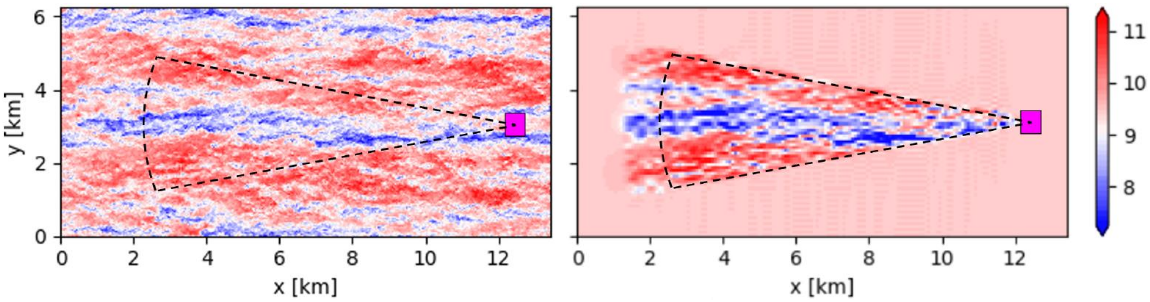

Figure 1: *Snapshot of the fine-grid reference flow field and coarse-grid reconstruction based on LiDAR measurements. Colours represent the instantaneous streamwise velocity [ms^{-1}].*

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[1] Alreweny et al., *Journal of Fluid Mechanics* **981**, A28 (2024)

[2] Janssens et al., *Computer Physics Communications* **296**, 109019 (2024)

[3] Wilson, *Boundary-Layer Meteorology* **85**, 35-52 (1997)