

Parallel-in-time multiple shooting using large-eddy simulation for flow reconstruction in the atmospheric boundary layer

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PDE-constrained optimization has become common in many engineering fields, yet the associated computational costs often remain a bottleneck. Very recently, Janssens and Meyers (2024) [1], following up on earlier work from Fang et al. (2022) [2], have proposed a multiple shooting algorithm suitable for large-scale PDE-constrained problems, with the objective of accelerating the computations by exploiting the time-parallelism enabled by the shooting decomposition. In this study, we further progress the multiple shooting paradigm towards problems governed by the three-dimensional Navier-Stokes equations in the fully turbulent regime, with applications in turbulence reconstruction in the atmospheric boundary layer (essential for numerical weather prediction).

For the flow reconstruction in the atmospheric boundary layer (ABL), we aim to reconstruct the initial flow field that minimizes the reconstruction error against the available flow measurements, where the ABL is modelled using large-eddy simulations (LES). The problem is first casted into a velocity tracking formulation, similar to Janssens and Meyers (2024), and solved using the time-parallel multiple shooting algorithm. Here, the time interval is subdivided into several windows that are processed parallel-in-time, with additional matching conditions at the interfaces to enforce continuity. The resulting equality constrained optimization problem is addressed using an augmented Lagrangian method, with limited-memory BFGS for the unconstrained inner problems.

The algorithm is tested for flow reconstruction on a coarse LES grid based on full field or LiDAR measurements collected from a fine-grid emulator. In either case, multiple shooting converges up to reasonable accuracy. For the full field cases, the measurements are used to initialize the shooting windows, resulting in satisfactory algorithmic speed-ups (~ 1). In the more realistic case of partial observations (such as LiDAR), algorithmic speed-ups are generally lower. However, the main advantage of the multiple shooting paradigm resides in the parallel-in-time execution of the forward and adjoint LES, offering strong potential for acceleration on modern HPC platforms and significantly accelerating the optimization. This approach demonstrates the viability of time-parallel optimization for large-scale turbulent flows and is, to our knowledge, the first application of multiple shooting in the context of LES of the turbulent ABL.

[1] Janssens and Meyers, Computer Physics Communications 296, 109019 (2024)

[2] Fang et al., Journal of Computational Physics 452, 110926 (2022)