Towards efficient scale resolving simulation for the prediction of industrial pollutant dispersion applications

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1 INTRODUCTION

Urban areas face significant challenges in managing gaseous pollutant emissions, which have direct implications for public health and urban planning. Predicting and managing the dispersion of pollutants is crucial for designing sustainable cities. In this context, Computational Fluid Dynamics (CFD) constitutes a powerful tool that can offer accurate predictions and provide insights on the mechanisms that drive dispersion.

The suitability of different computational methodologies for urban physics modelling applications has been a topic of extensive research and discussion over the last decades [1], [2]. In this context, our recent study [3] assesses how a Large Eddy Simulation (LES) model compares to the industry workhorse Reynolds Averaged Navier Stokes (RANS) turbulence modelling approach in predicting contaminants' dispersion over the Tokyo's Polytechnic University Atsugi campus. The numerical data were compared to wind tunnel experimental measurements available in literature [4]. The results of the study outlined the predominance of high-fidelity LES modelling in accurately reproducing complex flow patterns and predicting concentration distributions. However, one of the main outcomes was that the computational cost entailed in conducting LES simulations might be excessive in an industrial context where fast turnaround times are key, thus making RANS a more viable solution. The question that naturally arises from these observations is how can scale resolving simulations become more cost-effective.

Focused on addressing this point, the scope of the current study is to explore how the use of an implicit low dissipative pressure-velocity block-coupled solver, optimized to run at increased time-step size can impact the turnaround times and accuracy of scale resolving simulations.

2 METHODOLOGY

2.1 Numerical setup & data organizing

The study was aimed at replicating the wind tunnel experiment [4]. A 14 million cells hex-dominant mesh was created using HELYX®, an open-source CFD simulation software, and the Finite Volume Method (FVM) was used for solving the governing equations. A time-dependent inflow velocity profile, obtained by performing a LES precursor simulation of the actual wind tunnel geometry was used as inlet boundary condition. More details concerning spatial discretization, numerical setup and data organizing methodology can be found in [3].

2.2 CFD experiment outline

To sufficiently assess and quantify the potential benefits of the block-coupled solver, the performance of two segregated algorithms, namely PISO (Pressure-Implicit with Splitting of Operators) and transient SIMPLE (Semi-Implicit Method for Pressure Linked Equations), are also evaluated. The standard PISO algorithm operates by performing a predictor step to estimate the velocity field and then applying multiple corrector steps to adjust the pressure field and correct the velocity to ensure mass conservation. PISO is known to be particularly effective for transient simulations, as it provides better convergence and accuracy by repeatedly refining the solution within each time-step. The transient SIMPLE algorithm incorporates the iterative pressure correction of PISO with the robust handling of non-linearities typical of SIMPLE. For each time-step SIMPLE allows for multiple outer corrector steps similarly to PISO but can also performs additional inner iterations to stabilize the solution, making it suitable for transient scale resolving simulations with complex flows at larger time-steps. This hybrid approach of SIMPLE generally offers a balance between accuracy and computational efficiency, especially for cases where

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the flow exhibits significant transient behaviour or requires higher stability in the numerical solution. A known limitation for both these standard segregated pressure-velocity approaches, is the tendency to introduce relatively high numerical dissipation in the solution, as a result of discretization schemes, matrix preconditioning and the form of the momentum interpolation algorithm.

Contrary to the segregated algorithms, the block-coupled solver, as the name implies, solves the pressure and velocity fields simultaneously through coupling the momentum and continuity equations into a single block-matrix. This matrix is solved implicitly, meaning that the solution depends on both the current and the previous time-step. Through inherently enforcing mass conservation, this coupling offers enhanced stability thus allowing for larger time-steps and reduced corrector steps compared to the explicit methods.

At the outset of this study, an iterative process of fine-tuning and optimization of the convergence parameters of all three solvers was conducted. This process indicated that the PISO and transient SIMPLE algorithm reached optimal performance when operating under 3 pressure correction steps, whereas the block-coupled solver could perform well on just a single outer corrector step. Four time-steps were considered, namely 0.0005s, 0.001s, 0.002s and 0.003s, to evaluate the dependence of the results, leading to a total of 12 runs. All simulations were performed at ENGYS using 256 cores on an in-house high-performance computing cluster equipped with EPYC 9354 (Genoa) processors.

2.3 Measured quantities

The main quantity of interest, as defined in the original experiment [4], was the dimensionless concentration C/C_0, with C denoting the local concentration, and C_0 the reference concentration defined according to Eq. (1):

$$C_0 = \frac{q}{U_H H^2} \tag{1}$$

where q denotes the gas emission rate and U_H and H denote the reference velocity and reference height respectively. This quantity was measured at 15 probe locations. The predictions of these values were monitored at the corresponding locations inside the computational domain and were used for evaluating the accuracy of the simulations.

3 RESULTS

The results of the study can be summarized in Figure 1, Figure 2 and Figure 3. Figure 1 shows the Normalized Mean Square Error (NMSE) for the various algorithms at different time-steps. NMSE is defined based on the Eq. (2) below:

$$\mathrm{NMSE} = \frac{\overline{(C_o - C_p)^2}}{\overline{C_o C_p}} \tag{2}$$

where C_o denotes the observed value, C_p the numerically predicted value, n the number of predictions and the overbar symbol '-' denotes the average over the entire dataset. The plot highlights that SIMPLE and Coupled compare well with experiments in terms of mean concentration even at larger time-steps, whereas the accuracy of PISO tends to deteriorate.

Figure 2 shows the normalised mean concentration and its standard deviation obtained by different algorithms at all 15 measurement locations and at different time-steps. These graphs offer a more detailed comparison of the mean concentration predictions obtained by each algorithm. At the same time, they provide insights regarding the standard deviation of the predicted values. Finally, Figure 3 shows the runtimes times for each algorithm for all time-steps. This comparative graph underlines how PISO algorithm and the block-coupled solver are consistently faster than SIMPLE.

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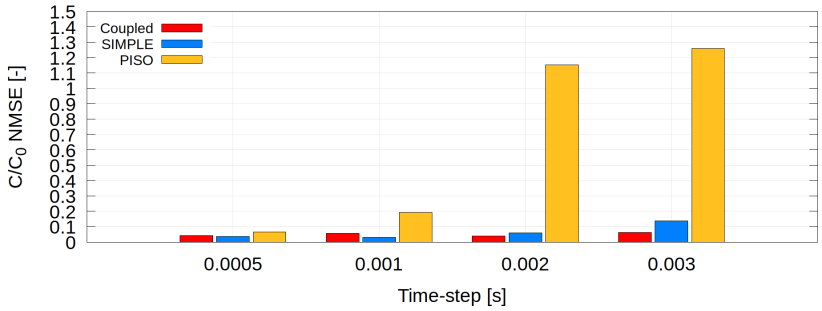

Figure 1. Comparison of the dimensionless concentration predictions' NMSE, for PISO, SIMPLE and Coupled solver for each time-step size.

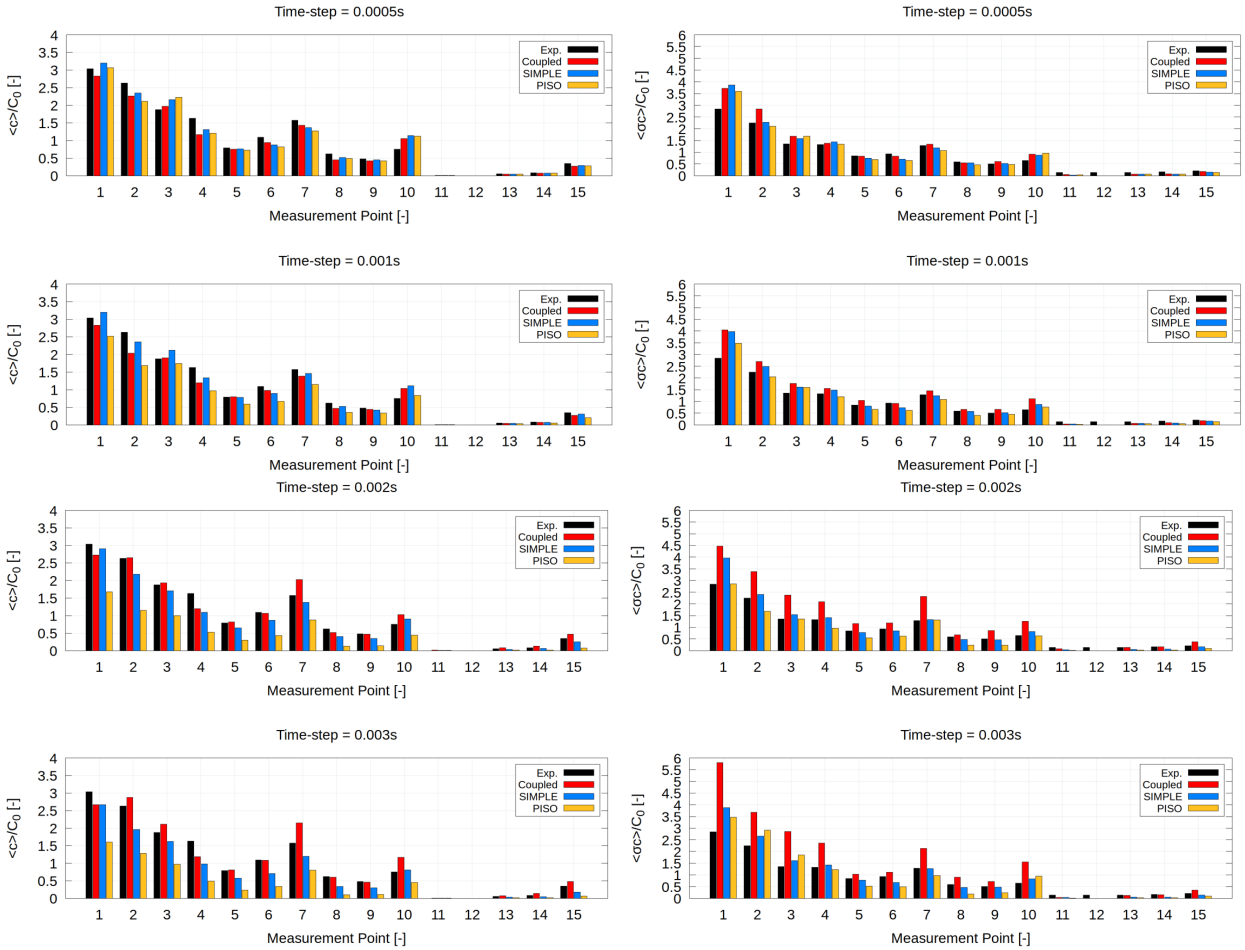

Figure 2. Mean normalized concentration (left column) and standard deviation (right column) at each measurement point for Coupled, SIMPLE and PISO at each time-step size.

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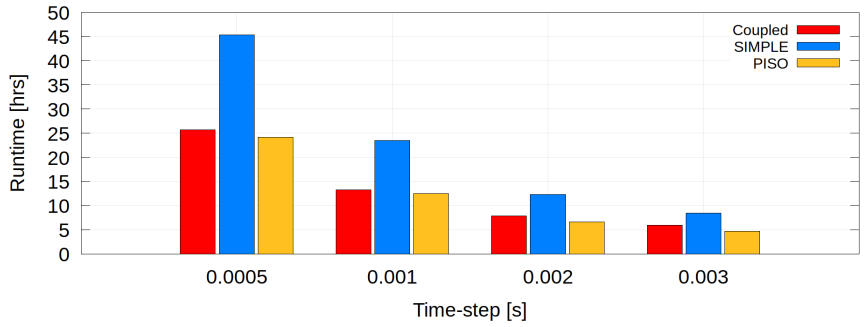

Figure 3. Comparison of the runtimes for Coupled, SIMPLE and PISO solver at different time-step sizes.

4 CONCLUSIONS & DISCUSSION

Results obtained so far indicate that although PISO yields the fastest turnaround times, the compromise in accuracy becomes significant as the time-step size increases. At the same time, SIMPLE yields consistently accurate results but at the cost of consistently being slower than PISO and coupled. The block-coupled solver, on the other hand, provides reasonably accurate predictions, comparable to those obtained by SIMPLE, but at a cost similar to PISO. The speed-up achieved through running coupled over segregated SIMPLE ranges from 43% to 30%. These observations underline how the block-coupled solver offers a good balance between accuracy and computational cost, which renders it as the most efficient approach and the overall best choice in the context of accurately predicting mean concentrations. However, it should be noted that, although the block-coupled solver offers good predictions of the mean concentration, the standard deviation of its predictions is consistently higher when compared to the segregated SIMPLE and PISO algorithms, especially for higher time-steps (i.e. 0.002s and 0.003s). Further investigations are required in this regard.

The conclusion that emerges from this study is that through significantly reducing the computational cost while simultaneously maintaining prediction accuracy in terms of mean quantities as compared to segregated algorithms, the implicit block-coupled solver can turn the scale resolving LES simulation from an impracticable to a more viable approach when running at larger time-steps. However, through coarsening the time-step size, resolution is sacrificed when looking at standard deviations. As such, a compromise in accuracy must be expected as a trade-off when trying to shorten the runtimes. The suitability of the block-coupled solver as an approach for obtaining high levels of accuracy at reduced computational cost depends on the nature of a particular study. If the objective is to predict mean concentration values, then the proposed solver constitutes a more efficient alternative to the standard segregated algorithms. However, if there is interest in accurately reproducing the whole transient nature of the flow, then sufficiently fine time-steps are a requirement, in which case there is less benefit to be gained from the block-coupled solver.

5 REFERENCES

[1] B. Blocken, "LES over RANS in building simulation for outdoor and indoor applications: A foregone conclusion?" *Building Simulation,* vol. 11, pp. 821-870, 2018.

[2] P. Gousseau, B. Blocken, T. Stathopoulos and G. van Heijst, "CFD simulation of near field pollutant dispersion on a higher-resolution grid: a case study by LES and RANS for a building group in downtown Montreail," *Atmospheric Environment,* vol. 45, pp. 428-438, 2011.

[3] A. Krassas, S. Renda, S. Mijorski, E. de Villiers and S. Capra, "Evaluating numerical models for the prediction of pollutant dispersion over Tokyo s' Polytechnic University campus," *Wind Engineering and Industrial Aerodynamics,* vol. 251, 2024.

[4] T. Tachibana, R. Yoshie, S. Nakayama, T. Kishida, K. Miyashita and R. Sasaki, "Comparison between field measurement and wind tunnel experiments of gas dispersion in an urban area and verification of similarity law.," *Wind Engineering and Industrial Aerodynamics,* vol. 47, pp. 39-52, 2022.

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