

ASSESSMENT OF LARGE EDDY SIMULATION FOR FLOW DYNAMICS IN URBAN-LIKE ENVIRONMENTS

D. FOLCH*, À. ALSALTI-BALDELLOU[†], G. COLOMER*, F. X. TRIAS* AND A. OLIVA*

* Heat and Mass Transfer Technological Center (CTTC)
Universitat Politècnica de Catalunya (UPC)
08222 Terrassa (Barcelona)
e-mail: david.folch@upc.edu, www.cttc.upc.edu

[†] Department of Civil, Environmental and Architectural Engineering
University of Padova
35131, Padova, PD, Italy
email: adel.alsaltibaldellou@unipd.it

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Summary. *We assess several LES models for turbulent flow simulations in urban environments, aiming ultimately at particulate pollutant dispersion. The methodology is progressively validated from canonical wall-mounted cube configurations to urban-like geometries and the CEDVAL benchmark. The TFA code and S3PQR models show reliable performance for the benchmark cases and promising results for more complex urban flows, even on coarse meshes. These results provide a basis for extending the methodology to realistic urban configurations and passive scalar transport.*

1 INTRODUCTION

Particle pollution is a major concern in urban environments. Effective urban design and evacuation planning require a thorough understanding of fluid dynamics around buildings. This study evaluates the performance of several Large Eddy Simulation (LES) models in order to apply them to urban configurations.

To validate the overall approach, we proceed step by step. First, we simulate the flow around a wall-mounted cube (WMC) in two distinct configurations — a channel flow and a boundary layer — to assess the reliability of the approach and perform a detailed comparison of the resulting flow fields and turbulence statistics. Then, as a proof of concept, we replace the obstacle with a different shape inspired by the urban landscape of Barcelona. Finally, we extend the simulations to a regular array of blocks (“buildings”) to investigate urban-canopy effects and compare the results with the CEDVAL wind-tunnel dataset [1].

The ultimate goal is to perform high-fidelity simulations of a realistic urban environment, incorporating passive scalar transport to model the dispersion of particulate pollutants.

2 LES MODELS

We are mainly interested in evaluating the S3PQR (namely, PQ, PR, QR) LES models [2]. We recall some of their main properties (ν_e denotes the eddy viscosity):

- 0) $\nu_e \geq 0$, locality and frame invariance;
- 1) $\mathcal{O}(y^3)$ near-wall behaviour;
- 2) $\nu_e = 0$ for two-dimensional flows in PR and QR;
- 3) $\nu_e \approx 0$ for the canonical axisymmetric flow (< 0.076)
- 4) good conditioning and low computational cost.

To date, these models have shown good overall performance for channel flow [3], homogeneous isotropic turbulence [2] (both forced and decaying), boundary layer [4], and wind farm [4] (with actuator-disk forces [5]). We have also tested several other well-known LES models: Smagorinsky [6], Verstappen’s [7], WALE [8], and Vreman’s [9].

3 NUMERICAL METHODOLOGY

In the previous computations, we used an in-house pseudospectral code [10]. Specifically for the periodic boundary layer, Spalart’s additional terms [11] [12] were employed to balance the energy.

In the present work, however, we adopt a different approach based on the finite-volume method implemented in Termofluids Algebraic (TFA).

TFA is a multi-physics CFD code designed for high-performance parallel computing [13]. It employs a finite-volume discretisation on unstructured (and structured) meshes with a collocated arrangement. The spatial discretisation is based on symmetry-preserving, kinetic-energy-conserving schemes. Pressure–velocity coupling is handled by a classical fractional-step (projection) method.

Time integration typically uses second-order explicit schemes, with the pressure gradient treated implicitly. Throughout this work, we have used an Adams-Bashforth time integration scheme and a CFL condition to determine the time step.

The following sections present the different configurations that are tested and validated one by one before proceeding to the urban simulations. As a general feature, a no-slip condition has been imposed at the walls. For the channel flow, a log-law streamwise velocity profile is prescribed at the inlet, whereas a free outflow condition is applied at the outlet. For the periodic boundary layer, energy is introduced through a body force [14].

4 VALIDATIONS

4.1 Wall-mounted cube in a channel flow

We first consider a wall-mounted cube in a channel flow. Our reference is [15]. The basic specifications are a $400 \times 200 \times 196$ mesh, domain dimensions of $6 \times 3 \times 17$ in the spanwise, wall-normal, and streamwise directions, respectively, and a friction Reynolds number $Re_\tau = 590$. The height of the cube is $h = 1.0$. Figure 1 shows the usual configuration of a wall-mounted cube.

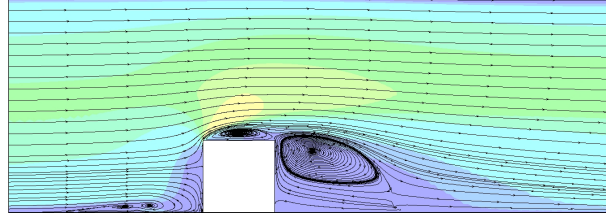


Figure 1: Reference [15] (with permission). Domain dimensions: $6 \times 3 \times 17$. WMC height $h = 1.0$

Using the same specifications, we focus on mesh dependence and LES model performance. In Figure 2 we show the results for two probe locations behind the cube, as in the reference [15]. For simplicity, only the PR model and the no-model case are displayed; the remaining S3PQR models yield similar results.

Regarding mesh dependence, the expected behaviour of the mean streamwise velocity profile is observed. The results improve when refining the mesh from $50 \times 50 \times 100$ to $200 \times 200 \times 400$ for the no-model case, and to $100 \times 100 \times 200$ for the LES model. Note that the LES model already matches the reference profile at lower resolution.

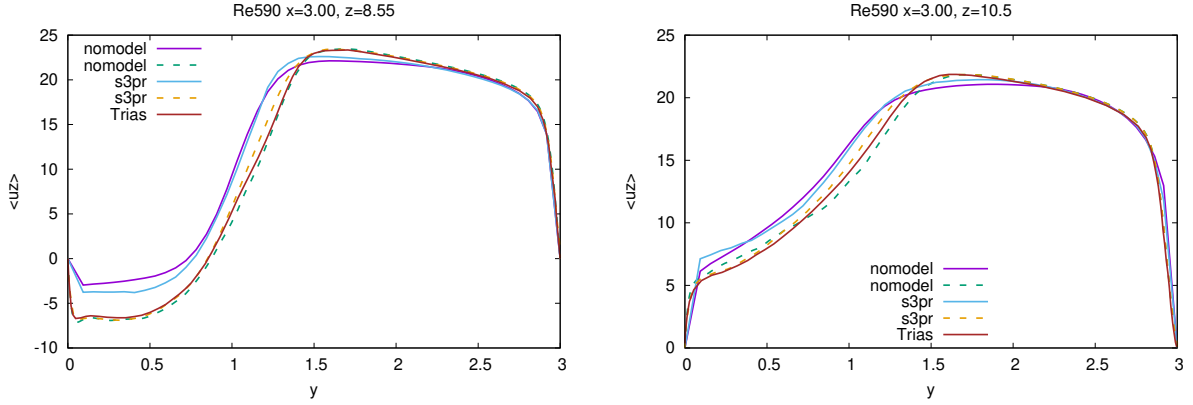


Figure 2: $Re_\tau = 590$; solid line: $50 \times 50 \times 100$; dashed line: $200 \times 200 \times 400$ no model, $100 \times 100 \times 200$ S3PR; brown line: Trias, reference [15]. **Left:** probe at $(3.0, y, 8.55)$. **Right:** probe at $(3.0, y, 10.5)$

For the mean Reynolds stress component $\langle ww \rangle$, Figure 3 again shows only the PR model and the no-model setup at the same two locations. The effect of increasing mesh resolution is visible; however, since these are second-order quantities, a longer integration time appears to be necessary. The overall behaviour agrees with that of the reference.

Figure 4 presents the global results for all S3PQR models, regarding the mean velocity and Reynolds stress. The performance is similar, as previously stated.

For a no-model simulation to be considered a Direct Numerical Simulation (DNS), the grid must adequately resolve the smallest relevant flow scales throughout the domain. As a first

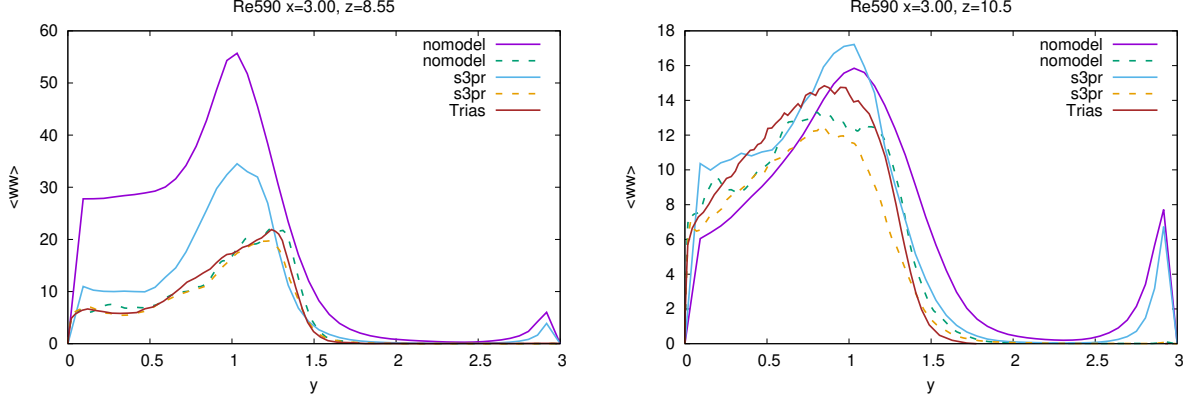


Figure 3: $Re_\tau = 590$; solid line: $50 \times 50 \times 100$; dashed line: $200 \times 200 \times 400$ no model, $100 \times 100 \times 200$ S3PR; brown line: Trias [15]. **Left:** $(3.0, y, 8.55)$. **Right:** $(3.0, y, 10.5)$

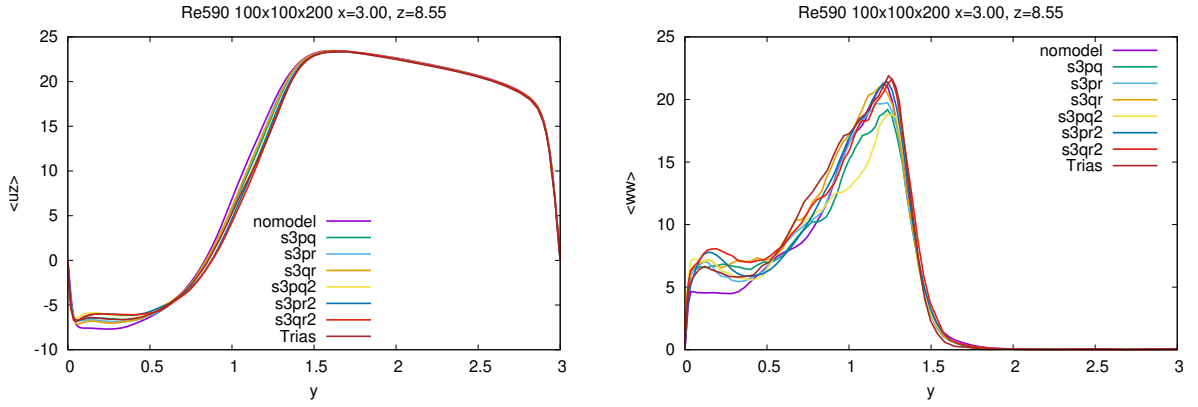


Figure 4: $Re_\tau = 590$, $100 \times 100 \times 200$ mesh; brown line: Trias [15]. There are two versions of the S3PQR models, see reference [2]. **Left:** normalized average streamwise velocity profile. **Right:** $\langle ww \rangle$

assessment, we have estimated the wall-unit spacing on three planes normal to the wall-normal direction at different positions around the wall-mounted cube. Although the estimated values suggest a sufficiently fine resolution over most of the analysed planes, a complete three-dimensional assessment is still required before the simulation can be classified as a DNS.

Figure 5 shows two of these planes, located at the bottom and the roof of the cube. The configuration corresponds to $Re_\tau = 590$, no model, $200 \times 200 \times 400$ mesh with geometric stretching near the cube and the walls.

The grid spacing in the wall-normal direction is less than $\Delta y^+ < 1.0$ over the whole plane, except in a few small regions near the edges, where the maximum value reaches $\Delta y^+ < 1.7$.

Figure 6 shows the third plane at half the cube height ($y = 0.5$). In this case, we examine the spanwise and streamwise directions. Away from the cube, the grid spacing is expected to remain

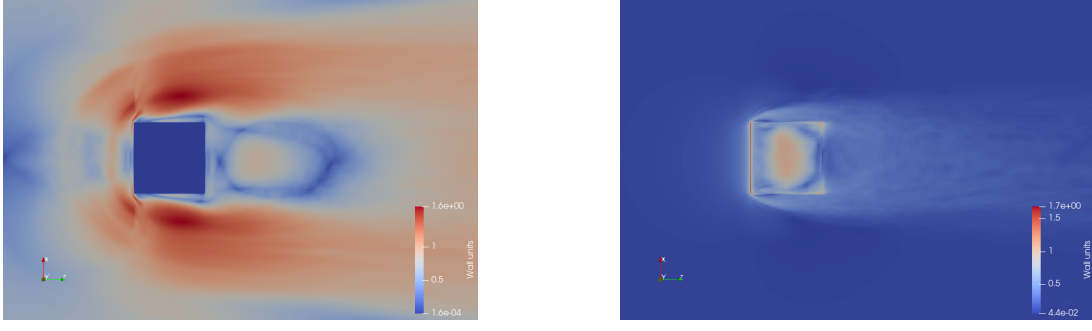


Figure 5: Left: bottom plane $\Delta y^+ < 1.6$. Right: WMC roof $\Delta y^+ < 1.7$

below one, with estimated maximum values near the edges of $\Delta x^+ < 1.7$ and $\Delta z^+ < 2.4$, respectively.

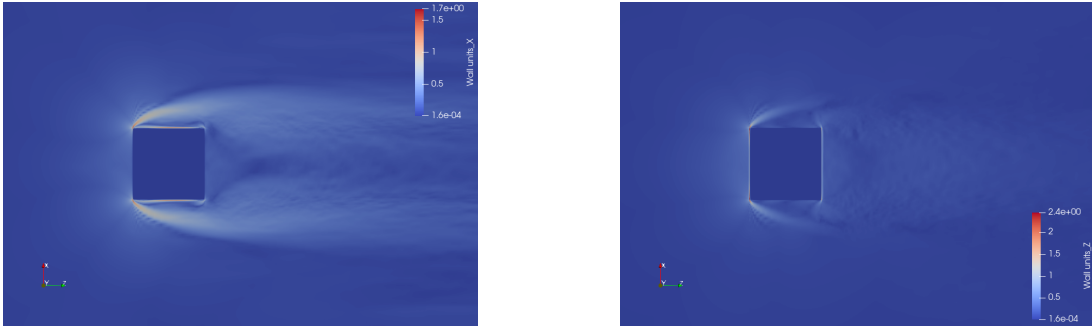


Figure 6: Left: spanwise direction $\Delta x^+ < 1.7$. Right: streamwise direction $\Delta z^+ < 2.4$

Further examination will be carried out to confirm whether the simulation can be considered a DNS.

4.2 Boundary Layer: periodic boundary conditions

If the ultimate goal is to simulate a real city, the natural choice is a boundary-layer configuration. In our previous studies [4] [10], we demonstrated the validity of the S3PQR models for a periodic boundary layer. Those simulations were performed with a pseudospectral code, and Spalart's extra terms [12] [11] were added to the Navier-Stokes equations to account for the periodicity of the domain. Two main changes in the present work require a new validation: the use of a finite-volume method and a different term to balance the momentum equations, as developed in [14].

We first recall some useful concepts for periodic boundary layers. Directly imposing periodic boundary conditions in the streamwise direction causes the boundary layer to decay. Energy must therefore be introduced into the system [14] (as is done, for example, in forced homogeneous isotropic turbulence) by means of an additional term(s) in the equations. It is

also necessary to define a Reynolds number that can be kept fixed. Two common choices are based on the displacement thickness or on the momentum thickness. Here we adopt the former.

The displacement thickness (δ^*) is defined as:

$$\delta^* = \int_0^\infty (1 - u/u_\infty) dy \quad (1)$$

where u_∞ is the free-stream velocity. Energy is introduced via a body force [14]:

$$f(t)y \frac{\partial \mathbf{u}}{\partial t} \quad (2)$$

where $f(t)$ depends on the desired δ^* , the instantaneous $\delta^*(t)$, a constant k , and the skin friction C_f :

$$f(t) := \frac{-k(\delta^* - \delta^*(t)) + \frac{1}{2}C_f(t)}{\delta^*(t)} \quad (3)$$

For reference, a "real" atmospheric boundary layer has a displacement thickness of the order of $\delta^* \sim 150m$. Consequently, the Reynolds number is of the order of $Re_{\delta^*} \sim 6 \cdot 10^7$.

To validate our finite-volume method (TFA), the energy-injection procedure and the LES models, we compare directly with one of the cases analyzed in [14], namely a periodic boundary layer at $Re_{\delta^*} = 2806$. We examine the streamwise average velocity and the root-mean-square (rms) quantities. For clarity, Figure 7 shows only the PR model together with the reference and the no-model results. All S3PQR models give similar results.

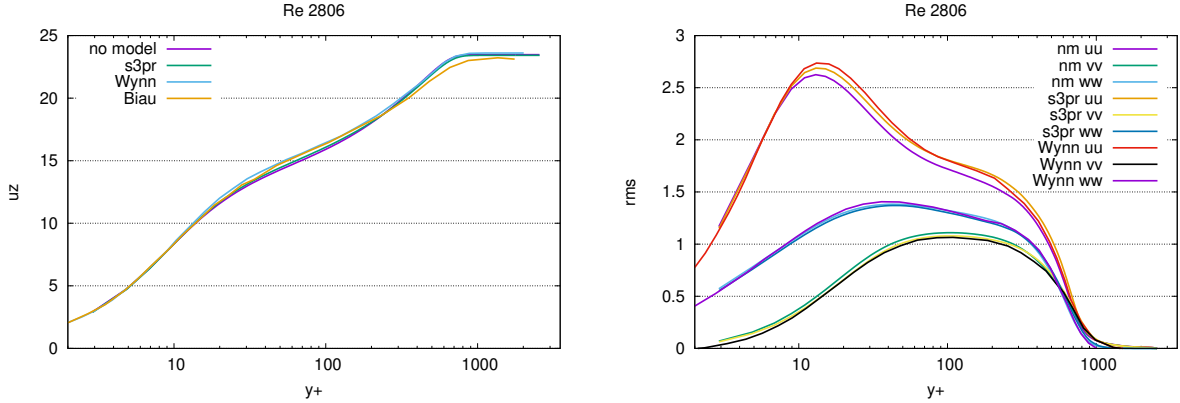


Figure 7: $Re_{\delta^*} = 2806$, $200 \times 400 \times 200$ mesh. **Left:** streamwise average velocity. **Right:** rms u^+ ; rms v^+ ; rms w^+ ; Wynn [14], Biau [14]

Reasonable agreement with the reference results is obtained for both the mean velocity and the rms values.

Following this validation, we analyse the behaviour of a wall-mounted cube inside a periodic boundary layer. At the time of writing, no suitable reference for a quantitative comparison

has been found, so the study remains qualitative. We therefore simulate a boundary layer that should resemble half of the channel flow considered earlier. That is, the boundary-layer thickness is roughly equal to the channel half-width. To obtain this heuristic equivalent case, we either integrate the log-law of the channel inlet profile or use similarity relations to estimate a theoretical displacement thickness. The Reynolds number finally chosen for the boundary layer is $Re_{\delta^*} = 1741$.

Figure 8 shows the qualitative behaviour of the wall-mounted cube flow inside the boundary layer compared with that obtained in the channel flow ($Re_{\tau} = 590$). The figure displays the average streamwise velocity profiles at the same two probe locations as before. The profiles do not match exactly, as expected; however, the algorithm handles the WMC in the periodic boundary layer without exhibiting any apparent numerical instabilities.

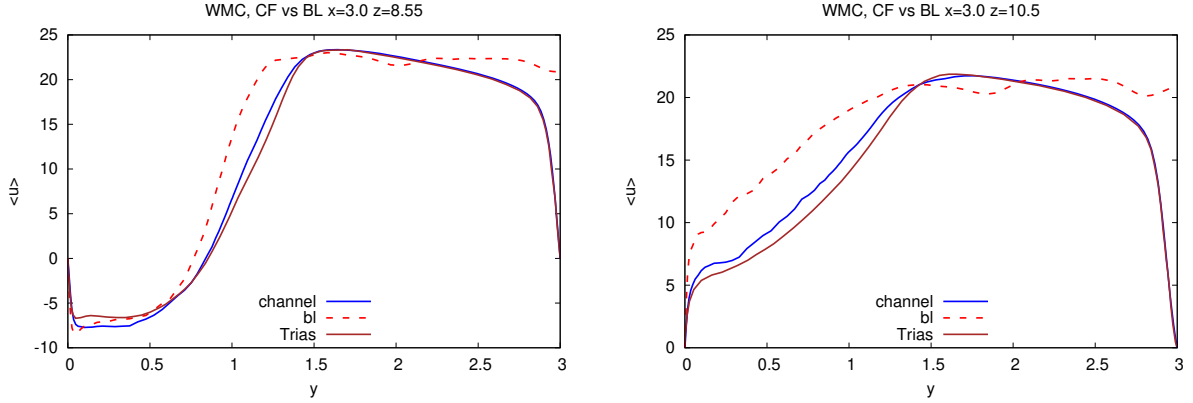


Figure 8: Average streamwise velocity profile. $100 \times 100 \times 200$ mesh. Comparison with Trias [15].

Left: $x = 3.0, z = 8.55$. Right: $x = 3.0, z = 10.5$

4.3 Changing the obstacle: an Illa de l'Eixample-inspired shape

To assess several aspects relevant to a future realistic urban simulation, we replace the obstacle in the flow. The objective is to identify and rule out possible inconsistencies when abandoning the already-validated wall-mounted cube. As a shape test, we choose a geometry similar to Barcelona's Illa de l'Eixample: a near-square block with flattened edges (see Figure 9):

The dimensions have been scaled proportionally so that the total distance between opposite sides equals one, thereby obtaining roughly the same volume and surface area as the original cube. The height is also set to one. The obstacle should therefore not be interpreted as a realistic building block.

Again, the analysis is mostly qualitative and is aimed at identifying any anomalous effects that might arise with alternative geometries. The results are compared with those for the wall-mounted cube in a no-model channel flow ($Re_{\tau} = 590$) and in a periodic boundary layer ($Re_{\delta^*} = 1741$), as before. Figure 10 shows the streamwise velocity average profiles: the first



Figure 9: Dimensions of the actual block: side of the larger square: 113 m. Size of the corner square: 14 m. Computation with side = 1.0 (as in WMC) scaled proportionally.

panel corresponds to the first probe location in a channel; the second panel to the second location in the boundary layer. Apart from the expected differences (somewhat larger than initially anticipated), the profiles obtained with the Illa-inspired shape remain physically reasonable and exhibit no significant numerical pathologies.

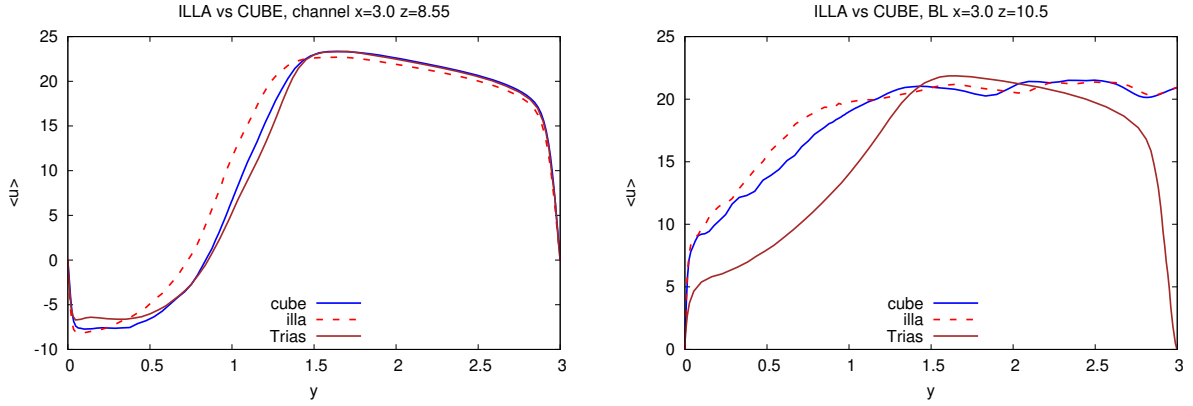


Figure 10: Average streamwise velocity profile. $100 \times 100 \times 200$ mesh. Trias [15]. **Left:** $x = 3.0, z = 8.55$, channel flow. **Right:** $x = 3.0, z = 10.5$, boundary layer

5 URBAN-LIKE ENVIRONMENTS: CEDVAL DATASET

The final step is the simulation of an urban canopy, i.e., an array of buildings. For comparison and validation, we adopt the CEDVAL dataset [1] from the University of Hamburg. Specifically, we consider the B1-2 flow in a finite array of square-shaped rings of buildings (aspect ratio I). The experiments were performed in a wind tunnel. All details, figures, and probe locations are provided in the reference. Figure 11 shows the general layout of the configuration.

As a first, rough approach, we start with a channel-flow configuration, with a domain size of $2m \times 3m \times 6m$. The wall-normal extent of the domain is chosen to be sufficiently large to

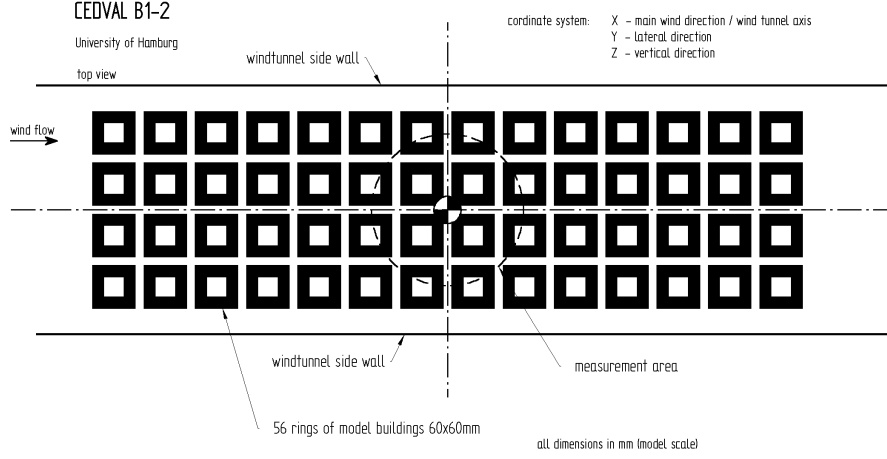


Figure 11: Layout of the CEDVAL B1-2 case (reproduced with permission).

minimise the influence of the upper wall. The Reynolds number given by CEDVAL is $Re_h = 14640$ based on the building height (60mm). In our channel configuration, this is equivalent to $Re_\tau = 37772$, with channel half-width of $H = 1.5\text{m}$, a viscosity of $1.5 \cdot 10^{-5}\text{m}^2/\text{s}$, and a friction velocity of $u_\tau = 0.37772\text{m/s}$, the latter two values being those prescribed by CEDVAL. At the inlet, we impose a power-law profile with the exponent provided by CEDVAL, as shown in Figure 12.

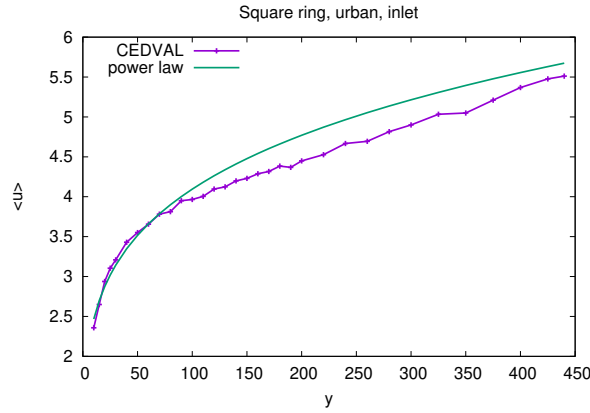


Figure 12: Inlet velocity profile on a $200 \times 200 \times 400$ mesh. CEDVAL profile and power-law approximation $u_z(y) = 3.66 \cdot (\frac{y}{60})^{0.22}$

Even with the relatively coarse mesh ($200 \times 200 \times 400$) for this Reynolds number and without wall models (for simplicity, as a crude approximation), meaningful results are obtained.

However, for realistic urban configurations at higher Reynolds numbers, wall-modelled LES approaches should be applied. The computation was performed with the PR LES model. Figures 13, 14, 15 display the mean streamwise velocity profiles at different positions and directions, compared with the CEDVAL data.

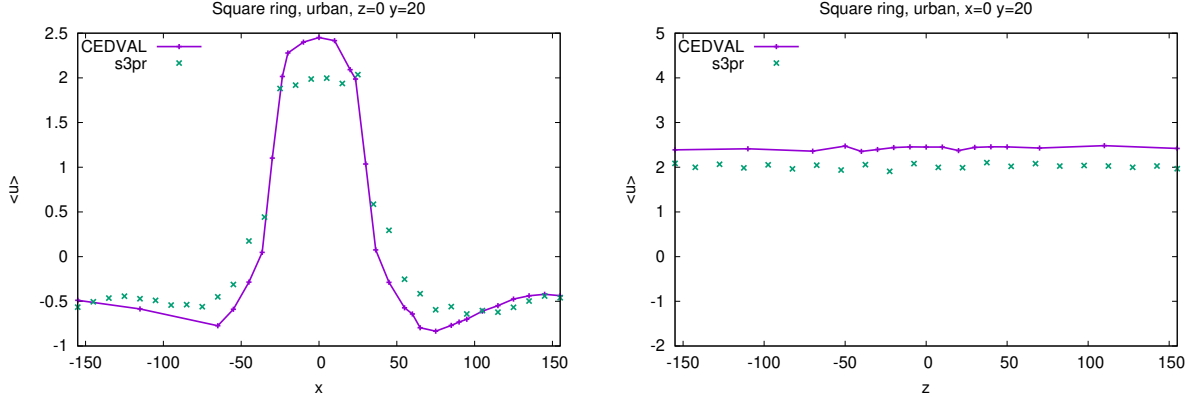


Figure 13: Mean streamwise velocity u_z in the spanwise (left) and streamwise (right) directions. $200 \times 200 \times 400$ mesh. Probe centre (0,20mm,0). Both directions span from -155mm to 155mm. CEDVAL and simulation data.

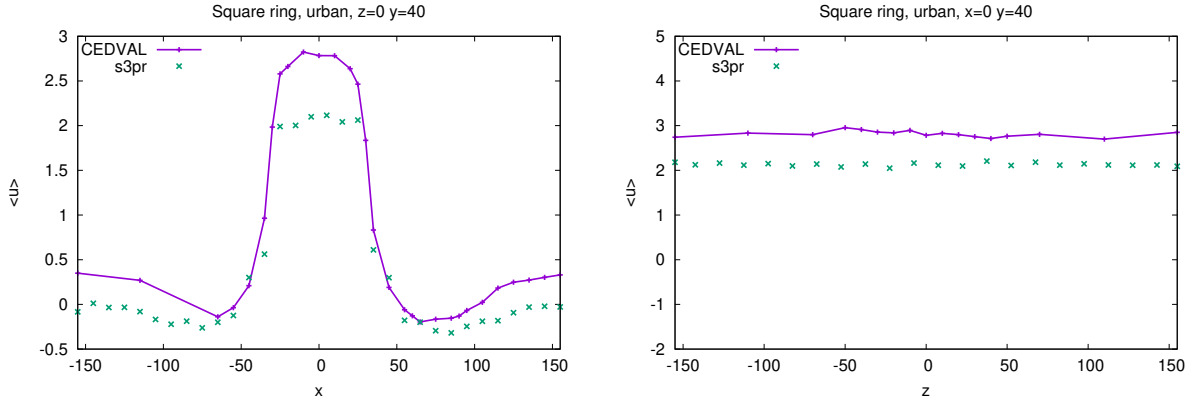


Figure 14: Mean streamwise velocity u_z in the spanwise (left) and streamwise (right) directions. $200 \times 200 \times 400$ mesh. Probe centre (0,40mm,0). Both directions span from -155mm to 155mm. CEDVAL and simulation data.

6 CONCLUSIONS

To simulate a realistic urban configuration, we have developed and validated a sequence of steps, obtaining promising results even with coarse meshes. The results indicate the reliable per-

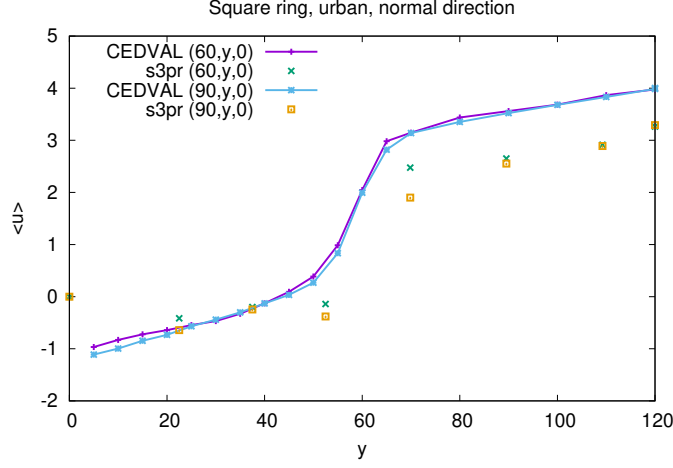


Figure 15: u_z mean streamwise velocity profiles in the wall-normal direction at two locations: $x = 60mm$, $x = 90mm$. $200 \times 200 \times 400$ mesh. CEDVAL and simulation data.

formance and versatility of the TFA code and the S3PQR LES models for benchmark cases such as the boundary layer and the wall-mounted cube in a channel flow. For the wall-mounted cube in a boundary layer and for the CEDVAL configuration, the results show reasonable agreement with the available reference data and support further development of the methodology.

Further work will involve completing and expanding the analysis to include all LES models and incorporating pollutant dispersion. As a related consideration, the possibility of improving LES models based solely on invariants of the velocity-gradient tensor (as is the case for all S3PQR models) remains open.

7 ACKNOWLEDGEMENTS

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