Summary

The Urban Co-Creation Data Lab (UCD Lab) project aimed to support decision-making at the municipality level to provide citizens with high quality services in the areas of micromobility, waste management, parking, pollution, and emergency. The project aimed at developing a new generation of public services in the context of smart cities exploiting supercomputing facilities and public and private data to analyse complex combinations of large datasets in areas of public interest. The analytical model presented in this document was developed for the city of Lisbon regarding pollution and was made publicly available to any interested person or institution. The UCD Lab was co-financed by CEF Telecom, the EU instrument to facilitate cross-border interaction between public administrations, businesses and citizens, and the project beneficiaries were: Universidade Nova de Lisboa, Município de Lisboa, Agência para a Modernização Administrativa, I.P., NEC Portugal - Telecomunicações e Sistemas, S.A, and Barcelona Supercomputing Center - Centro Nacional de Supercomputación.

Service description

Although this service can be applied to any urban geometry, it has been used to simulate two use cases in different areas in the city of Lisbon:

1. The propagation of natural gas after a disruption in the natural gas network in Alcântara area (Lisbon), with a temporal frequency of 1 minute to 15 minutes, in an area of 1 Km^2, calculated from the location of the incident
2. The propagation of nitrobenzene after a train accident in Roma-Areeiro train station area (Lisbon), with a temporal frequency of 1 minute to 15 minutes, in an area of 1 Km^2, calculated from the location of the incident

In Table 1 are presented the coordinates of the incidents for each use case.

Table 1. Coordinates of the incidents for the use cases of Alcântara and Roma-Areeiro. The coordinates are projected in the ETRS89 / Portugal TM06 (EPSG: 3763) coordinate system.

Use case	**Y**	**X**
1 - Alcântara	-106559,43952	-90388,247875
2 – Roma-Areeiro	-101946,9944	-87149,50364

Analytical model

Input data

In Table 2 the datasets necessary to develop the analytical model for #4 Pollution use cases are presented.

Table 2. Datasets necessary for the development of the analytical model for #4 Pollution use case.

Dataset	**Source**	**Open data**
Building geometry (2.5D)	Lisbon City Council (CML)	No
Digital Terrain Model	Lisbon City Council (CML)	Yes
Weather data	Portuguese Institute for Sea and Atmosphere (IPMA)	No

Modelling

Computational Fluid Dynamics is used to perform the wind flow predictions. In particular, wall-modelled Large Eddy Simulation (WMLES) is applied to take accurately into account the spatial and temporal resolutions of both use cases while dealing with the presence of sizeable solid wall areas. Wall modelling for LES (WMLES) allows overcoming the unfeasibility of the explicit resolution of city-sized solid wall areas. The main advantage of this strategy was to keep the reliability and accuracy of an LES prediction while circumventing the costs of the explicit wall resolution. In Figure 1 it is presented the isometric view of a WMLES for the area of Alcântara, and a horizontal section of the WMLES velocity is shown in Figure 2.

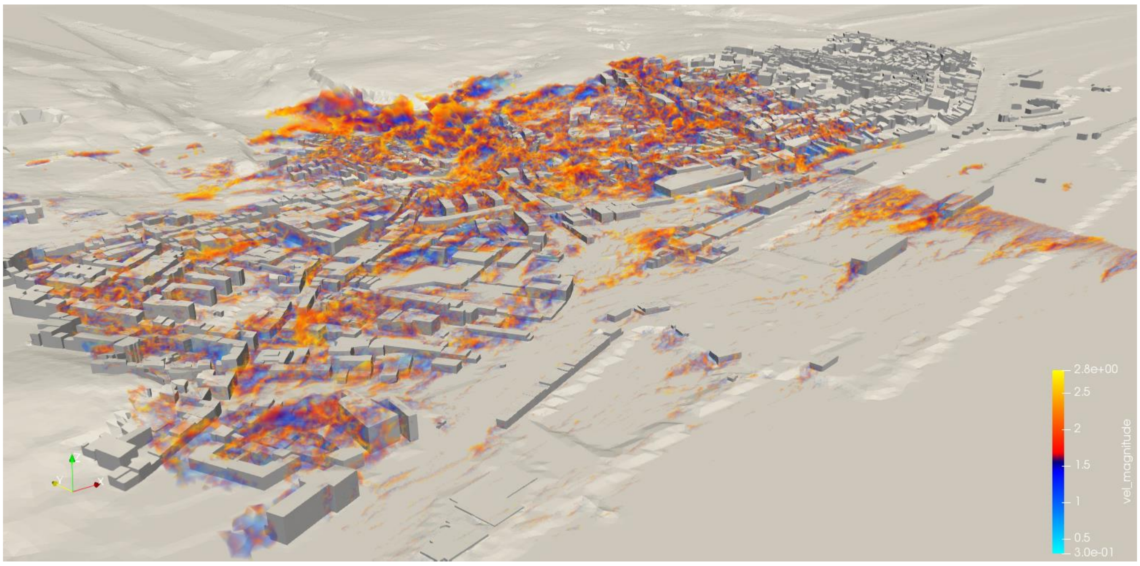

Figure 1. Isometric view of a wall modelled LES simulation in Alcântara. Contours of the velocity magnitude are plotted.

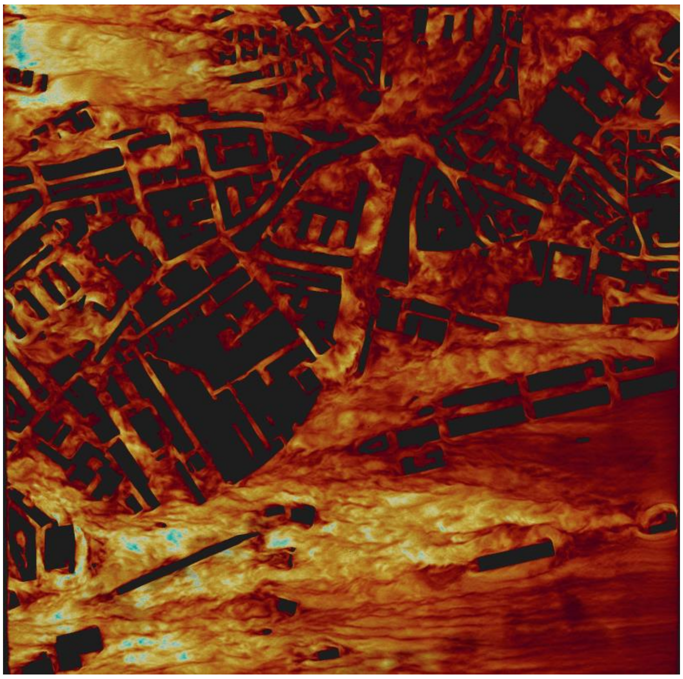

Figure 2. Horizontal section of the WMLES velocity field at pedestrian level in Alcântara area.

The wind flow resolution through WMLES was carried out with Alya, an existing in-house HPC code (Vázquez et al., 2016) developed at CASE Department.

The physical and mathematical model implemented in Alya is based on the numerical resolution of the spatially-filtered incompressible Navier-Stokes Equations:

$$\frac{\partial \overline{u}}{\partial t} + (\overline{u} \cdot \nabla)\overline{u} = \nabla \cdot [2(\nu + \nu_{sgs})S(\overline{u})] - \nabla \tilde{p}$$

$$\nabla \cdot \overline{u} = 0$$

where $\bar{u}$ is the filtered velocity field, $\bar{p}$ is the filtered pressure, ν is the fluid molecular viscosity, and ν_{sgs} stands for the subgrid viscosity. This is a suitable model to characterize the ABL physics (García-Sánchez, van Beeck, & Gorlé, 2018; Kurppa et al., 2018; Owen et al., 2020).

To close the formulation, a proper subgrid model was used to provide the ν_{sgs}. For the present modelling approach, the Vreman model was used given its proven reliability in modelling atmospheric boundary layers (Owen et al., 2020):

$$\nu_{sgs} = c\sqrt{\frac{B_\beta}{\alpha_{ij}\alpha_{ij}}}$$

$$\alpha_{ij} = \nabla\overline{u}$$

$$B_\beta = \beta_{11}\beta_{22} - \beta_{12}^2 + \beta_{11}\beta_{33} - \beta_{13}^2 + \beta_{22}\beta_{33} - \beta_{23}^2$$

$$\beta_{ij} = \Delta_m^2 \alpha_{mi}\alpha_{mj}$$

where c is a model constant while Δ_m is the grid characteristic length-scale.

On the other hand, to deal with the difficult near-wall physics, a wall model based on an equilibrium atmospheric boundary layer profile with roughness is used. This approach has proven to be suitable for atmospheric boundary layers (Owen et al., 2020) and urban flows (García-Sánchez et al., 2018).

$$u_x(y) = \frac{u_\tau}{\kappa} ln\left(\frac{y + y_0}{y_0}\right)$$

being u_x the wall-parallel velocity component, y stands for the wall distance, u_τ is the skin friction velocity, κ is the Von Kármán constant, and y_0 is the wall roughness height.

Finally, the transport of the pollutant substance within the atmospheric flow has been modeled as a passive scalar through a filtered advection-diffusion equation:

$$\frac{\partial\overline{c}}{\partial t} - \nabla\cdot(\overline{uc}) = \nabla(D + D_{sgs}\nabla\overline{c}) + S$$

where $\bar{c}$ is the relative substance concentration ($\bar{c} = 1$ represents pure substance), D is the diffusivity, D_{sgs} is the subgrid diffusivity due to the unresolved scales, and S stands for any substance source. To determine the diffusivity coefficients, a constant Schmidt number has been applied. Again, this approach has been validated to model the transport of pollutant substances in urban environments (Gousseau, Blocken, Stathopoulos, & van Heijst, 2015).

To summarize, the variables that will characterize the micrometeorology and the dispersion problem are the wind velocity field, the pressure, and the pollutant substance concentration at each point of the high-resolution computational grid.

To deal with the complex issue of the boundary conditions for a time-resolved turbulent flow, a novel strategy has been developed for the present simulations. The approach is based on prescribing periodic boundary conditions in all domain's wall-parallel directions. The wind motion is enforced through the geostrophic pressure gradient provided by WRF, which is imposed as a source term to the model. This creates a natural and straightforward coupling between the mesoscale and microscale simulations through a single vectorial value (Figure 3). At the same time, the proper resolution of the turbulent time scales throughout the computational domain is ensured by this method since this approach is widely used for DNS and LES of canonical wall-bounded turbulent flows (Lozano-Durán & Jiménez 2014).

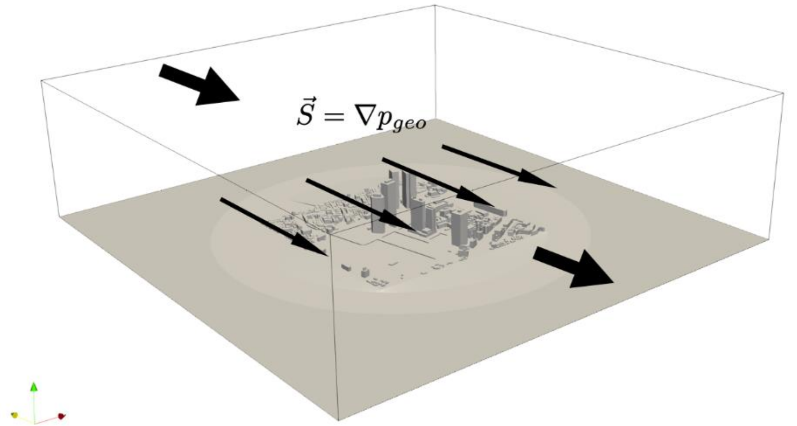

Figure 3. Wind flow enforcement scheme.

Model validation

An a priori validation test has been carried out to ensure that the global modeling strategy performed successfully. The main objective of the test was to ensure that the periodic strategy combined with the physical and numerical model was able to reproduce realistic velocity profiles upstream of the urban area. To achieve this, the downstream perturbed atmospheric boundary layer must recover the original logarithmic profile along the periodic loop. For that reason, the urban area of Shinjuku (Tokyo) has been used to validate the strategy. Its geometry is particularly challenging for the model due to the height of the buildings present in this area, severely disrupting the boundary layer equilibrium profile (Figure 4).

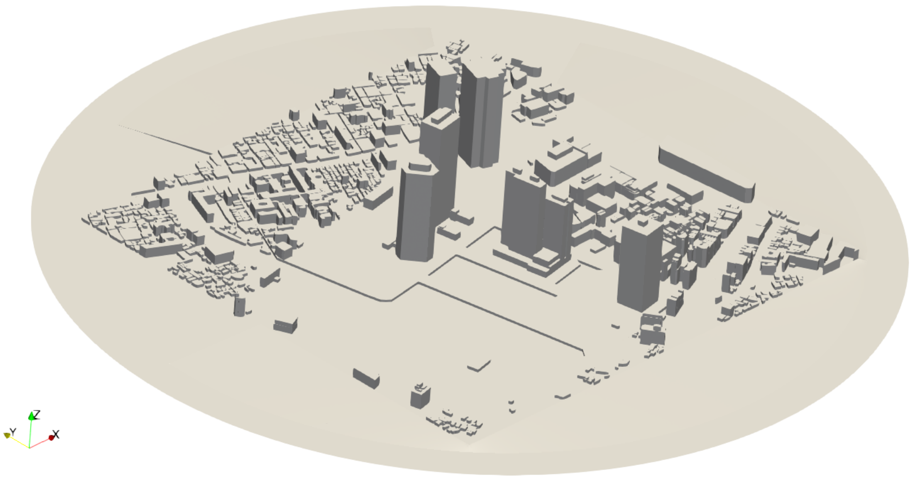

Figure 4. Shinjuku (Tokio) urban area geometry.

The tests consisted of simulating a periodic ABL flow through Tokyo's Shinjuku urban area and determining the necessary streamwise domain length to recover the original ABL logarithmic profile upstream of the urban geometry such that the perturbations introduced by the urban geometry have dissipated along the periodic loop (Figure 5).

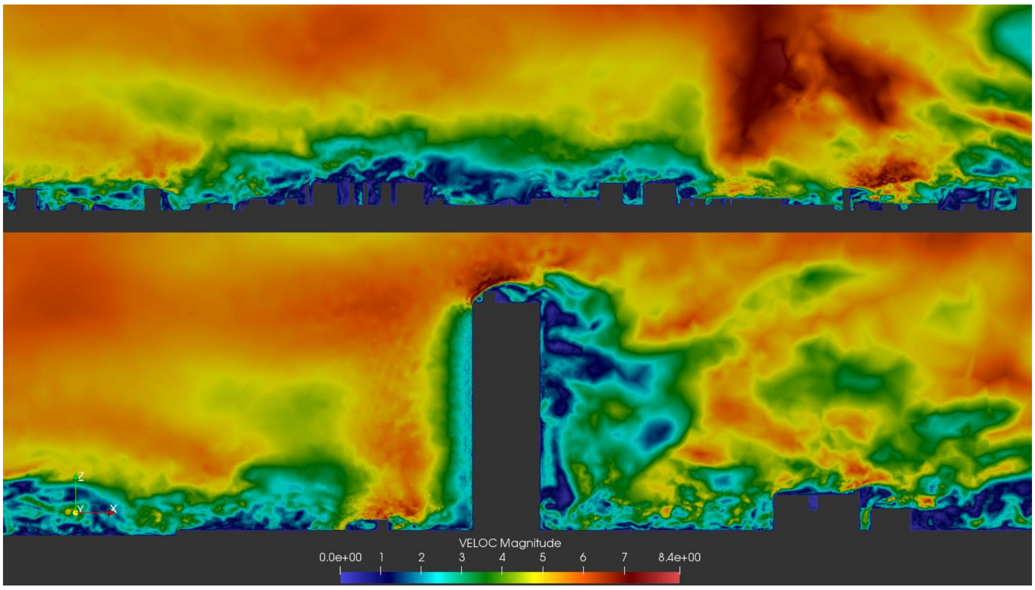

Figure 5. Shinjuku urban area ABL. Top: mildly perturbed ABL featuring small-building urban geometries. Bottom: Strongly distorted ABL due to the presence of tall buildings.

Specifically, three domain sizes were tested, 3L, 5L, and 10L being L the urban area horizontal length (1Km). On the other hand, the wall model roughness was set at $y_0 = 0.1\ m$. Below, the mean velocity profiles upstream and downstream of the urban area are displayed for the 5L and 10L tests (Figure 6).

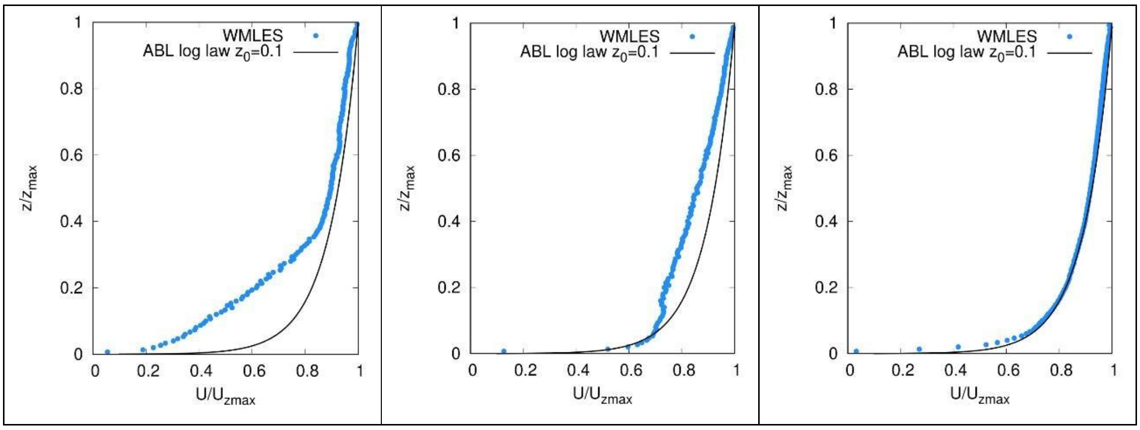

Figure 6. left: downstream average velocity profile, middle: upstream velocity profile for the 5L domain length, right: upstream velocity profile for the 10L domain length. Dotted blue: WMLES results, solid black line: analytical reference results.

The tests revealed the need to extend the computational domain in the streamwise direction up to a 10L length to allow the boundary layer to recover. Nevertheless, according to the obtained results, we could conclude that the modelling strategy could reproduce the real physics provided that a sufficient streamwise domain length is prescribed. The required length will depend on the particular urban geometry and the degree of distortion that it introduces to the ABL.

References

García-Sánchez, C., van Beeck, J., & Gorlé, C. (2018). Predictive large eddy simulations for urban flows: Challenges and opportunities. *Building and Environment*, *139*, 146–156. https://doi.org/https://doi.org/10.1016/j.buildenv.2018.05.007

Gousseau, P., Blocken, B., Stathopoulos, T., & van Heijst, G. J. F. (2015). *Near-field pollutant dispersion in an actual urban area: Analysis of the mass transport mechanism by high-resolution Large Eddy Simulations*. *114*, 151–162. https://doi.org/10.1016/j.compfluid.2015.02.018

Kurppa, M., Hellsten, A., Auvinen, M., Raasch, S., Vesala, T., & Järvi, L. (2018). Ventilation and Air Quality in City Blocks Using Large-Eddy Simulation—Urban Planning Perspective. *Atmosphere*, *9*(2). https://doi.org/10.3390/atmos9020065

Lozano-Durán, A. and Jiménez, J. (2014). Effect of the computational domain on direct simulations of turbulent channels up to *Re*τ= 4200. *Physics of Fluids*, Vol. 26, pp. 011702

Owen, H., Chrysokentis, G., Avila, M., Mira, D., Houzeaux, G., Borrell, R., … Lehmkuhl, O. (2020). Wall-modeled large-eddy simulation in a finite element framework. *International Journal for Numerical Methods in Fluids*, *92*(1), 20–37. https://doi.org/https://doi.org/10.1002/fld.4770

Vázquez, M., Houzeaux, G., Koric, S., Artigues, A., Aguado-Sierra, J., Arís, R., … Valero, M. (2016). Alya: Multiphysics engineering simulation toward exascale. *Journal of Computational Science*, *14*, 15–27. https://doi.org/https://doi.org/10.1016/j.jocs.2015.12.007