Best Practice Guide on Pollutant Dispersion Simulations with the Commercial Tool „ ANSYS Fluent“ at CERN

U. Kaeuflin, M. Battistin, Dr S. La Mendola, Prof Dr-Ing B. Leitl
CERN, Switzerland – University of Hamburg, Germany

Abstract

Large Eddy Simulations (LES) are of raising interest for numerous engineering applications in which an accurate flow prediction is necessary. This paper searches for the optimum mesh resolution in numerical simulations reliably predicting dispersion of pollutants in the lower part of the Atmospheric Boundary Layer (ABL). For the dispersion of pollutants, turbulent quantities have been assessed at several distances from the release point and compared to each other. Areas close to release points located at low altitudes are given a particular importance, because air pollutant concentrations can be too high for people present at such places. To achieve a realistic prediction of the flow and pollutant concentrations close to populated areas, LES are preferred over the Reynolds-Averaged Navier Stokes (RANS) models (Vita et al, 2020). A mesh resolution of 0.5 m is recommended at distances from the release point shorter than 40 m. Near the release point, physical effects like building downwash and horizontal plume enlargement due to the downstream wake region of buildings have a direct impact on pollutant concentrations and particle trajectories. In built-up areas at intermediary distances where the dispersion of the plume is directly influenced by buildings in their given constellation and where the energy production is high, a mesh resolution of 1.5 m is suggested. In areas where the plume is already dispersed and geometrical obstacles are rare, a mesh resolution of 3 m and more is sufficient. In these areas, the dissipation of energy and the transport of particles (mean quantities) that determine the flow are less affected by the mesh size.

Introduction

Simulating an atmospheric boundary layer (ABL) flow with Large Eddy Simulations (LES) is a challenging and demanding task. The alternative approach of using LES is mainly found in research so far (Vasaturo R et al 2018), but best practice guides (BPGs) do not exist at present (Vita et al, 2020). To encourage practitioners to use LES and to harmonise LES for ABL flows in the future, turbulence characteristics are investigated for five different grid resolutions in a pollutant release scenario.

At CERN (Conseil Européen pour la Recherche Nucléaire), a project called FIRIA (Fire-Induced Radiological Integrated Assessment) was launched in 2018 to develop a risk assessment methodology that aims at predicting radiological consequences of fires potentially developing inside some of the Organisation's research facilities.

Computational Geometry

Local-scale pollutant dispersion in built-up areas does not only depend on the structure (topographical and geometrical) of the immediate surrounding area, but also on topographical variations and presence of buildings far upwind of the release point. For the pollutant dispersion simulations the CERN site, located between Geneva (CH) and Saint-Genis-Pouilly (FR), was used (Figure 1).

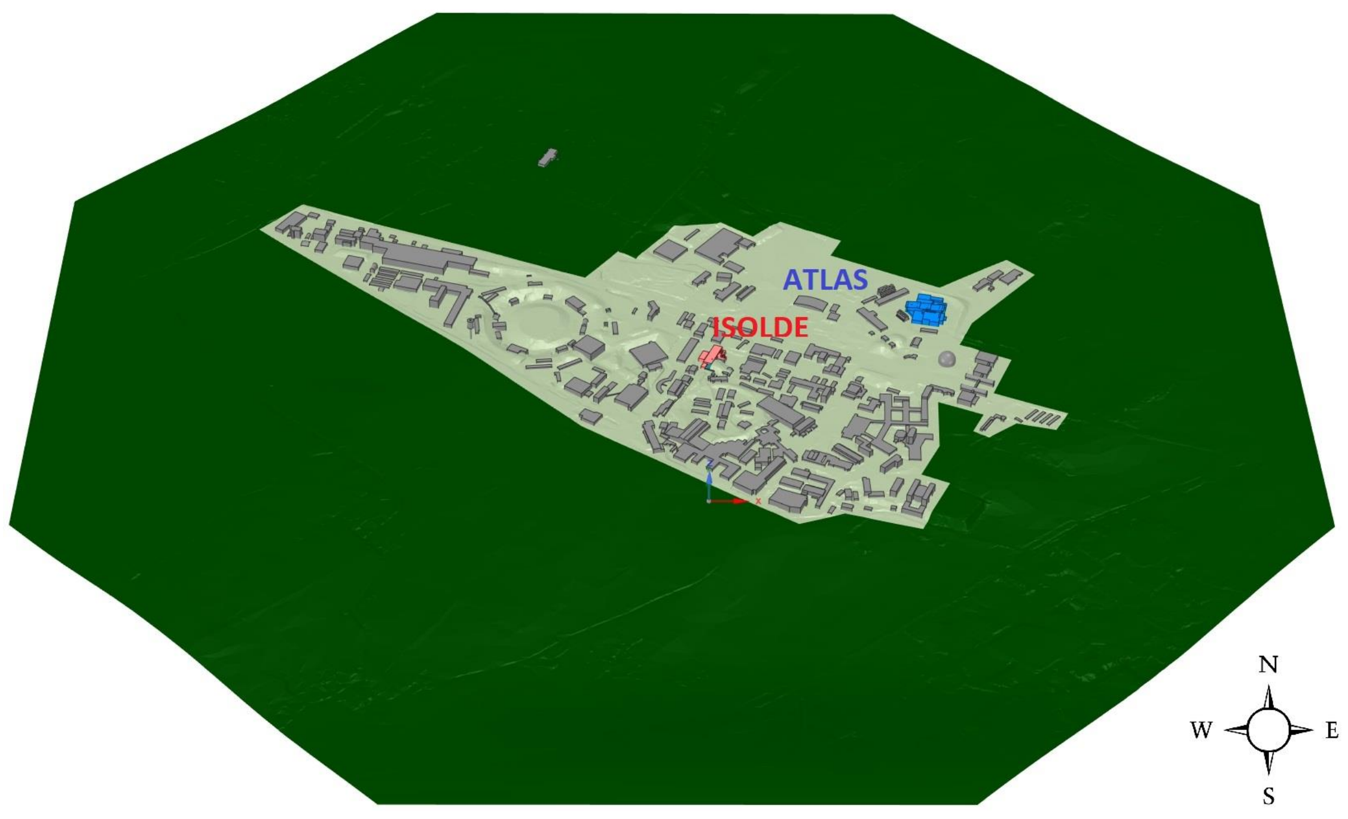

Figure 1: Polyhedral shaped domain including topography model, CAD buildings (grey, red, blue).

A digital terrain model was used to integrate topographic elevations and CAD modelled buildings were connected to one single domain (Figure 1). The domain has a polyhedral shape and a total size of 3×3km² with a height of 500m. A relaxation of the domain sides was achieved by changing altitude values on the domain sides.

Meshing

An unstructured polyhedral mesh was used to have several degrees of freedom, i.e. to adapt the mesh to the geometry and to refine regions of interest. For the mesh refinement study, five different meshes were created with ANSYS Fluent Meshing module: very coarse (2.2M cells), coarse (4.3M cells), medium (9.8M cells), fine (16.1M cells), and very fine (21.6M cells). Depending on the coarseness level, several parameters vary with sizing functions. The maximum global size for the polyhedral cells ranges between 50m and 100m, and the minimum global size and the size function for special buildings is set to 0.5m to resolve the buildings of interest and their surrounding areas.

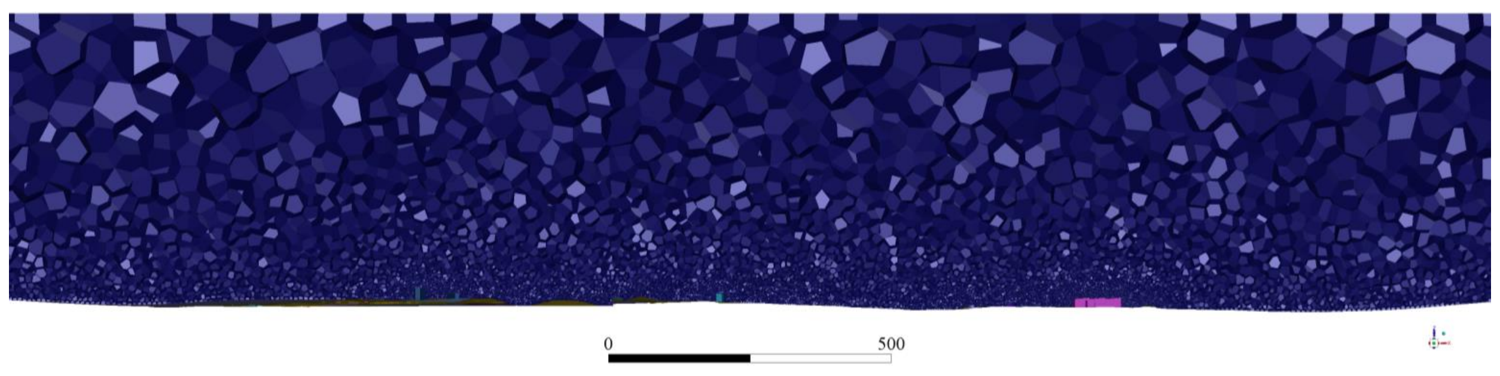

Figure 2: Polyhedral cells display in a cut-plane through the full domain for the very coarse refinement level.

Boundary Conditions

Monin-Obukhov similarity theory as described in Dyer (1974) was used to define the velocity profile of the neutral ABL flow. A terrain roughness value of z_0=1m was chosen (suburbs, villages and forests) (Stull, 2000). The Synthetic Turbulence Generator (Shur and Spalart et al, 2014) was used to add fluctuations to the mean velocity terms at the inlets. For the top of the domain and the sides of the domain pointing in the wind direction, velocity inlets were used. At the outlets, simple pressure outlets have been defined. At all the walls (ground and buildings), a no-slip condition was applied. Two wind directions have been evaluated: wind blowing into south (S) and wind blowing into north-east (NE) direction. Downwind planes (40m, 100/110m, 200m, 300m, 400m) have been defined perpendicular to the wind direction to track the pollutants and to analyse turbulence characteristics.

Numerical Methods

The in ANSYS Fluent implemented LES with second-order implicit time-dependent solution formulation and the Wall-Adapting Local Eddy-viscosity (WALE) model, with CW = 0.325, was used (Nicoud and Ducros, 1999). A time step between 0.1 s and 0.2 s was chosen to make sure that the Courant-Friedrichs-Lewy (CFL) condition of CFL < 1 is satisfied.

Results

Mean velocity magnitude and turbulent kinetic energy (TKE) have been calculated from the exported time dependent velocities. The atmospheric flow is mainly disturbed close to buildings where velocity layers are separated. It could be observed that values for TKE were changing drastically with the mesh resolution: The finer the mesh, the more fluctuations are resolved and therefore the TKE increases. In LES, eddies smaller than the grid size are sub-grid modelled and only the part which can be resolved is seen in the figures due to its fluctuations in the time dependent velocity values.

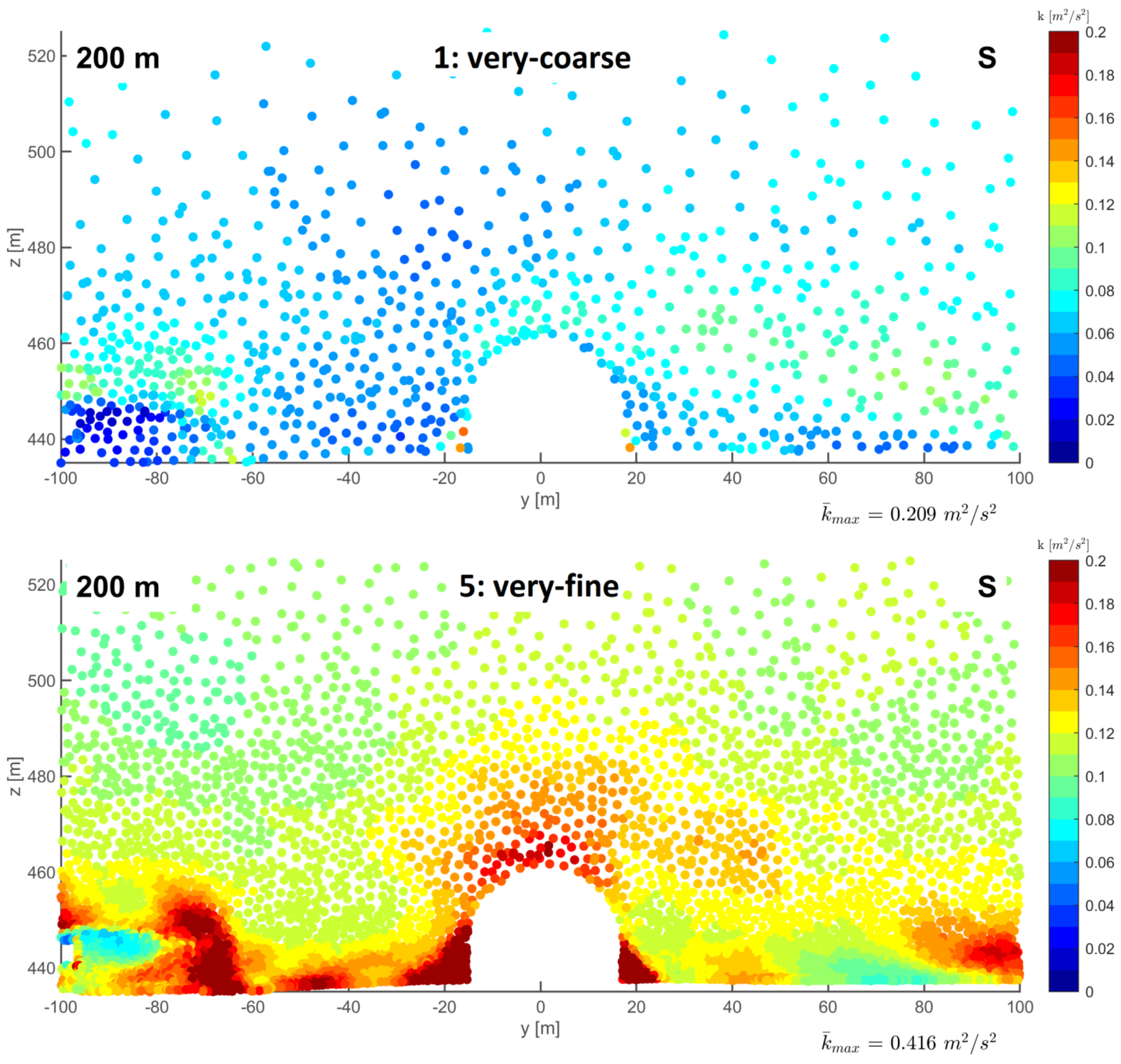

Figure 3: TKE coloured on perpendicular planes. Example for very-coarse and very-fine mesh sizes in the wind direction towards south at 200m distance from the release point.

Conclusions

According to the study, it is possible to give recommendations for future flow predictions at CERN and generally for similar simulation setups. To predict the movement and dispersion of pollutants through the air in the ABL, two quantities are of major importance: The mean velocity, which affects the transport of particles and therefore also the time, a particle rests at a certain location; and TKE, which has an impact on the plume size.

Local mesh refinements are required close to the release point of the pollutants and in the surrounding region for high-density areas. At distances far from the release point, the mesh size is not as important because the initial shape of the plume is already well resolved in a finer mesh.

Before setting up the simulations it is important to define whether the aim of the investigation is to figure out the area, affected by the plume, or concentration values at certain locations. Predictions with larger cell sizes (very coarse to medium mesh) are more conservative in terms of maximal pollutant concentrations, though the difference is rather small (1-5%). However, to establish emergency evacuation plans, it is recommended to use in general a finer mesh, since turbulent fluctuations are stronger and therefore the affected area is bigger (1-5%). But when considering computational costs the medium mesh size can be recommended, as the difference from medium to very fine mesh is marginal.

The investigation also shows that the finer the mesh, the more realistic the flow prediction and therefore the expectation of concentration. Recommended mesh sizes are: 0.5m close to the release point on the ground and in direct nearby area, a ground sizing of 1m and a surround body-of-interest with 3m resolution in high-density area and a ground resolution of 3m in far distance from source, where no production of energy is present.

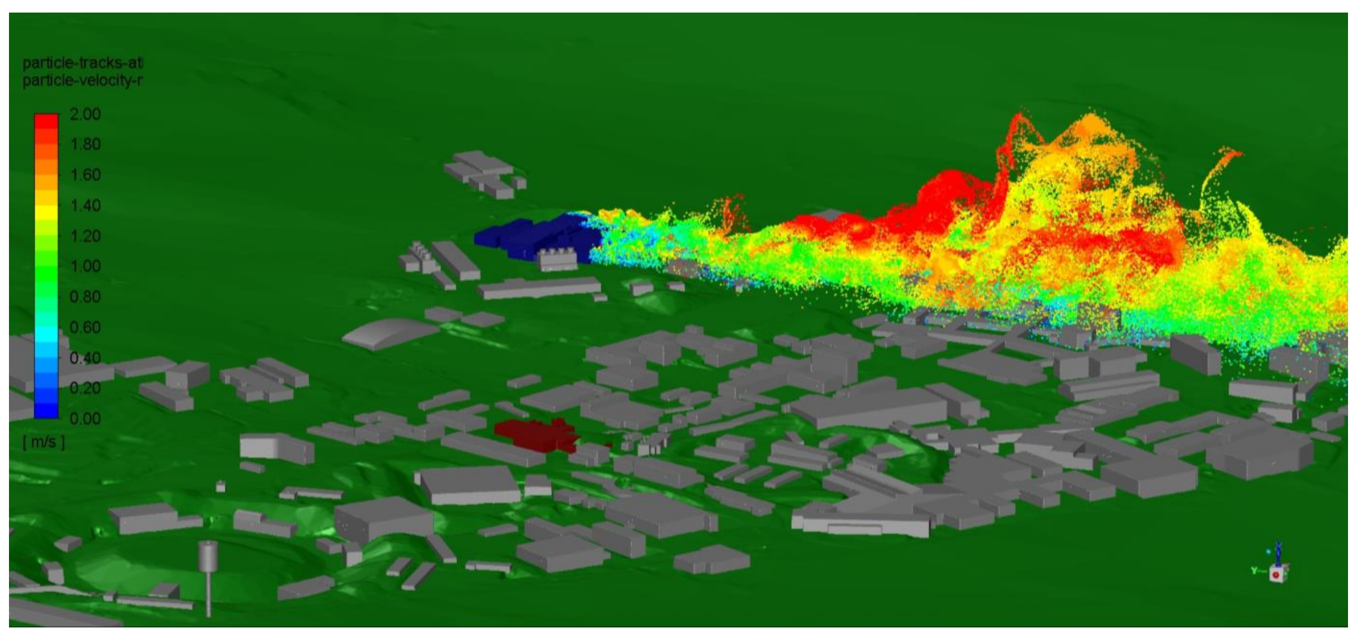

Figure 4: Lagrangian particle dispersion at a total simulation time of 3056s, particles coloured with velocity (0-2m/s).

References

1. Vita G, Salvadori S, Misul DA, Hemida H, 2020: Effects of Inflow Condition on RANS and LES Predictions of the Flow around a High-Rise Building, Fluids, 5(4), 233
2. Vasaturo R, Kalkman I, Blocken B, van Wesemael P J V, 2018: Large eddy simulation of the neutral atmospheric boundary layer: performance evaluation of three inflow methods for terrains with different roughness. Journal of Wind Engineering & Industrial Aerodynamics, 173, 241–261.
3. Dyer A J, 1974: A review of flux profile relationships. Boundary-Layer Meteorology, 7, 363–372.
4. Stull R B, 2000: Meteorology for Scientists and Engineers. Brooks/Cole, Pacific Grove, California, 2nd Edition.
5. Shur M L, Spalart P R, Strelets M K, Travin A K, 2014: Synthetic Turbulence Generators for RANS-LES Interfaces in Zonal Simulations of Aerodynamic and Aeroacoustic Problems; Flow Turbulence Combust, 93: 63.
6. Nicoud F and Ducros F, 1999: Subgrid-Scale Stress Modelling Based on the Square of the Velocity Gradient Tensor.Flow. Turbulence and Combustion, 62(3). 183–200.

Contact Details

U. Kaeuflin: uwe.kaeuflin@cern.ch
M. Battistin: michele.battistin@cern.ch
S. La Mendola: saverio.la.mendola@cern.ch
B. Leitl: bernd.leitl@uni-hamburg.de

HARMO20, Tartu, Estonia
20th International Conference on Harmonisation within
Atmospheric Dispersion Modelling for Regulatory Purposes