

# **Increasing high-fidelity modelling efficiency with automated setup and validation of methodologies**

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## **1 INTRODUCTION**

CFD requires a significant time investment to get accurate, realistic results. The task of the work undertaken here is to significantly reduce the time taken to conduct high-fidelity modelling of chemical plumes through the use of automation. In order to correctly model downstream dispersion, in particular near field dispersion, a good prediction of the flow field is important. Both convection and diffusion processes of the pollutants should be simulated accurately. Convection and diffusion are driven, in urban areas, by large and small turbulent eddies, respectively. Computational Fluid Dynamics (CFD), in the form of Large Eddy Simulation (LES) will be used to resolve the energetic eddies generated within the urban boundary layer. This will make use of Palm4U, an LES code designed for simulation of urban boundary layers. It is possible to run simulations at near real time with small grids ( $O(1m)$ ) and suitable computing power. To drastically reduce the time required an automation tool will be created. This will include the entire setup process, which includes downloading terrain and building data, creating the mesh file, setting up boundary conditions and generating the required input files.

## **2 METHODOLOGY**

In order to accurately predict downstream concentrations, particularly nearfield dispersion, an accurate prediction of the flow field is required, because the mean flow field and turbulence play significant roles in the downstream development and dispersion of plumes. Palm4U [1] will make it practically possible to adhere to the requirements for simulating urban flow fields, providing accurate results. LES in Palm4U is capable of running CFD simulations at close to, if not at real time, through the application of finite differencing over cartesian grids with horizontal uniform grid spacing, the use of the Fast Fourier Transform or multigrid approaches to solve the Poisson equation, and the use of the efficient synthetic inflow turbulence generation [2]. Palm4U can provide results comparable to that of FVM CFD codes such as OpenFOAM [e.g. 4-7].

In reducing total simulation time it was decided to create a tool to automate the meshing and setup of the simulations. When using Palm4U, setup and meshing time can amount to a significantly larger portion of the time taken to complete a simulation. Automating the procedure will significantly reduce overall time to complete a simulation from start to finish, while maintaining accuracy.

## **3 AUTOMATION TOOL**

The aim of the current project will use Python to create the geometry used in the fluid domain from the Ordnance Survey (OS) BHA data set (Building Height Attribute). and OS 5m resolution terrain data. The code will then produce the `_topo` file (the topography of region to be investigated). To compliment topology creation, the setup tool creates the run files required by Palm4U. Palm4U requires 4 files to run a simulation. The control file (`_p3d` & `_p3dr`) contains runtime parameters, grid size and data output parameters. Inflow conditions (`_iprf`) provide vertical profiles of mean velocities, Reynolds stresses and integral length scales. Synthetic turbulence generation method [2] uses these profiles to generate inflow turbulence for LES. This part of the project will automate the entire setup and meshing of the simulation. In order to run, only these 4 files would need to be uploaded to an HPC facility or computer powerful enough to run the simulation.

### **3.1 Outline of the automation process**

The current framework is to generate very-large scale geometries specifically for use in Palm4U. For example, Figure 1 shows a (16km by 16km) region of London, with a resolution of 5m. The axes here are grid index, specifically required by the `_topo` file. Interpolated regions are created to allow the flow

to develop and provide a smooth transition to the real terrain and buildings. This smoothing region is 1km in the coincident boundary normal direction. The contour is coloured by ALS (Above Sea Level) height (m). This methodology has shown success in creating geometries for current research projects, such as Bristol for the ASSURE project and the City of London for the FUTURE project. Results of which have been presented at the Urban fluid mechanics special interest group meetings [6].

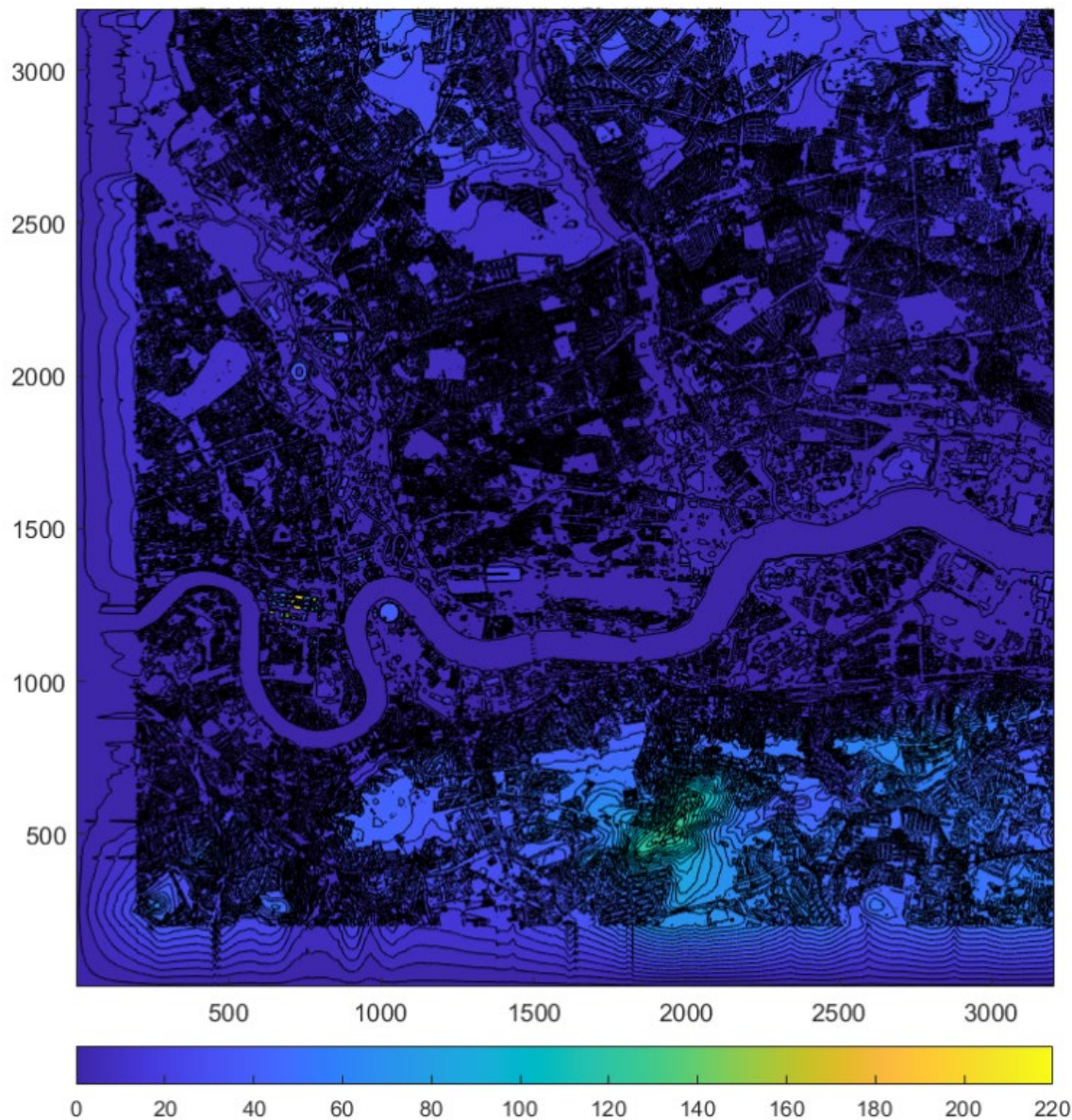


Figure 1: 16km by 16km region with a resolution of 5m, coloured by height (m) above sea level (ASL) for the region centered just north of London City Airport

The input of the data can be any resolution terrain data, here DTM 5 (Digital Terrain Model) with a 5m resolution is used, interpolated onto a 1m grid. The terrain within the domain is created first, which can also be used to compare the effects of buildings on the flow over complex terrain. Building heights are collected from the Ordnance Survey BHA data set (Building Height Attribute). To add buildings, a small region around each building is created, if the building is present within a certain cell, the absolute height of the building is applied to the terrain cell. It is possible to define a minimum, maximum or range of heights for buildings included. This is important when analyzing the effect of building heights. The terrain can also be altered through a multiplying factor to assess the impact of terrain height on flow

within and above the urban canopy [4,7]. The output is interpolated onto a grid with resolution required for simulation.

One of the challenges of CFD for urban atmospheric flows is the inflow conditions. The wind direction within the urban boundary layer usually changes significantly within short time scales, e.g. 15 minutes [8]. This makes modelling scalar dispersion difficult due to the increased horizontal spreading of the plume, which decreases the mean concentrations downstream, but increases the width of the plume.

### 3.2 Current Progress

The automation tool take lat/long data for finding the domain centre and defining which buildings are to be included within the domain. The code automatically converts lat/long to eastings/northings and loads the appropriate terrain and building data from the database. Once the grid size is selected, the code then interpolates the terrain data on the new grid with the chosen domain size and resolution. The building creation uses a search function to check which grid points are within the building's perimeter. The cells within the perimeter have the building's ASL height applied to them. The terrain array and building array is rotated separately if required, and a method is used to rotate the buildings without interpolation, so that the plan area of all buildings are conserved and no data is lost.

A GUI has been created to make the input of data simple, fast and efficient. The GUI allows for users with less experience to utilise Palm4U with appropriate setup parameters, inflow conditions and grid sizes, as these are preselected within the code. The GUI displays the final topography files so that no extra steps are required to check the created topography.

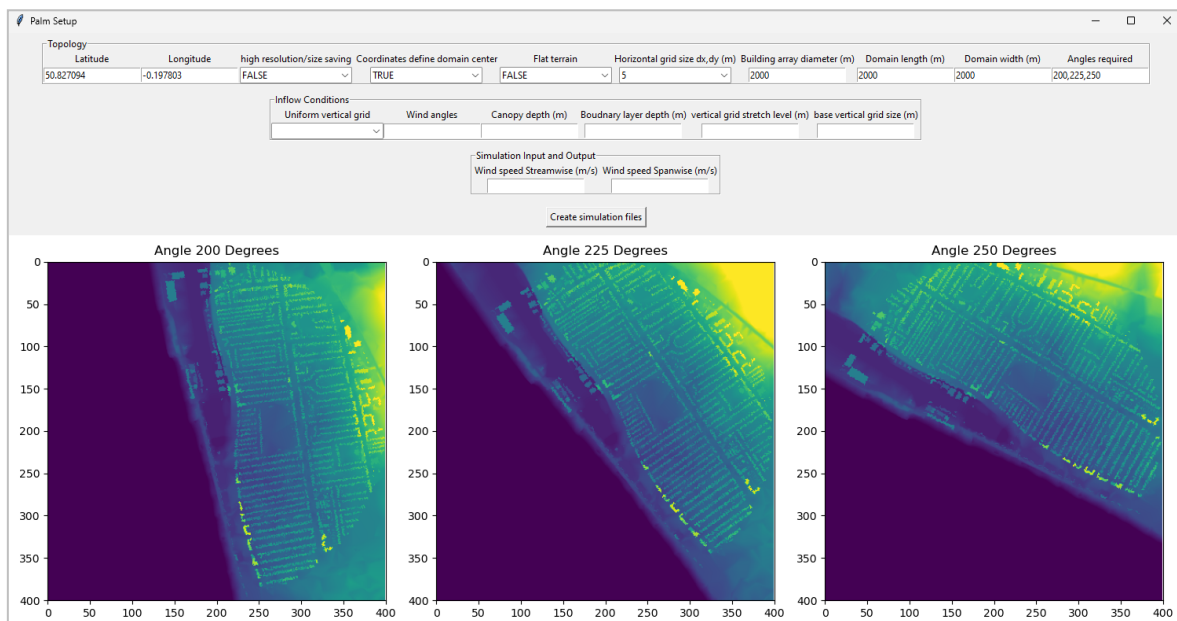


Figure 2: PALM4U Setup tool GUI, post topology creation, showing the three wind angles requested (wind is left to right in each image)

## 4 PLANNED WORK

The final work package of the 2-years project combines the approaches to carry out a case study to demonstrate the new capability. Field study data (e.g. ASSURE project) will be used to compare to the final data set created using the data driven approach. Dispersion data from field studies are available for Southampton [3] and Bristol [6,9], both from sensor networks. These data sets will be used to validate the methodology proposed here. The data generated through DA will be used to assess the uncertainty of the upstream wind direction compared with the field study results.

Data assimilation has been used to gain knowledge of upstream boundary [10]. Thus it will be possible to quantify the uncertainty in applied boundary conditions. This will lead to a more accurate representation of the upwind condition and thus a more accurate representation of a real world scenario

with a better prediction of downstream dispersion from the source release location. The results will be able to identify sharp changes in the local wind and scalar concentration from changes in the upstream wind direction.

#### ACKNOWLEDGEMENT

MC acknowledges a grant from Royal Academy of Engineering (ICRF2324-7-144), ZTX acknowledges a grant support from NERC (grant number NE/W002841/1).

#### REFERENCES

- [1] Maronga et al.(2015) The Parallelized Large-Eddy Simulation Model (PALM) version 4.0 for atmospheric and oceanic flows: model formulation, recent developments, and future perspectives. *Geoscientific Model Development*, 8(8), 2515-2551.
- [2] Xie ZT and Castro IP (2008) Efficient generation of inflow conditions for large eddy simulation of street-scale flows. *Flow, turbulence and combustion*, 81, pp.449-470
- [3] Bulot, Florentin MJ, et al. ((2019) "Long-term field comparison of multiple low-cost particulate matter sensors in an outdoor urban environment." *Scientific reports* 9.1 1-13.
- [4] Coburn M (2023) "High fidelity modelling of neighbourhood-scale environments." *PhD Thesis*, University of Southampton.
- [5] Coburn M, Xie ZT, and Herring SJ. (2022) "Numerical Simulations of Boundary-Layer Airflow Over Pitched-Roof Buildings." *Boundary-Layer Meteorology* 185.3: 415-442.
- [6] Coburn M, Xie ZT, and Herring SJ (2022) "LES for wind environments and dispersion at Bristol City", Urban Fluid Mechanics Special Interest Group. <https://www.urbanfluidmechanics.org/meetings/metofficereading-sept-1-2-2022>.
- [7] Coburn M et al. (2023) "Impact of Local Terrain Features on Urban Airflow." *Boundary-Layer Meteorology*, 189, 89–213.
- [8] Xie, ZT (2011) Modelling street-scale flow and dispersion in realistic winds—towards coupling with mesoscale meteorological models. *Boundary-layer meteorology*, 141, 53-75.
- [9] Matthews JC (2024) Sensor measurements and large-eddy simulation of point source plumes over a complex urban terrain, *14th UK Conference on Wind Engineering*, Southampton, 4-6th September 2024.
- [10] García-Sánchez, C., D. A. Philips, and C. Górlé (2014) "Quantifying inflow uncertainties for CFD simulations of the flow in downtown Oklahoma City." *Building and environment* 78, 118-129.