Metamodelling for micro-scale atmospheric pollutant dispersion large-eddy simulation

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Abstract:

In atmospheric dispersion problems, mapping pollutant concentrations within the first tens or hundreds of meters from the emission point source still remains a modelling challenge. Computational fluid dynamics (CFD) approaches provide relevant insights into turbulent flow and pollutant concentration patterns in complex terrain such as urban and mountainous areas [1]. At the forefront of CFD approaches, large-eddy simulations (LES) are a promising way to represent time and space variability of turbulent atmospheric flows and to assess public short-term exposures [5]. LES are subject to uncertainties due to the intrinsic variability of environmental factors, among whom the large-scale meteorological forcing and the emission source characteristics [2].

The design of metamodels for LES could help handling multiple scenarios of atmospheric pollutant dispersion. Coupling CFD approaches and metamodels for atmospheric dispersion problems is the subject of active research. For instance, polynomial chaos expansions have been used to represent how uncertainties associated with the inlet wind profile affect the averaged pollutant concentration field over a urban area [3, 4]. Gaussian process regressions have also been coupled to proper orthogonal decomposition (POD) to reduce the dimension of the pollutant concentration levels simulated by LES to a limited number of principal components [4].

The objective of this study is to provide an exhaustive metamodel-to-metamodel comparison to design an efficient and accurate metamodelling strategy to synthetise the turbulent flow information provided by LES and their associated uncertainties. We present a proof of concept on a simplified but representative flow configuration (2-D flow around a surface-mounted cube) using the AVBP LES code (http://www.cerfacs.fr/avbp7x/). Three physical parameters – the inflow velocity (representative of the upstream atmospheric forcing that is imposed as boundary condition in LES) and the point-source emission position – are uncertain. We analyze the influence of these three uncertain parameters on time-averaged LES fields (mean and fluctuations), which are represented as principal components using POD. Different parametric families of metamodels (linear and ridge regressions, matching pursuit, random forest, gradient boosting and gaussian processes) are considered to represent the relationship between each principal component and uncertain parameters, each offering specific advantages in terms of regularity, parsimony and robustness.

Considering the spatial flow patterns, a multi-metamodel approach is chosen. We focus our study on the concept of champion metamodels; one champion metamodel being selected for each principal component based on the strength of its local Q_2 performance metrics. The robustness of the resulting multi-metamodel approach is evaluated with respect to the size of the LES training set and its associated noise. Results show that for sufficiently statistically-converged quantities of interest, metamodels can succeed in synthesizing LES information (see example in Fig. 1). The next step is to extend this approach to more realistic flow configurations (3-D test case, field-scale campaign). Ultimately, metamodels – more competitive in terms of computational time —

could motivate the use of LES for alerting the public to toxic pollution exposure during major environmental disasters (e.g. industrial accidents, wildfires).

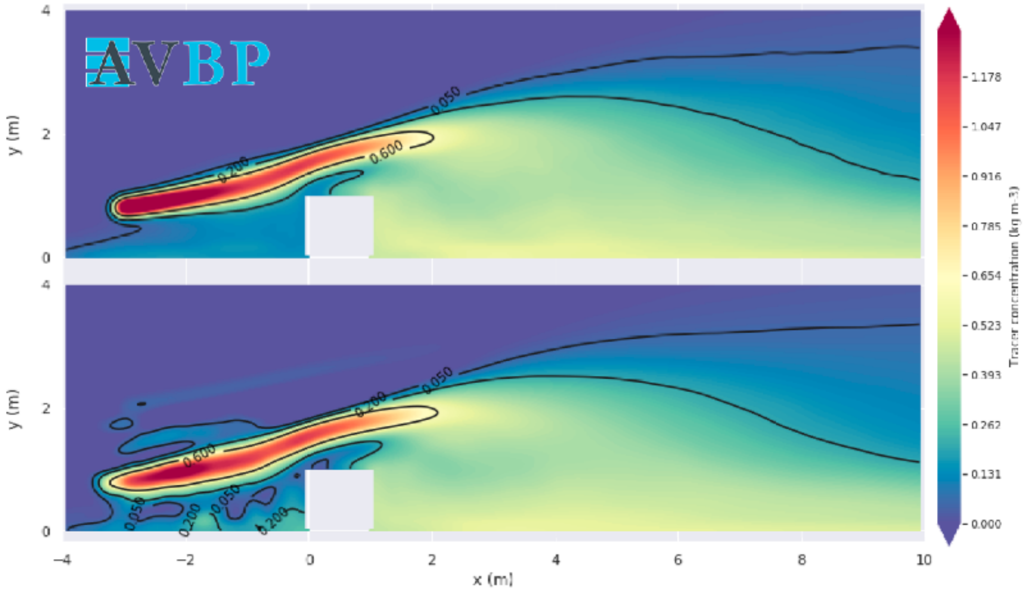

Figure 1: Comparison of a predicted average plume concentration in the 2-D flow test case around a surface-mounted cube (white square) obtained by the LES approach (top panel) and the champion metamodel approach (bottom panel) for inlet wind velocity equal to 2.13 $\mathrm{m\,s^{-1}}$ and tracer point-source emission located at (-3.08 m, 0.79 m). This scenario is not used in the training process.

References

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Short biography – After graduating from INSA Toulouse with a specialization in applied mathematics, Bastien Nony started his thesis at Cerfacs in October 2019 in collaboration with LIMSI (CNRS/Université d'Orsay). The objective is to give access to high-fidelity simulations of atmospheric dispersion over complex terrain (in urban areas for instance) and represent associated uncertainties in the event of accidental dispersion.