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A NEW APPROACH TO COUPLING FLOW AND DISPERSION CFD SIMULATIONS IN A LARGE URBAN AREA AND BUILDINGS OF INTEREST

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Abstract: In a built environment, exposure to air pollution is a major environmental problem. Near-field dispersion of pollutants involves the interaction of plumes with the flow disturbed by buildings. The phenomenon involves both meteorological and aerodynamic aspects of buildings. ARIA/ARIANET in collaboration with CEA has developed the PSWIFT & PSPRAY models in the Parallel-Micro-SWIFT-SPRAY (PMSS) system. The PSWIFT model is a mass-conserving diagnostic atmospheric model. The PSPRAY model is a 3D stochastic Lagrangian dispersion model of pollutants in the atmosphere. They are optimized for use on an urban scale, and allow simulations on large domains, such as the city of Paris, with computation times acceptable for an operational application. To obtain acceptable computation times, only mass conservation is imposed, and the influence of buildings is described geometrically in the PSWIFT model. A RANS model such as Code_Saturne allows to overcome these limitations. Indeed, the flow inside and outside buildings as exchanges at the interfaces are computed explicitly. In order to keep the computation time acceptable for the modeling of an urban area, the RANS model is not used for the whole study area. The approach proposed here consists in using PMSS for the modeling at the scale of the district and Code_Saturne on a nested domain and focused on a building of interest. While a first coupling was implemented between the two models, a new approach and first results are presented here. The flow in the nested domain encompassing the building of interest is computed by Code_Saturne on an unstructured mesh. The flow in the whole urban domain is then computed by PSWIFT on a regular mesh accounting for Code_Saturne output. The question arises of choosing the right interpolation method when moving from one mesh (unstructured for Code_Saturne) to another (structured for PSWIFT). The paper deals with this issue by comparing and discussing the flow and turbulence characteristics interpolated by PSWIFT and simulated by Code_Saturne for a choice of meteorological conditions around a railway station in Paris city (France). Then, dispersion computations are carried out with PSPRAY using PSWIFT flow both in the urban environment and in the building of interest, for fictitious releases outside and inside the station.

Key words: *indoor-outdoor transfer, 3D Lagrangian dispersion model, 3D mass-consistent model, micro-scale, Code_Saturne, Micro-SWIFT-SPRAY, urban environment*

INTRODUCTION

Industrial accidents as well as malevolent actions could result in atmospheric releases of noxious species, especially radionuclides or toxic chemicals. There is an increasing demand for modelling and decision-support systems dedicated to emergency preparedness and response. The challenge is to provide the most precise and reliable evaluation of the spatial and temporal distribution of the gases and/or airborne particles, in computation times consistent with a crisis management situation. The Parallel Micro-SWIFT-SPRAY (PMSS) modelling system developed by ARIA Technologies, ARIANET, and the CEA is an intermediate quick response capability to simulate the micro-scale processes.

Infiltration of pollutants inside buildings is a key process to estimate health effects risks due to hazardous releases, especially in urban areas. Outdoor dispersion models like PMSS (Armand *et al.*, 2010) or the emergency response code ALOHA from US-EPA, compute the infiltration inside buildings with macroscopic methods, deriving analytical indoor concentrations from the outdoor concentrations. These methods are mainly based on an infiltration / exfiltration time scale that can be, in practice, complex to estimate. This time scale is linked with the building's air exchange rate which is the number of times per hour that the volume of air within the building is completely replaced by fresh air when doors and windows are closed. Moreover, in many accidental situations (e.g. fires) or terrorist actions, hazardous releases can occur indoor, in large semi-enclosed buildings, such as industrial facilities or public places (as railway stations or institutional buildings) which are typically the kind of buildings with an infiltration time scale that is difficult to estimate and even could not be relevant because of large openings.

To predict in detail the atmospheric dispersion and the sanitary consequences inside and outside, CFD models appear to be a possible solution. They are often used for both outdoor and indoor dispersion modelling. But the large calculation time of CFD is a significant disadvantage for operational application. The system proposed previously by Nibart et al. (2011) limits the use of CFD to the indoor flow modeling. The indoor and outdoor dispersion is done by the short response model PMSS. A coupling method has been developed between PMSS and the CFD model Code_Saturne. This paper firstly sums up the previous coupling algorithm and presents its limitations. Then improvements of the method that were partially possible thanks to PMSS and Code_Saturne are detailed. Lastly, an application on a realistic case in a dense urban area is presented.

PREVIOUS WORK

The previous coupling strategy was based on a nesting approach: an outer domain includes an inner domain discretized at a better spatial resolution. CFD model was used only for the flow in the inner domain that contains both the main target building in which indoor flow is computed and the very near outdoor environment of this building. This 3D flow, meaning wind, temperature, and turbulence fields, was stored in the same format as PSWIFT. The outer domain flow was computed with PSWIFT. The dispersion was simulated by PSPRAY in both the inner and outer domains, considering the best spatial resolution fields according to each Lagrangian particle position.

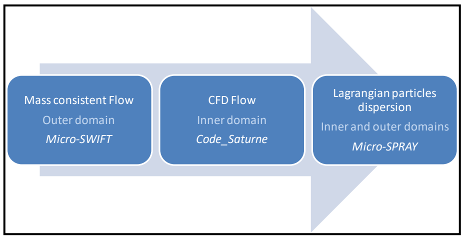

Figure 1: Indoor/outdoor coupling: workflow.

To perform this coupling, dedicated features had been developed. The standard output format of Code_Saturne is Ensight format which is not compatible with PSPRAY. This incompatibility is not only a matter of format but also of basic structure: Code_Saturne is based on a regular unstructured grid solver whereas PSPRAY requires structured wind fields as input. To deal with this issue:

- The mesh used by Code_Saturne was structured and obtained thanks to a translator tool, especially developed, that converts PSWIFT mesh (potentially topography and buildings aware) into IDEAS “unv” format which is one of the available input formats of Code_Saturne.
- A specific writer, based on PSWIFT source code, has been implemented into Code_Saturne to write the 3D field in the same format as PSWIFT.

These elements have been used successfully but lead to the three following limitations. Using regular structured grids for Code_Saturne is a significant decline. It implies a projection of obstacles (buildings) on the grid instead of cells relying on exact obstacles geometry and it makes difficult to increase spatial resolution in specific zones. The second limitation is the use of a specific version of Code_Saturne and not a standard one because of the writers. This increases the amount of work to manage the maintenance and update of the whole chain and decreases the portability of the solution. The last limitation concerns the flow itself. Code_Saturne modeling on the inner domain is initialized with data from the outer domain of PSWIFT. There is no feedback from the inner domain to the outer domain and the impact of buildings on the flow (recirculation zone, wake zone, etc) may be discontinuous around the two domains.

The nesting capability of PSPRAY was initially developed for the coupling. It was limited to two nesting levels and only one domain per level. The very first version of this feature is now generalized in PSPRAY. It is possible to consider several levels and several domains per level. Spatial parallelization is also compatible with this generalized nesting but limited to the deeper level. It has been notably successfully used, sometimes with Code_Saturne flow coupling, in downscaling system (Oldrini et al. (2016)) or for Jack Rabit II validation that implied multiple length scale (Gomez et al., 2021).

PRELIMINARY DESCRIPTION OF THE COUPLING

We present our new approach to the coupling between Code_Saturne and PMSS. For the example, the building of interest is the "Gare du Nord" in Paris (France). The weather is stationary although a succession of stationary states could have been considered. The buildings seen by Code_Saturne and PMSS are identical. A simplified 3D geometric model for the neighborhood of Gare du Nord is created using ArcGIS and then SALOME pre-processor for Code_Saturne. This geometry is discretized with a 3D unstructured grid shown in Figure 2 (left panel), which consists of 441,953 tetrahedral elements with a maximum mesh size of $25m$. The mesh size is $10m$ for elements touching the ground and further refined to $5m$ for elements on the exterior wall of Gare du Nord and $2.5m$ for elements on the interior. Elements near the 6 entrances on the facade have a small mesh size of $0.5m$ to accurately capture the air flow into the station.

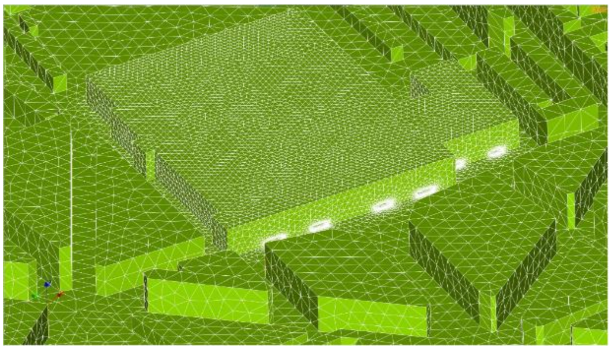
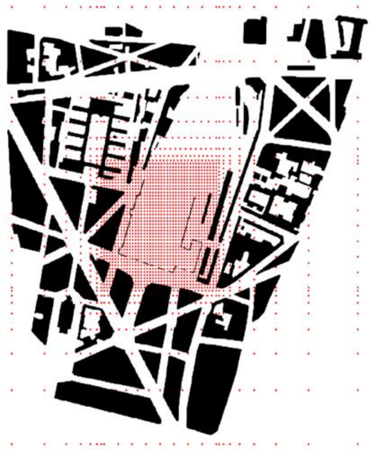

Figure 2: Simplified 3D geometry around Gare du Nord and 3D unstructured mesh generated with SALOME (left). Horizontal locations of vertical profiles extracted from the Code_Saturne simulation (right).

A steady-state 3D CFD simulation is performed on this grid using Code_Saturne, an open-source, general-purpose, finite-volume-based, unstructured CFD solver which solves the Navier-Stokes equations coupled with turbulence models. The standard 2-equation $k - \varepsilon$ turbulence model (Launder and Spalding, 1974) is used for this study with a 2-scale log law wall function. The incoming wind is at 240° south-west with a magnitude of $3.485m/s$ at $z = 10m$. An inlet boundary condition is assigned to the south, west and roof boundary faces with prescribed vertical profiles of velocity, temperature, turbulent kinetic energy (TKE) and turbulent kinetic energy dissipation rate (ε) that correspond to a neutral meteorological condition of Pasquill stability class D. Advective zero-gradient outlet boundary condition is assigned to the north and east boundary faces, and the ground (including all buildings) is modeled as rough walls with a characteristic roughness of $0.1m$. Gravity and Coriolis force are both neglected.

There are two points to emphasize here about the coupling. Once a steady-state solution is obtained in Code_Saturne, flow variables are extracted in the form of vertical profiles which are then used as initialization data for the mass-conserving PSWIFT solver. In order not to degrade the flow calculated by Code_Saturne, we avoid the creation of analytical zones around the buildings for the creation of recirculation zones, wakes or street canyons. This is an important difference with the standard way of using PSWIFT and is possible because the flow is forced by Code_Saturne. For this new coupling, PSWIFT interpolates the turbulence estimated by Code_Saturne. This also avoids double counting of turbulence. In this study, 40×40 vertical profiles are extracted within a $300m \times 300m$ square region surrounding Gare du Nord to recover detailed flow features near the station. As we move further away from Gare du Nord, the distance between two profiles becomes larger with an expansion ratio of 1.5. A total of 2435 vertical profiles are extracted. Figure 2 (right panel) shows the locations on the X-Y plane of all extracted profiles marked by red dots.

PSWIFT RESULTS

A nested PSWIFT approach is tested in the current study in order to allow enhanced grid resolution in the region of interest (RoI). The inner domain in the current study is defined by a $300m \times 300m$ square surrounding Gare du Nord with a grid resolution of $1m \times 1m$ instead of $2m \times 2m$ which corresponds to the grid resolution outside the RoI. In the context of nested PSWIFT approach, the outer domain is denoted by Nest 1 and the RoI by Nest 2 (Nest 2 $\subseteq$ Nest 1).

In Figure 3, we compare the velocity field around Gare du Nord computed by PSWIFT in Nest 1 with the original Code_Saturne solution. This comparison shows that, by initializing PSWIFT with vertical profiles extracted from the CFD solution, the mass-conserving PSWIFT manages to recover satisfactorily the original velocity field from the CFD simulation. Flow features such as convective acceleration, flow separations, vortices, etc. are observed in the PSWIFT simulation which are impossible to capture without solving the momentum equations. We observe that the solution in Nest 2 remains globally consistent with the solution in Nest 1 with slight improvement in regions where strong velocity gradients are present (e.g., immediately in front of Gare du Nord) when compared with the Code_Saturne solution. The similarity between the two grid resolutions is important since it implies that the numerical methods in PSWIFT is consistent and that we can expect a minimal level of discontinuity across nest boundaries when using this velocity field for dispersion modeling in PSPRAY.

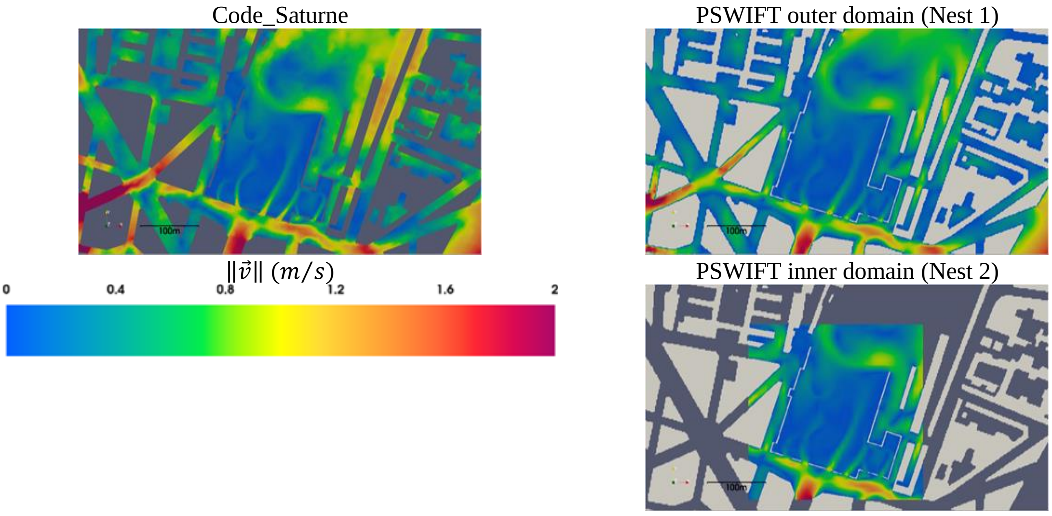

Figure 3: Velocity field comparison between Code_Saturne and PSWIFT at 2m above ground.

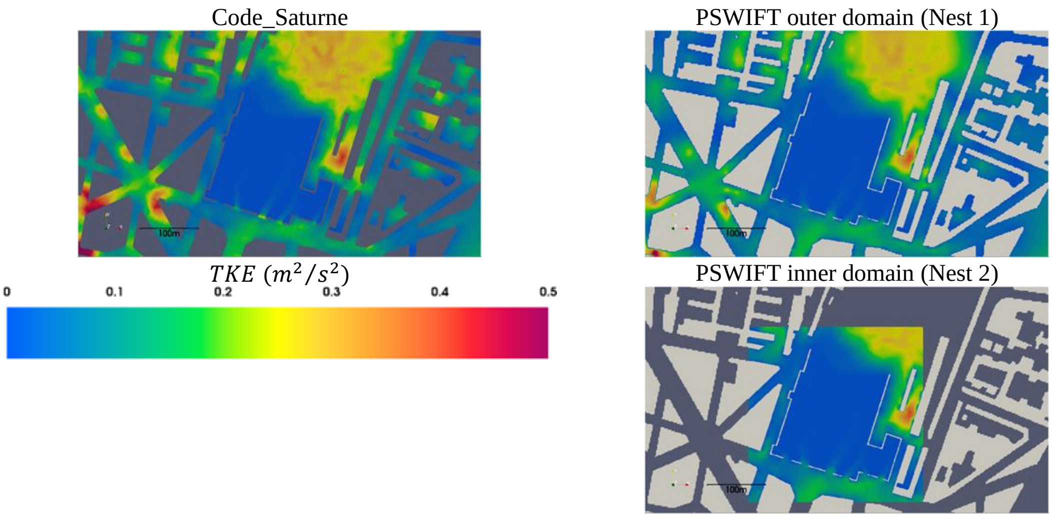

Figure 4: TKE field comparison between Code_Saturne and PSWIFT at 2m above ground.

The same analysis is also performed on the turbulence kinetic energy (TKE) field. As shown in Figure 4, PSWIFT recovers the TKE field from Code_Saturne which is obtained by solving the two-equation $k - \varepsilon$

turbulence model. In the presence of Gare du Nord, the PSWIFT simulation in Nest 1 reproduced the increase in TKE due to air inflow from the southern façade, as well as the highly turbulent wake region in the north. This level of detail is only made possible for PSWIFT by coupling with a Navier-Stokes solver with turbulence modeling capabilities. The TKE field remains consistent from Nest 1 to Nest 2.

PSPRAY RESULTS

The flows obtained in the two nests with the PSWIFT model forced by Code_Saturne are then used by the Lagrangian particles dispersion model PSPRAY. Two stationary releases of a neutral gas are considered. The first release P1 is placed outside Gare du Nord in front of the southern facade, the release P2 is placed within Gare du Nord and both sources are at $1m$ above ground. The concentration near the ground is shown in Figure 5. The numerical particles emitted from P1 enter and fill Gare du Nord by the 6 entrances in the facade following the main flow pattern. The concentration of P2 particles is at its highest level within Gare du Nord and their propagation is bounded by the solid walls. In both cases, the particles exit Gare du Nord via the northern opening and quickly dissipate into the highly turbulent wake region then propagate further downstream. The two concentration fields remain consistent from Nest 1 to Nest 2, which is the result of the grid consistency demonstrated by the PSWIFT solver as we mentioned in the previous section.

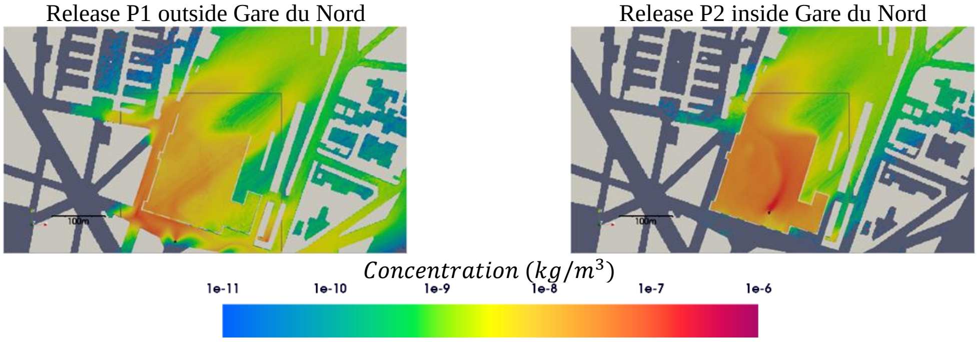

Figure 5: Dispersion modeling of releases P1 and P2 in a nested PSPRAY simulation. Positions P1 and P2 are marked by the black dot.

CONCLUSION

A coupling between PMSS and Code_Saturne had been developed to model indoor and outdoor dispersion in the surrounding neighborhoods of a building of interest. In this work, we have detailed the limitations to the historical implementation of the coupling and an update is suggested. This one benefits from the standard versions of PMSS as well as Code_Saturne. It requires no development other than an extraction of vertical wind and turbulence profiles from Code_Saturne. Note that the impact of buildings on the flow is not analytically described in PSWIFT, since it is already considered by Code_Saturne. The turbulence in the two nested domains is an interpolation of the one calculated by Code_Saturne. This new coupling shows no discontinuity at the interface between the inner domain, historically modeled by Code_Saturne, and the outer domain modeled by PSWIFT. The dispersion with PSPRAY finally shows that a plume can easily enter and leave a train station without having to estimate the building's air exchange rate.

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