23rd International Conference on
Harmonisation within Atmospheric Dispersion Modelling
for Regulatory Purposes
15-19 September 2025, Hamburg, Germany

EXTENDED ABSTRACT

High-Resolution Urban Atmospheric Modeling Using PALM4U Coupled With MOLOCH: Toward the Development of a Digital Twin for Cities

Lippin Pauly[1], Tony Christian Landi[1], Francesca De Santi[2], Rita Cesari[1], Fabrizio Roccato[1], Tommaso Sorgente[2], Oxana Drofa[1], Silvia Trini Castelli[1]

[1] CNR - Institute of Atmospheric Sciences and Climate (ISAC)
[2] CNR - Institute for Applied Mathematics and Information Technologies (IMATI)

Abstract:
As part of the Urban Intelligence Science Hub (UISH) project, a high-resolution urban modelling framework has been developed to support the creation of digital twins of Italian cities, with Catania selected as a pilot site. The system integrates the regional-scale meteorological model MOLOCH with the building-resolving LES model PALM4U through an offline nesting approach, enabling the transfer of synoptic variability down to the urban canopy scale.
A heatwave event in July 2023, coinciding with a Saharan dust intrusion and elevated PM concentrations, was simulated to demonstrate the system's potential. Three PALM4U domains with resolutions of 40 m, 10 m, and 2 m were nested within MOLOCH, reproducing key features of Catania's urban microclimate. Preliminary results highlight the ability to capture neighbourhood-scale contrasts in temperature, ventilation corridors, and pollutant hotspots. This work demonstrates the feasibility of the MOLOCH–PALM4U coupling as a tool for high-resolution urban climate and air-quality studies. Beyond the Catania case, the framework supports the development of digital twins to inform scenario testing and mitigation strategies in Mediterranean cities.

Key words: *Digital twin cities; Urban atmospheric modeling; Large-Eddy Simulation (LES); PALM4U; MOLOCH regional model; Heatwave; PM10 dispersion.*

INTRODUCTION AND OBJECTIVES

Urban microclimates are shaped by complex interactions between synoptic weather, local morphology, and anthropogenic activities. Increasing heat stress and air pollution episodes in Mediterranean cities raise urgent needs for reliable simulations of air flow, pollutant dispersion, and thermal comfort at fine scales. Large-eddy simulations (LES) are capable of resolving the turbulent flows and recirculation phenomena that govern microclimate variability in cities, including street-canyon dynamics, flow disturbances, and thermal contrasts. However, LES models cannot operate in isolation and require realistic boundary conditions from mesoscale drivers that provide non-stationary and synoptic variability.
In Italy, the MOLOCH nonhydrostatic mesoscale model is successfully used in operational forecasting and research for severe convective events, urban meteorology, and turbulence parameterization studies (Davolio et al., 2020; Trini Castelli et al., 2020). Its integration with PALM4U offers a novel opportunity to generate urban-scale simulations rooted in an established forecasting chain. While PALM4U has been widely applied with mesoscale drivers such as COSMO and WRF, the present study represents one of the first couplings with MOLOCH, which is developed and maintained in-house at CNR. This approach ensures continuous availability of boundary conditions, adaptation to Italian-specific topography and emission patterns, and the possibility of refining source codes for targeted improvements.
This work is conducted within the "Digital Twin for Air" (DTAir) task of the Urban Intelligence Science Hub (UISH) Project at CNR. The project aims to develop dynamic urban replicas—digital twins—integrating atmospheric and environmental modelling to support decision-making. Catania was chosen as a pilot city due to its dense urban fabric, complex coastal topography, and vulnerability to heatwaves and Saharan dust episodes. The objectives of this study are to demonstrate the feasibility of the MOLOCH–PALM4U coupling, evaluate its performance in reproducing key urban processes, and highlight its potential

as a tool for digital twin development. In addition, a specific goal of this research is to develop, test, and apply an original scaling tool for the Italian territory, designed to be transferable to different urban contexts across the country.

METHODOLOGY

The modelling chain is based on CNR-ISAC operational forecast suite (GLOBO–BOLAM–MOLOCH). For this study, MOLOCH outputs at ~1.25 km horizontal resolution were used to provide meteorological initial and boundary conditions to PALM4U. Figure 1 illustrates the multi-scale downscaling approach from MOLOCH chain to PALM4U, showing the progressive refinement of resolution and the coupling between mesoscale and microscale processes. An offline coupling was implemented to drive PALM4U with meteorological fields from MOLOCH, while within PALM4U a sequence of nested domains at 40 m, 10 m, and 2 m resolution was applied to progressively refine the flow fields down to the building-resolving scale.

PALM4U, an open-source LES model developed at Leibniz University Hannover, has been widely recognised in international collaborations for its ability to simulate urban meteorology, air quality, and bio-meteorological parameters. It has been successfully validated for urban canopy flows, pollutant dispersion, and urban heat island effects (Resler et al., 2021). While PALM4U is often used with COSMO or WRF, its integration with MOLOCH offers unique advantages: boundary conditions that are natively consistent with CNR operational forecast chain, improved adaptation to Italian orography and emission inventories, and the flexibility to customise the coupling within an in-house modelling environment. The static driver for PALM4U was generated from OpenStreetMap building and road data, complemented with land-cover classifications suitable for urban applications. The RRTMG radiation scheme was applied to account for radiative fluxes, while a Synthetic Turbulence Generator was used to produce realistic turbulent inflow conditions. Pollutant emissions were parameterised based on traffic intensity and mapped onto the street network. For this study, the PALM4U chemistry module was activated in passive mode, allowing the transport and dispersion of PM10 to be simulated as a tracer. This configuration accounted both for anthropogenic emissions and for the Saharan dust contribution during the event.

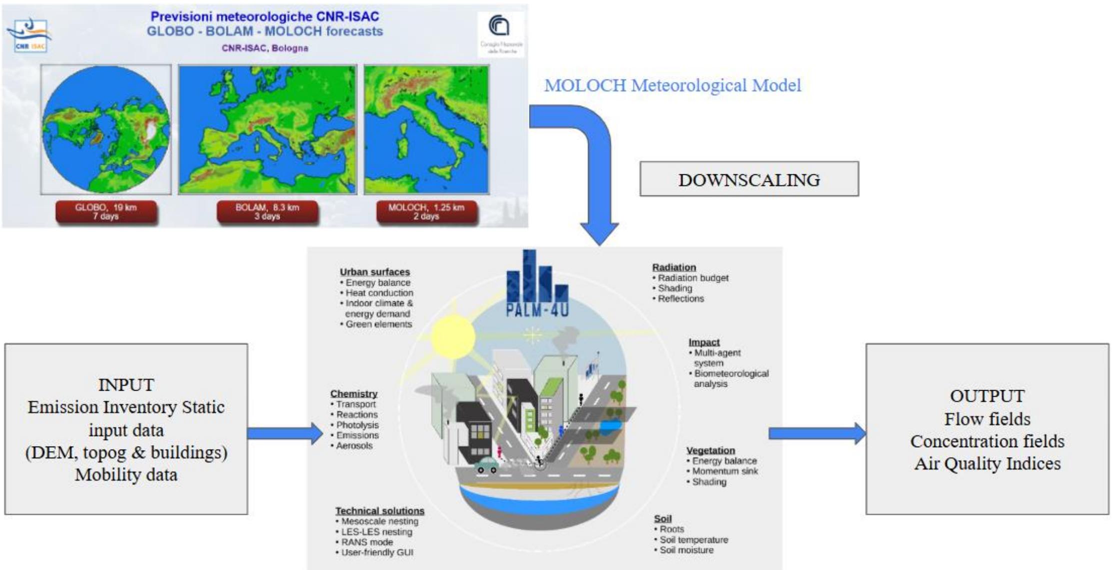

Figure 1. Schematic representation of the downscaling approach from MOLOCH to PALM4U.

RESULT AND DISCUSSION

The coupled MOLOCH–PALM4U system was applied to Catania for a six-hour simulation beginning at 03:00 local time on 23 August 2023. This period coincided with a severe heatwave and a Saharan dust intrusion, leading to exceptionally high background concentrations of PM10.

The horizontal and vertical temperature fields reveal pronounced spatial variability across the city as shown in Figure 2 and 3. Hotspots correspond to areas of limited ventilation and high building density, illustrating the model's capacity to reproduce intensified urban heat island effects. Wind simulations highlight the crucial role of urban morphology in shaping local circulation (Figure 4). PALM4U captured channelling along major transport corridors, stagnation in enclosed courtyards, and recirculation within complex canyon geometries. Such detailed structures are essential for assessing ventilation efficiency and for evaluating mitigation strategies such as ventilation corridors or urban greening.

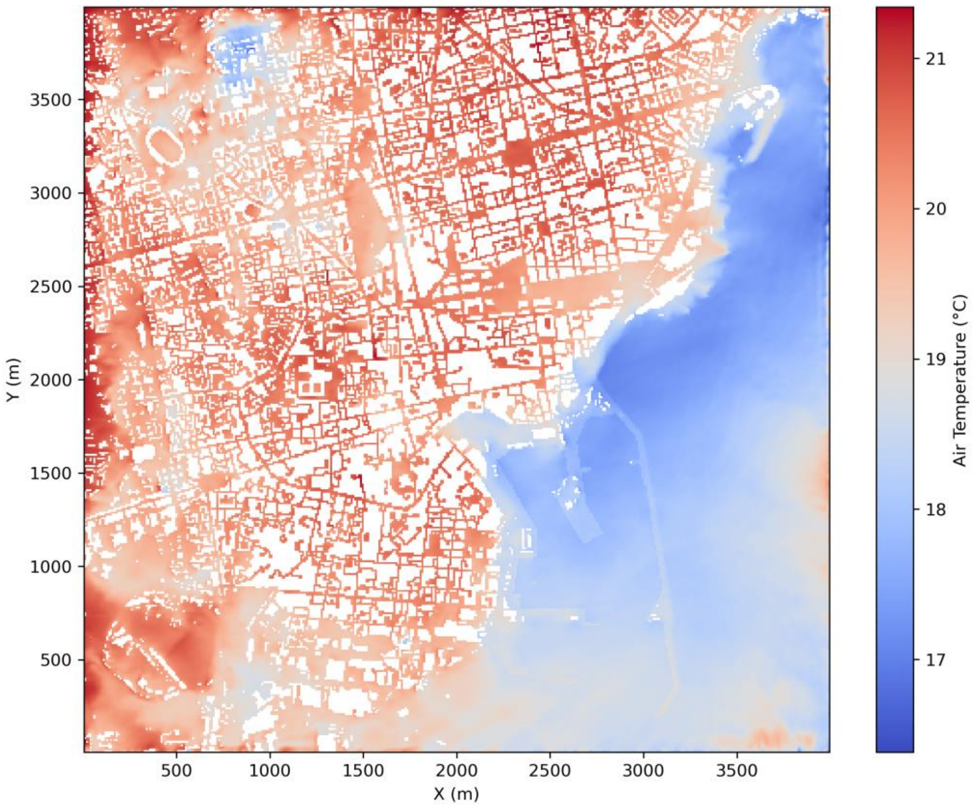

Figure 2. Simulated near-surface air temperature (15m agl) for Catania during the 23 August 2023 at 4 am

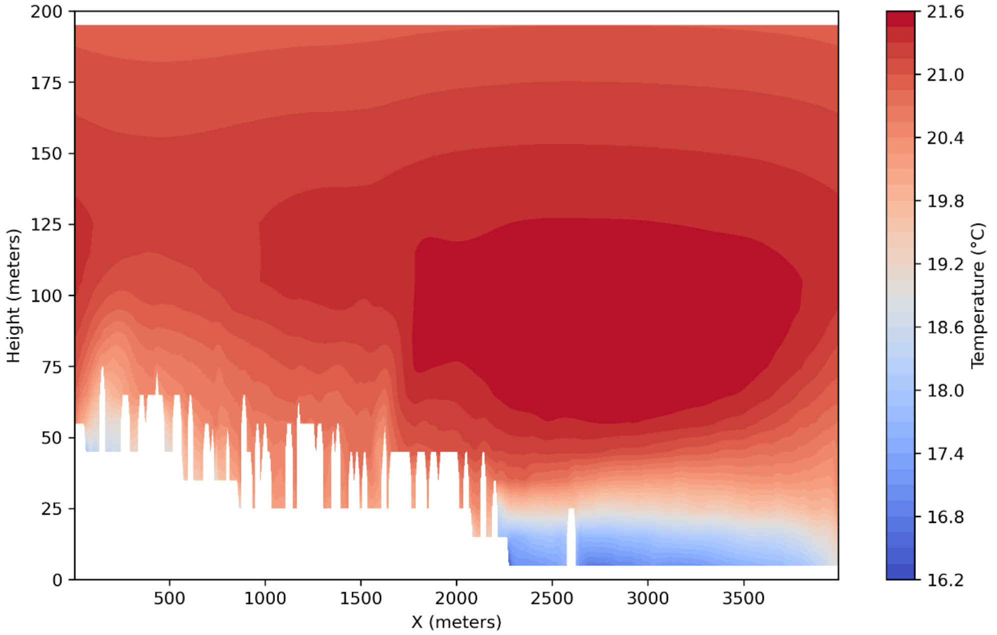

Figure 3. Simulated air temperature (at section y=1335 m) for Catania during the 23 August 2023 at 4 am

Dispersion results were evaluated in a separate PALM4U test run in which cyclic boundary conditions were applied to the meteorological fields. This configuration allowed the passive tracer module to be tested independently of the mesoscale–microscale coupling. As shown in Figure 5, the simulation reproduced reasonable pollutant accumulation patterns, with elevated concentrations along major traffic corridors and hotspots in poorly ventilated districts. While synoptic-scale dust transport was not included in this setup, the experiment confirmed the ability of PALM4U to represent fine-scale dispersion of traffic-related PM10 when parameterised through road-type emissions. This tracer test provides a foundation for extending the coupled MOLOCH–PALM framework toward full multi-scale air-quality applications.
Beyond reproducing individual fields, the system demonstrated the benefits of multi-scale coupling: MOLOCH provided realistic synoptic forcing, while PALM4U resolved fine-scale canopy flows and pollutant patterns. This integration offers a physically consistent basis for urban digital twins, enabling scenario testing under different meteorological and emission conditions. The results confirm that the coupled framework is not only a research tool but also suitable for operational applications to support urban planning, climate adaptation, and air-quality management.

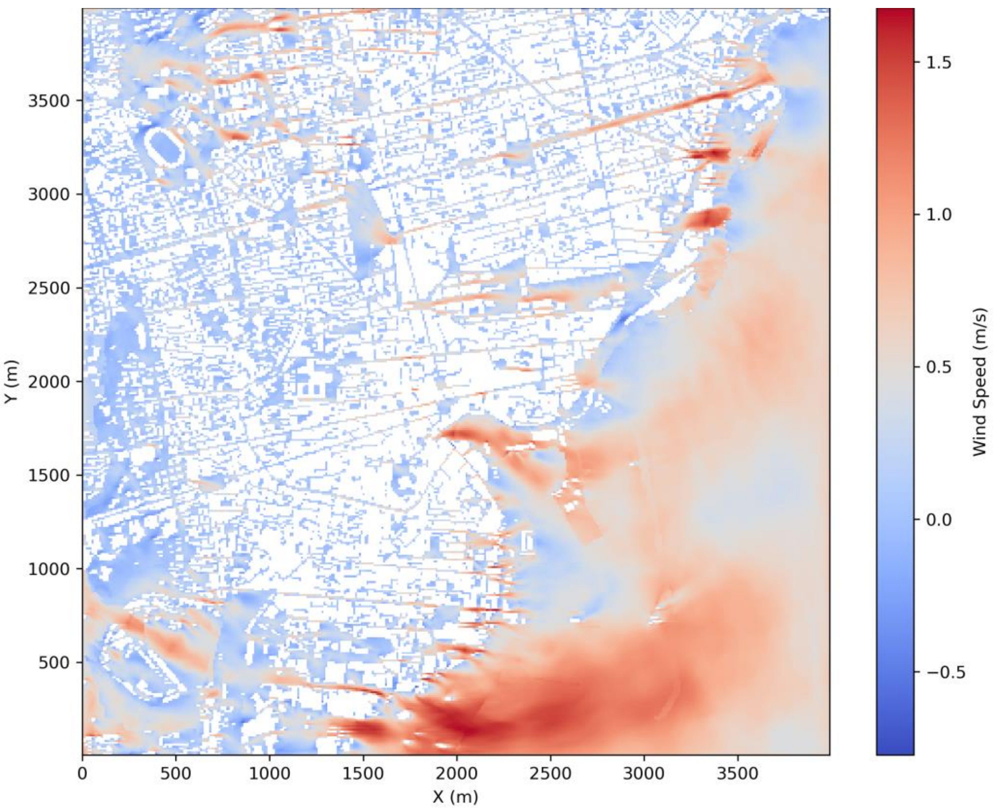

Figure 4. Simulated windspeed (at 10m agl) for Catania during the 23 August 2023 at 4 am

CONCLUSION AND RELEVANCE

This study has demonstrated the successful coupling of MOLOCH and PALM4U as a multi-scale framework for urban climate and air-quality applications. Using Catania as a pilot case, the system reproduced essential features of the urban microclimate during an extreme heatwave and Saharan dust event, including neighbourhood-scale thermal contrasts, ventilation patterns shaped by building morphology, and pollutant accumulation in poorly ventilated districts. The results confirm that harmonised mesoscale–microscale modelling can provide physically consistent and operationally relevant information, bridging the gap between synoptic meteorology and building-resolving simulations. By leveraging MOLOCH's established role in Italian forecasting together with PALM4U's advanced LES capabilities, the approach is tailored to national conditions while contributing to international efforts on model inter-comparison and harmonisation.

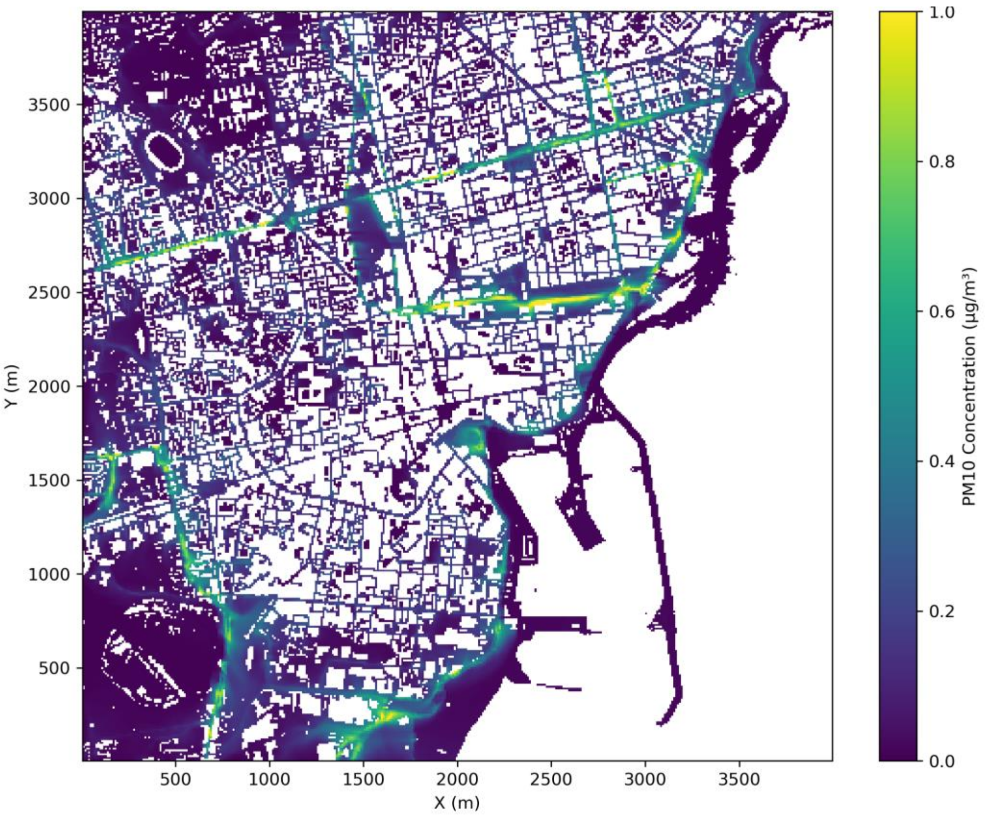

Figure 5. Simulated PM10 concentration (at 2m agl) from a standalone PALM4U tracer test, for Catania during the 23 August 2023 at 6 am

Beyond scientific advances, the framework directly supports the development of urban digital twins, enabling scenario testing for climate adaptation, air-quality management, and sustainable city planning. As such, it aligns with the overarching goals of the HARMO community: to promote robust, interoperable modelling systems that can serve both research and regulatory needs.

ACKNOWLEDGEMENT

This work was carried out as part of the Urban Intelligence Science Hub (UISH) initiative by the National Research Council of Italy (CNR) , with support from ISAC, IMATI, and local authorities in Catania. The authors thank the developers of PALM4U and acknowledge the support of the CINECA HPC facilities used during model development and testing.

REFERENCES

Davolio, S., M. Mazzetti, A. Moscatello, F. Siccardi, A. Boni, F. D'Andrea and G. Piana, 2020: The Piedmont flood of November 1994: a testbed of forecasting capabilities of the CNR-ISAC meteorological model suite. Bull. Atmos. Sci. Technol., 1(3), 263–282.

Resler, J., M. Belda, P. Krč, M. Eben, M. Benešová, T. Vlček, L. Derbek, A. Maronga, B. Kanani-Sühring, F. Ketelsen and S. Sühring, 2021: Building-resolving urban modelling with PALM: Evaluation in Prague-Dejvice. Atmosphere, 12(5), 620.

Trini Castelli, S., D. Anfossi, G. Tinarelli, M. Martilli, L. Mortarini and L. Brusasca, 2020: Evaluation of the turbulence parametrization in the MOLOCH meteorological model. Q. J. R. Meteorol. Soc., 146(726), 124–140.