



**Barcelona
Supercomputing
Center**

Centro Nacional de Supercomputación

Physics-Constrained Deep Learning for Downscaling Atmospheric Chemistry Simulations

The Role of Auxiliary Forcings and
Model Architecture

EGU General Assembly - May 2026

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The Need for High-Res Air Quality Data

Problem

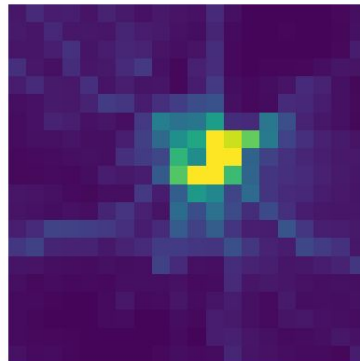
Current operational forecasts of air pollutant **too coarse** (10km).

- Chemical Transport Models (CTMs) too computationally expensive.

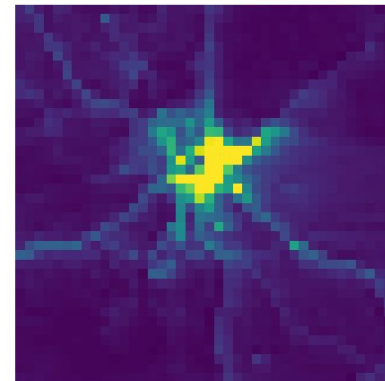
Our approach

- Produce training data by running CTM at both 10km (LR) and 5km (HR) resolution.
- **Train neural network** to learn LR \rightarrow HR.
- Ensure physically meaningful results through:
 - **Hard constraints** (mass conservation, inter-variable relations)
 - Conditioning on **auxiliary data** (e.g., meteo, emissions, topography)

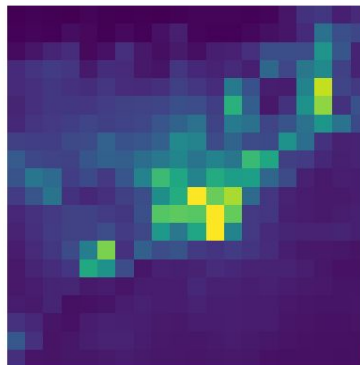
Madrid - NO2 at 10km



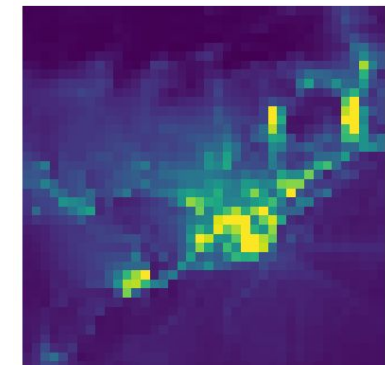
Madrid - NO2 at 5km



Barcelona - NO2 at 10km




Barcelona - NO2 at 5km



Dataset and Problem Setup

Training data:

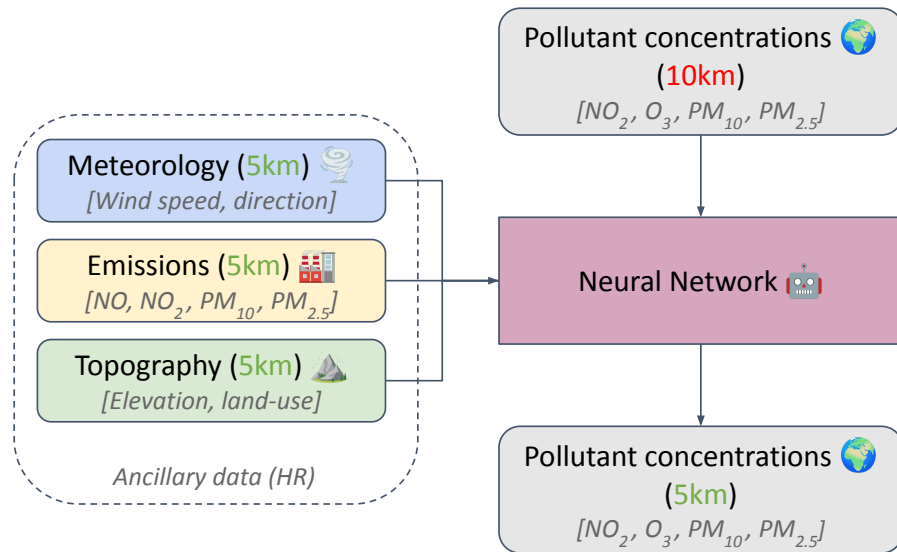
- CTM: MONARCH (in-house)
- Domain: Iberian Peninsula 
- Period: 2021-2023 (hourly)
- Size: ~72,000 paired samples

Inputs:

- **Pollutant concentrations** (LR) – NO_2 , O_3 , PM_{10} , $\text{PM}_{2.5}$
- **Meteorology** (HR) – Wind speed, Wind direction
- **Emissions** (HR) – NO , NO_2 , PM_{10} , $\text{PM}_{2.5}$
- **Topography** (HR) – Elevation, Land-use


Targets:

- **Pollutant concentrations** (HR) – NO_2 , O_3 , PM_{10} , $\text{PM}_{2.5}$



Dataset and Problem Setup

Training data:

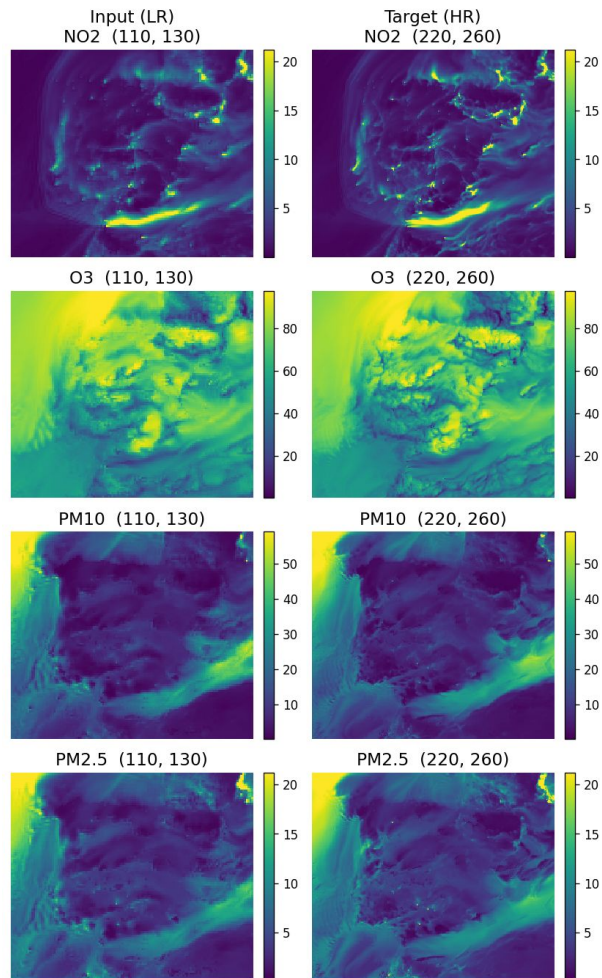
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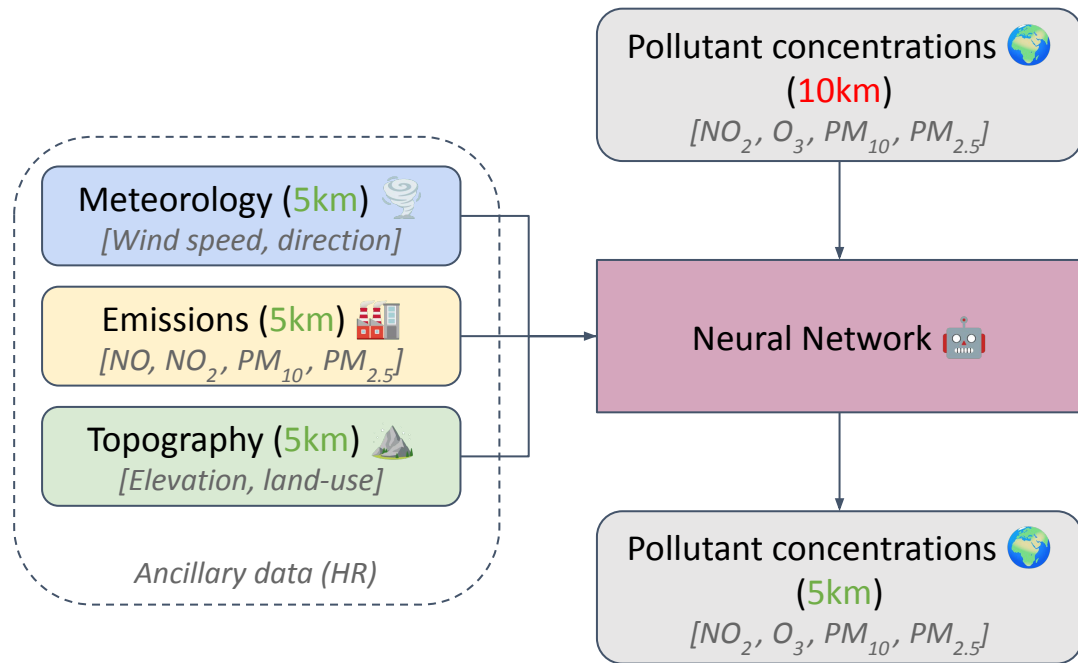
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Dataset and Problem Setup



Key Insight: This is Not Image Super-Resolution

The Structural Mismatch Problem

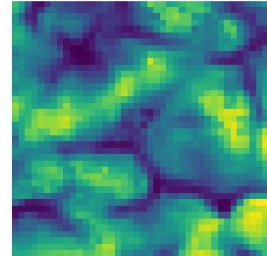
LR and HR simulations use **different resolution forcings** – so they are **qualitatively different fields**, not just blurry/sharp versions of each other.

- LR run: valleys / hotspots smoothed out
- HR run: fine spatial structure present

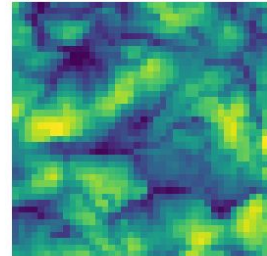
Implication: No 1-to-1 pairing: same boundary conditions
≠ same field

Our approach: Decompose into two sub-problems

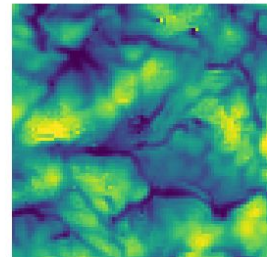
LR (110 x 130)



HR-pooled (110 x 130)

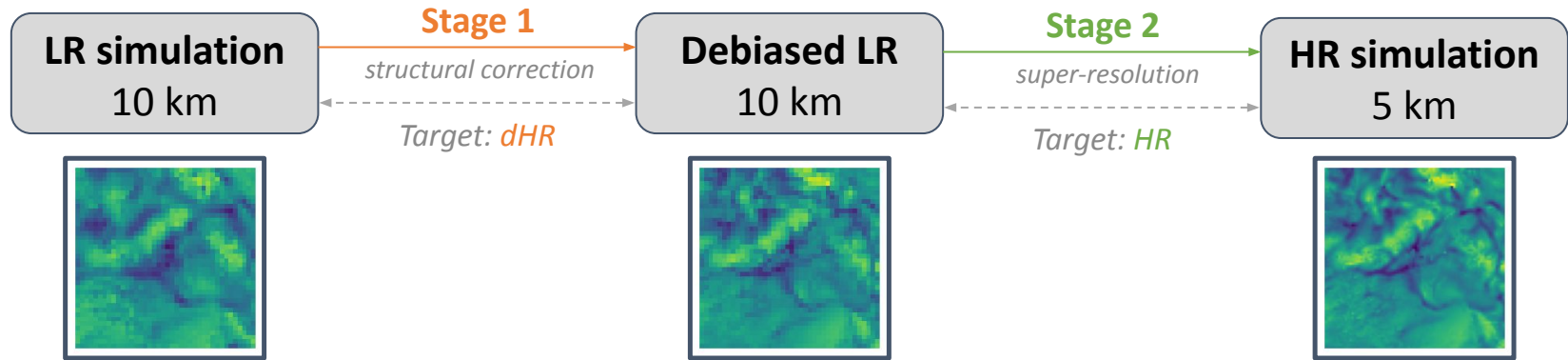


HR (240 x 280)



Problem Decomposition

Break the problem into two subproblems:



Results: Super-Resolution (Step 2)

Architectures explored:

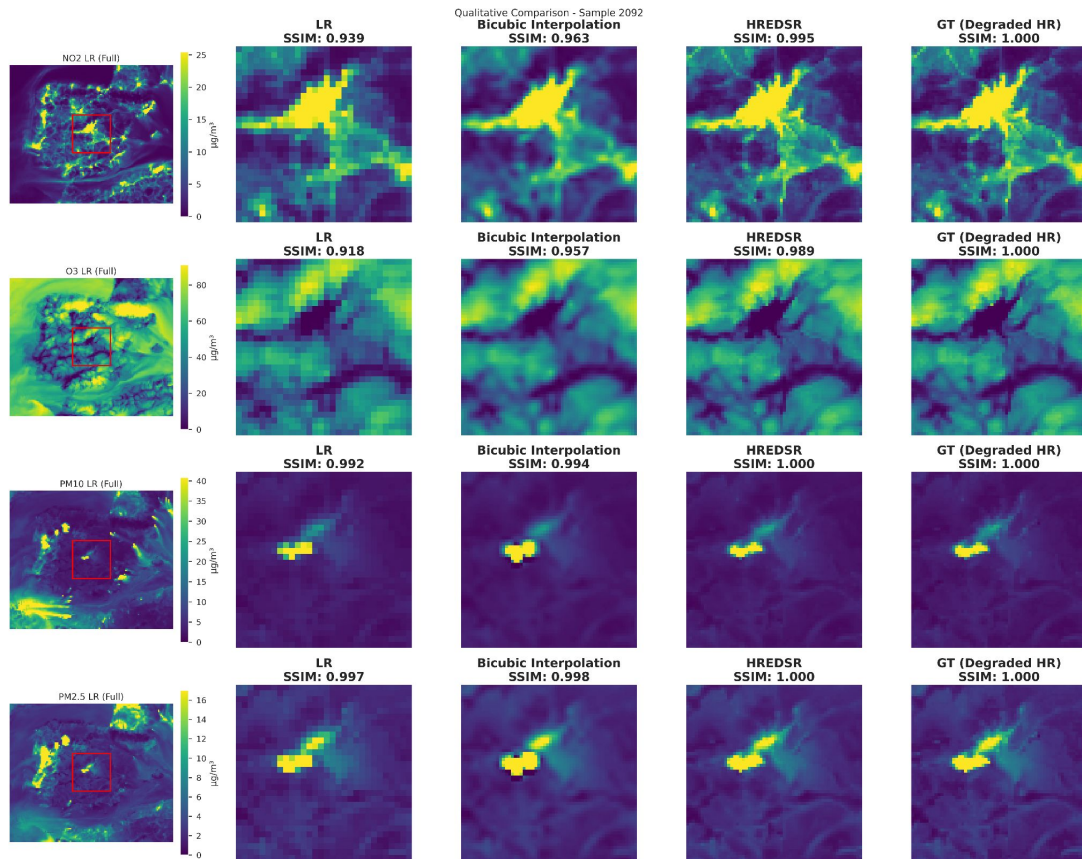
Bicubic (baseline), MLP, CNN, EDSR, RCAN, HREDSR (ours)

Best result: HREDSR + multcl

- SSIM = 0.992
- nRMSE = 4.9%
- Nearly indistinguishable from ground truth

Key findings:

1. **Physical constraints** are effective regularizers.
2. **Residual learning** > direct learning



Results: Super-Resolution (Step 2)

Architectures explored:

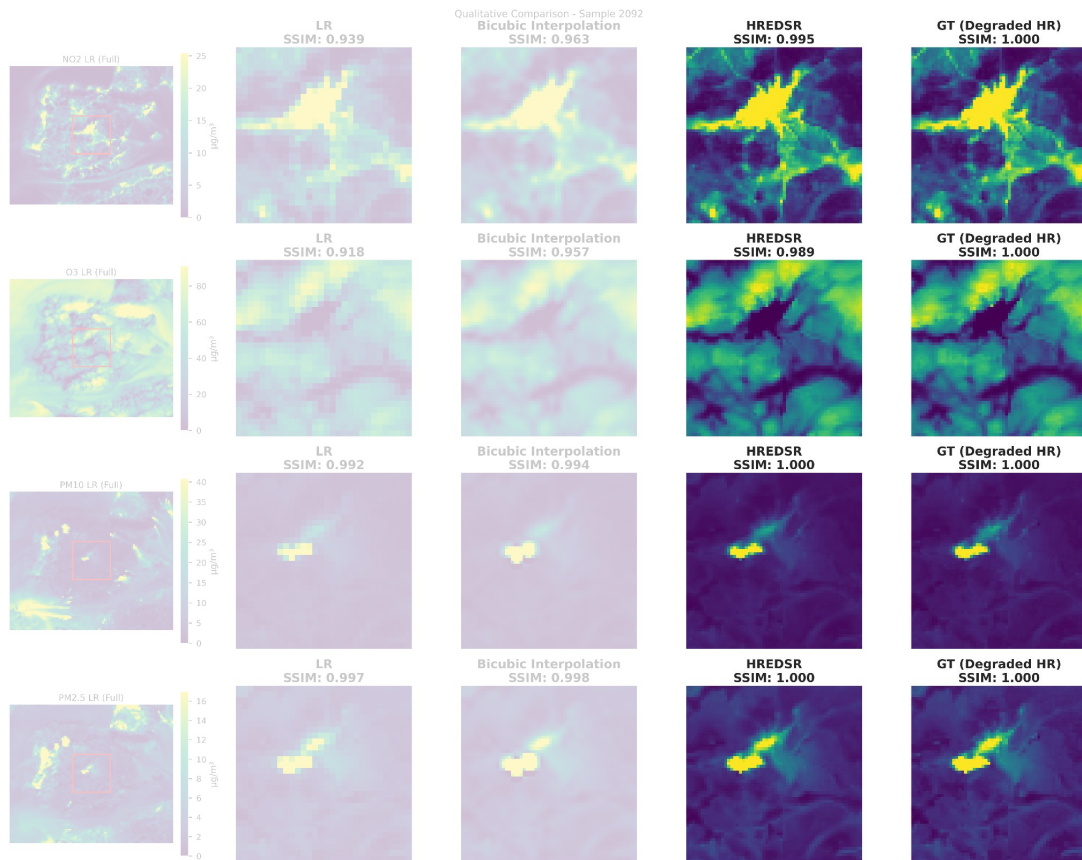
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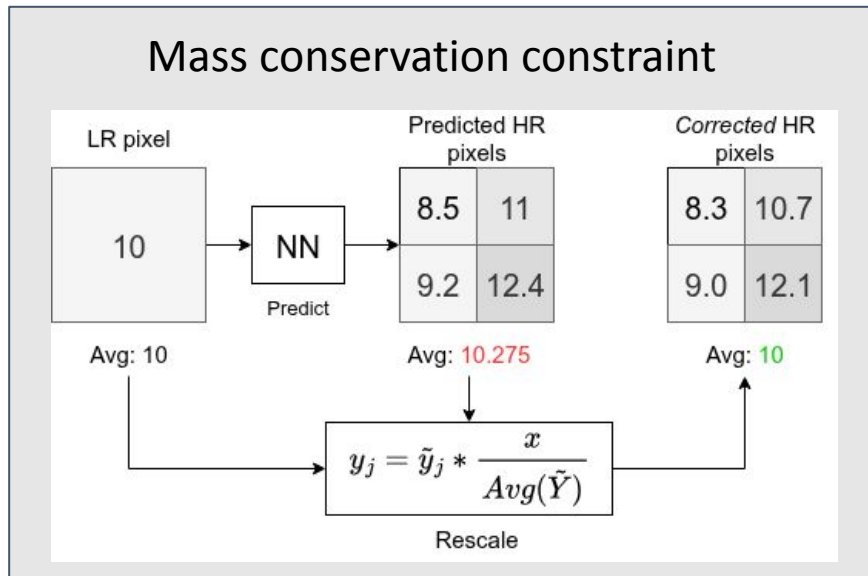
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Key findings:

1. **Physical constraints** are effective regularizers.
2. **Residual learning** > direct learning



Results: Structural Correction (Step 1)

The challenge:

- No perfect 1-to-1 pairing of LR \leftrightarrow dHR fields
- Same boundary conditions can lead to **different spatial structures** depending on simulation history
- Inherently a **many-to-many** relationship

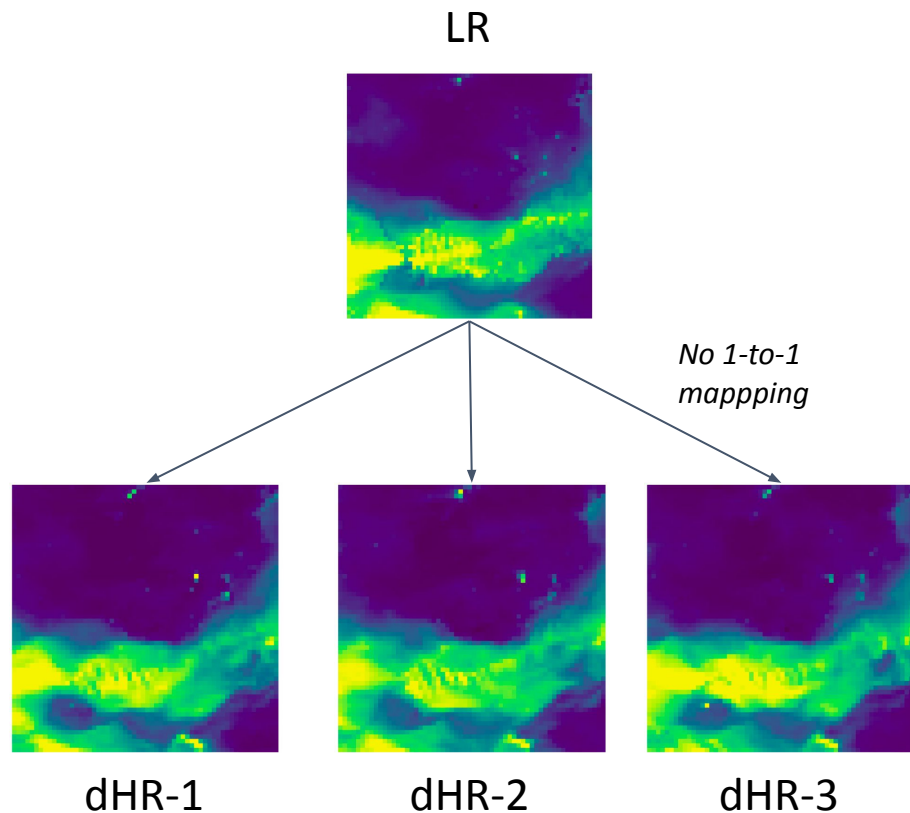
→ Deterministic models are fundamentally limited here (*oversmoothing*)

Solution: conditional generative models

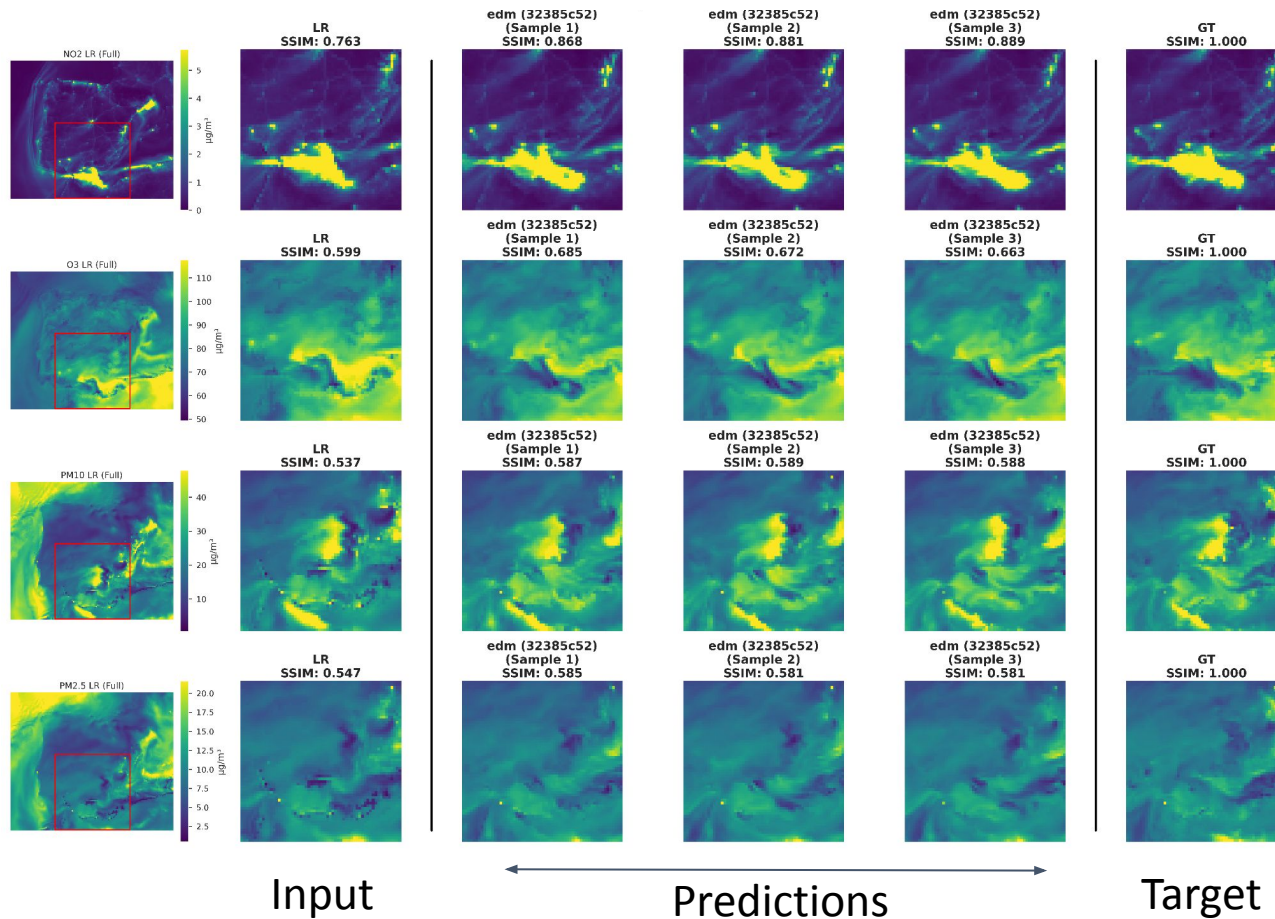
Architectures evaluated:

Deterministic (HREDSR), GAN, Flow Matching, DDIM-diffusion, **EDM-diffusion (best)**

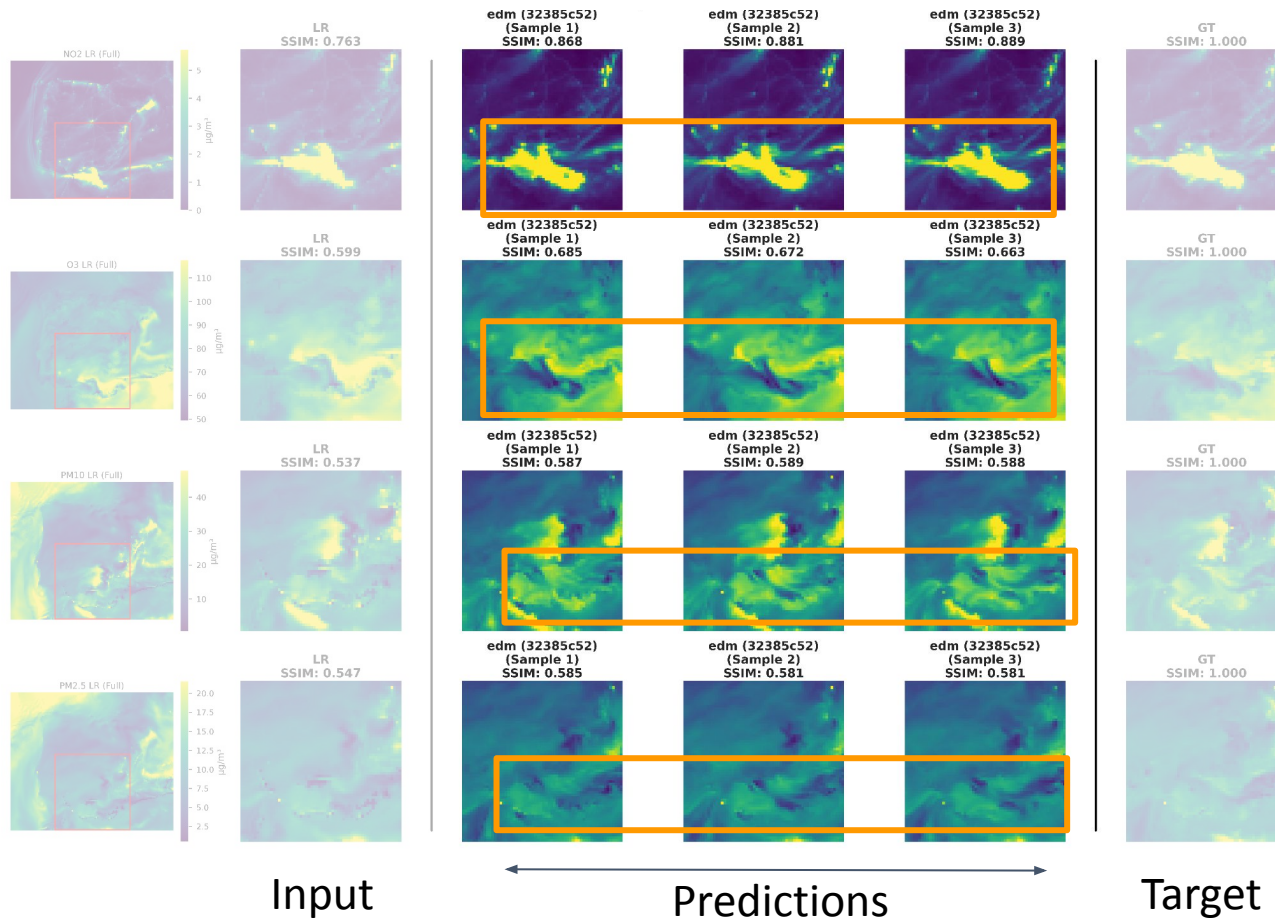
- CRPS: 1.18, nRMSE 27.23%



Results: Structural Correction (Step 1)



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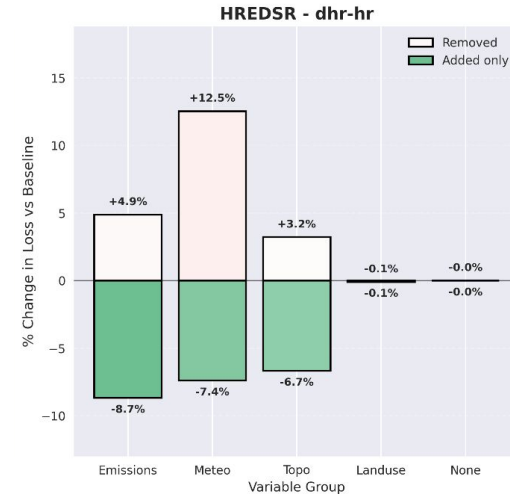
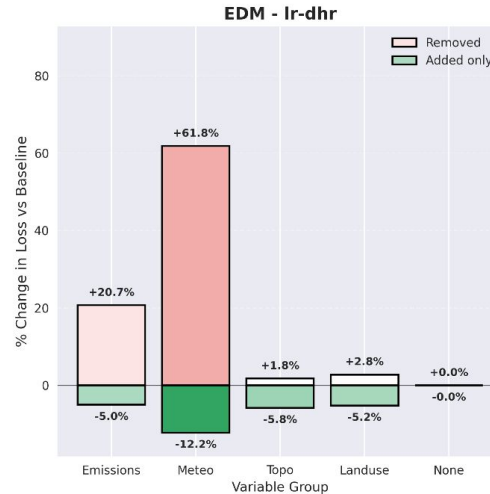


What Actually Helps? Role of Auxiliary Forcings

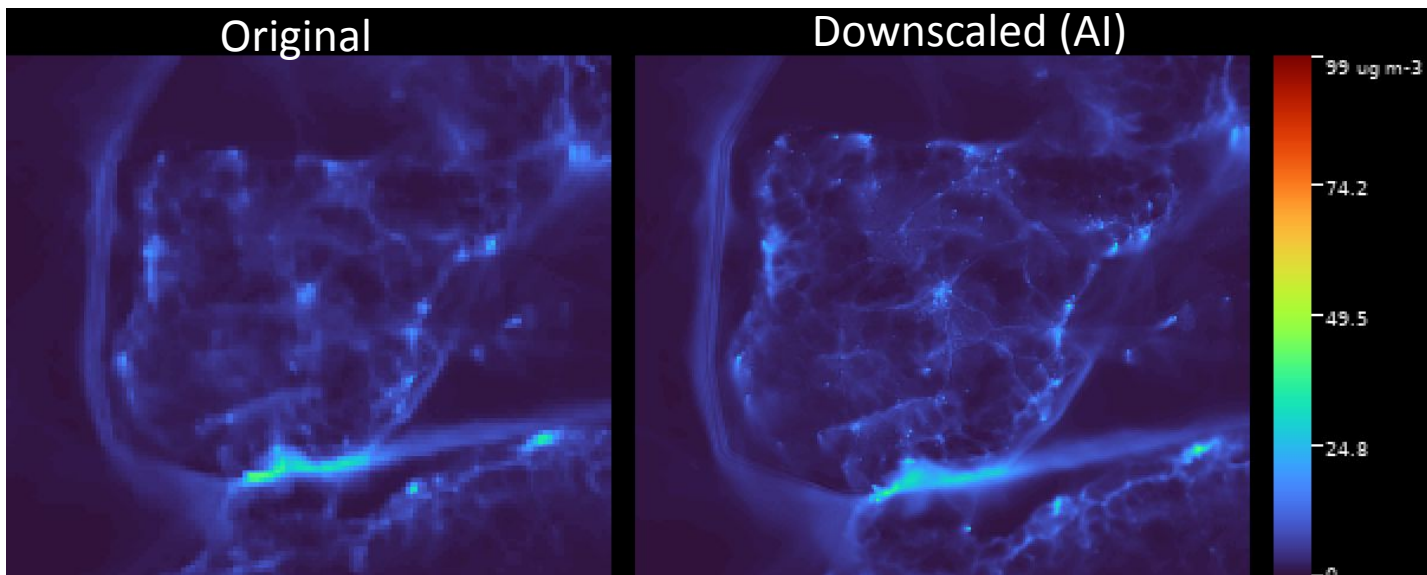
Ablation study: remove/add one group of auxiliary variables at a time (for both stages).

Importance:

1. **Meteorology** – Wind drives transport and dispersion of pollutants: dominant effect for all species
2. **Emissions** – Especially for NO_2 (near-source species); less so for O_3 and PM_{10}
3. **Elevation** – Helps when added *alone*. Otherwise already captured by meteo.
4. **Land use** – Minimal benefit. Likely redundant



Thank you



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1. *The work is part of the R&D project **AIRE**, funded by the grant "Proyectos de Investigación en el Ámbito de la Inteligencia Artificial – 2025", Grant AIA2025-163866-C21 funded by MICIU/AEI/10.13039/501100011033.*
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3. *This project is part of the **Recovery, Transformation and Resilience Plan** (Plan de Recuperación, Transformación y Resiliencia, PRTyR) funded by the European Union - NextGenerationEU)"*
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Other findings

1. SR models can be **much simpler than emulators** -- you only need to learn diffusion of aerosols, which is a much simpler process than learning complex temporal dynamics and interactions between variables.
2. **Physical constraints** (e.g., mass conservation, $PM_{2.5} < PM_{10}$) are effective regularizers that improve performance across the board (i.e., different model complexities).
3. **Univariate models only marginally better than multivariate models** (does not justify the increased computational cost and complexity).
4. **Two-stage pipeline** better than one-stage pipeline -- EDM-HREDSR combination best balance between CRPS and RMSE.

BACKUP



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