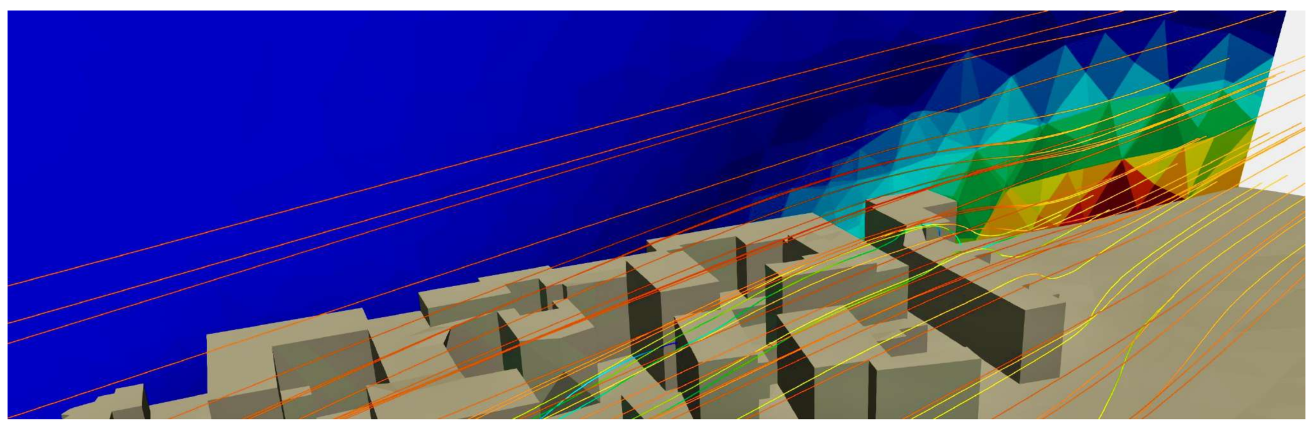
ROM for Large-scale Modelling of Urban Air Pollution

Moaad Khamlich [1], Giovanni Stabile [1], Gianluigi Rozza [1], László Környei[2], Zoltán Horváth[2]

[1] Mathlab, Mathematics Area, International School of Advanced Studies (SISSA), Trieste, Italy
[2] Széchenyi István University, Department of Mathematics and Computational Sciences, Gyor, Hungary

Introduction

In this work, we introduce a **reduced order model (ROM)** to describe the evolution of urban air pollutants. The underlying model is the transport-diffusion equation, where the convective field is given by the solution of the Navier-Stokes equation, and the source term is an empirical time series.
We developed a hybrid technique based on **POD with interpolation (POD-I)** coupled with Galerkin Projection (POD-G) in order to preserve the advantages of both approaches. Our data-driven method exploits a feedforward neural network to recover nonintrusively the convective reduced-order operator needed for the online evaluation.



Streamlines of the velocity and a cross section of the concentration field.

Problem Formulation

The **transport-diffusion equation** is a linear partial differential equation, which takes the form:

$$\frac{\partial c}{\partial t} - \nu \Delta c + \nabla \cdot (\mathbf{u} c) = f; \tag{1}$$

where $c(\mathbf{x}, t) : \mathbb{R}^n \times [0, +\infty) \to \mathbb{R}$ is the unknown function, which can be thought of as the concentration of a pollutant such as NO_2.
Specifically, the quantity $c(\mathbf{x}, t)dV$ represents the mass present at time t in an infinitesimal neighborhood of the point $\boldsymbol{x}$. Consistently, the mass of pollutant present in volume V at time t is given by :

$$\int_V c(\boldsymbol{x}, t) dV. \tag{2}$$

The term "$\nabla \cdot (\mathbf{u}c)$" models the convective transport effect, that is, the transport of the pollutant due to the motion of the fluid in which it is immersed.

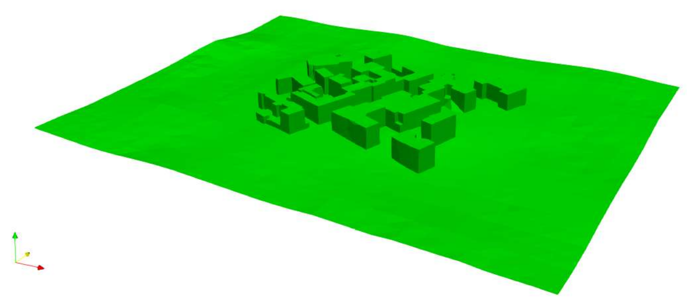
In particular, since we are working within the turbulent regime, we considered the steady **Reynolds Averaged Navier-Stokes** (RANS) equations:

$$\begin{cases} \nabla \cdot (\overline{\mathbf{u}} \otimes \overline{\mathbf{u}}) - \nabla \cdot 2(\mu_L + \mu_T) \nabla^{\mathbf{s}} \overline{\mathbf{u}} = -\nabla \overline{p} & \text{in } \Omega \times [0, T] \ , \\ \nabla \cdot \overline{\mathbf{u}} = \mathbf{0} & \text{in } \Omega \times [0, T] \ . \end{cases} \tag{3}$$

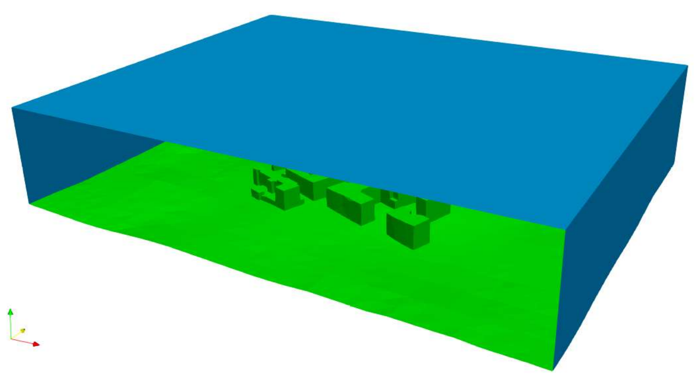
The eddy viscosity μ_T needs then an appropriate turbulence model. For the present work, we used the **k-ϵ model**, which consists in adding two PDEs describing the transport of turbulent kinetic energy (k) and turbulent kinetic energy dissipation rate (ϵ).
In addition, we consider the following boundary conditions:

$$\begin{cases} \overline{\mathbf{u}} = \mathbf{0} & \text{on } \Gamma_{FrontAndBack} \cup \Gamma_{Ground} \ \times [0, T], \\ \overline{\mathbf{u}} = (\mu_1 \cos(\mu_2), \mu_1 \sin(\mu_2), 0) & \text{on } \Gamma_{In} \times [0, T], \\ (\nu \nabla \overline{\mathbf{u}} - p\boldsymbol{I})\boldsymbol{n} = \mathbf{0} & \text{on } \Gamma_{Out} \times [0, T]. \end{cases} \tag{4}$$

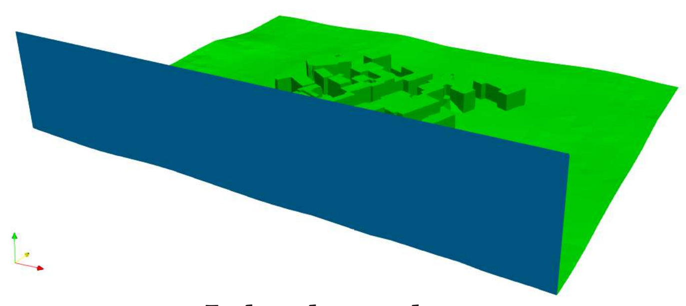
The parameter under consideration is $\boldsymbol{\mu} = (\mu_1, \mu_2)$, which codifies the inlet velocity condition.



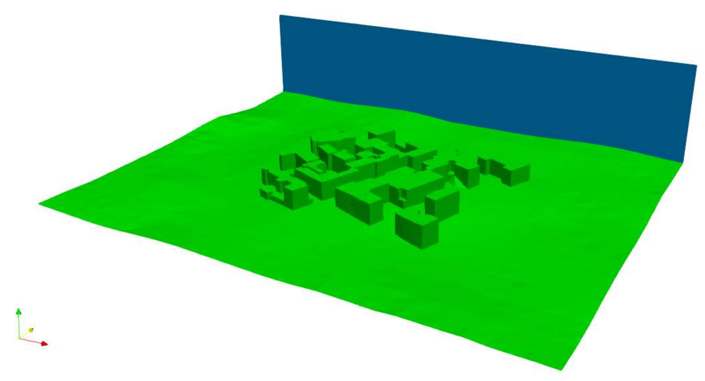
Ground boundary



Front and back boundary



Inlet boundary



Outlet boundary

Reduced order model

We employed the **Reduced Basis** (RB) method. The POD modes are used to approximate the solution $c(t, \boldsymbol{\mu})$ for any new value of the parameter with a linear combination:

$$c(t, \boldsymbol{\mu}) \approx \sum_{i=1}^{N_s} a_i(\boldsymbol{\mu}, t) \phi_i(x), \tag{5}$$

where $a_i(\boldsymbol{\mu}, t)$ are the parameter dependent coefficients and $\phi_i(x)$ are the parameter independent basis functions.
The coefficients of Eq. 5 are then obtained solving:

$$\boldsymbol{M_r} \dot{\boldsymbol{a}} - \nu_T \boldsymbol{B_r} \boldsymbol{a} + \boldsymbol{C_r} \boldsymbol{a} = \boldsymbol{f_r}(t), \tag{6}$$

where each term inside Eq. 6 is obtained by Galerkin projection:

$$\begin{cases} (\boldsymbol{M_r})_{ij} = (\phi_i, \phi_j)_{L_2(\Omega)}, & (\boldsymbol{B_r})_{ij} = (\phi_i, \Delta \phi_j)_{L_2(\Omega)}, \\ (\boldsymbol{C_r})_{ij} = (\phi_i, \nabla \cdot (\mathbf{u}(\boldsymbol{\mu}) \phi_j))_{L_2(\Omega)}, & (\boldsymbol{f_r})_i(t) = (\phi_i, f(t))_{L_2(\Omega)}. \end{cases} \tag{7}$$

POD-NN [1] and POD-DEIM [4]

The complexity in the treatment of the Eq. 6 concerns the convective term and the empirical source term, for which we employed the following strategies:

- The reduced order convective matrix C_r is obtained using the POD-NN approach, that is:

$$(\boldsymbol{C_r})_{ij}(\mu) = \sum_{i=1}^{N_\phi} (\phi_i, \nabla \cdot (u_k \Psi_k \phi_j))_{L_2(\Omega)}; \tag{8}$$

  where the coefficients u_k are the output of a feedforward NN.

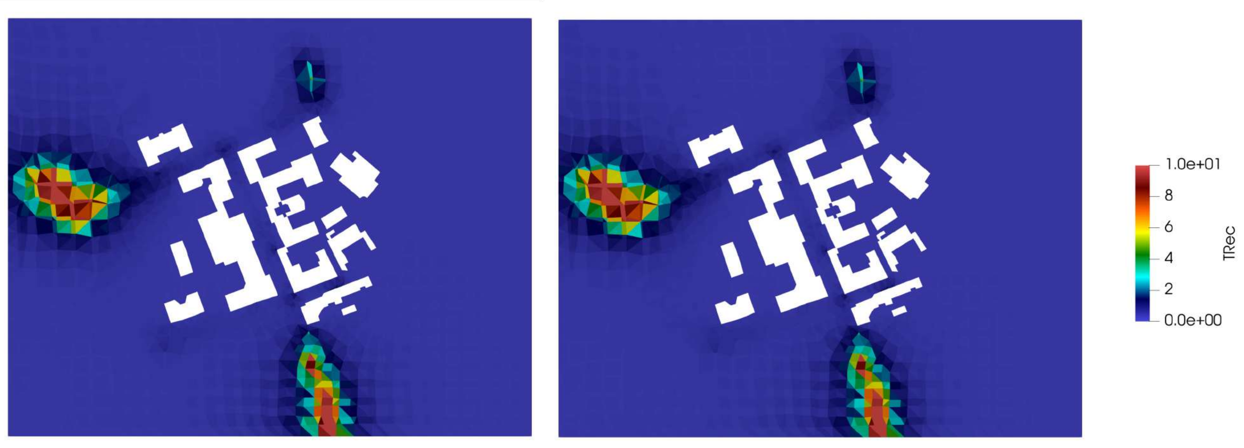
- The DEIM is employed for the source term $f(t)$, which is approximated as:

$$f(t) \approx \sum_{i=1}^{N_{DEIM}} p_i(t) \chi_i(\boldsymbol{x}); \tag{9}$$

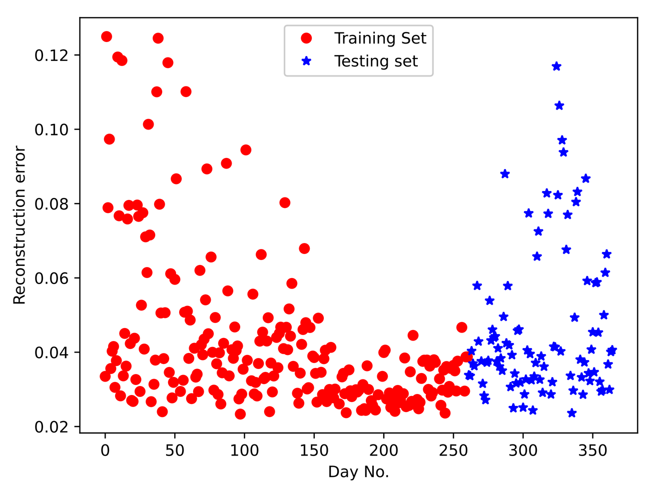
  where the coefficients are determined with a point-wise evaluation of the function f in judiciously chosen **magic points** $\boldsymbol{q}_i$.

Numerical Results

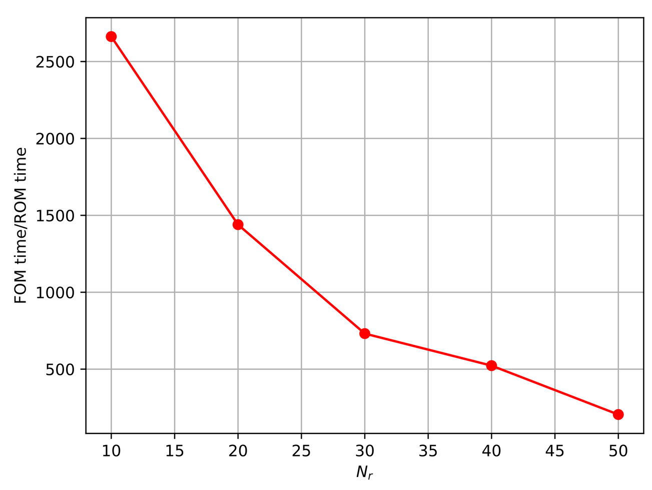
- **Mesh**: main campus of the University of Bologna, with 40k cells.
- **Numerical Discretization**: The offline phase was conducted using the finite volume method. The libraries employed are OpenFoam and ITHACA-FV [3].
- **Dataset**: Syntetic emission data using the fastrace traffic model and 1 year long empirical measurements for the inlet velocity condition.



Offline (left) and Online (right) solution for Day 20, $t = 7500$s.



Average daily reconstruction error for both training and testing datasets.



Speed-up w.r.t the number of basis functions.

References

[1] J. S. Hesthaven and S. Ubbiali. Non-intrusive reduced order modeling of nonlinear problems using neural networks. *J. Comput. Phys.*, 2018.
[2] M. Khamlich, G. Stabile, G. Rozza, L. Kornyei, and Z. Horváth. ROM for large-scale modeling of urban air pollution. *In preparation*, 2022.
[3] G. Stabile and G. Rozza. ITHACA-FV - In real Time Highly Advanced Computational Applications for Finite Volumes. `http://www.mathlab.sissa.it/ithaca-fv`.
[4] G. Stabile, M. Zancanaro, and G. Rozza. Efficient geometrical parametrization for finite-volume-based reduced order methods. *International Journal for Numerical Methods in Engineering*, 2020.