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Acceleration of simulations by application of a kernel method in a high-resolution lagrangian particle dispersion model

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Scope

The use of **microscale** atmospheric dispersion models in **long-term studies** and **forecasting systems** is growing.

→ Constraint of computational **resources and time**

→ Implementation and test of an **alternative method to compute concentration** in a **microscale Lagrangian Particle Dispersion Model** to **reduce the overall simulation time**

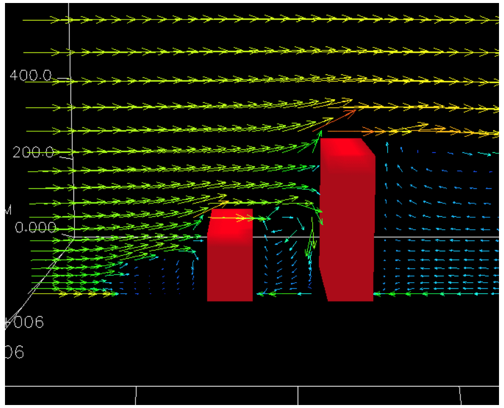
PMSS model

Parallel Micro – SWIFT – SPRAY

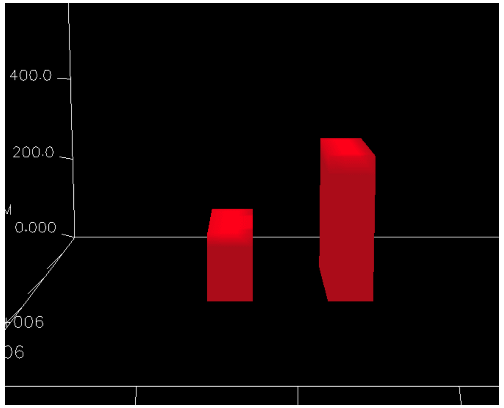
- code designed to perform simulation at microscale

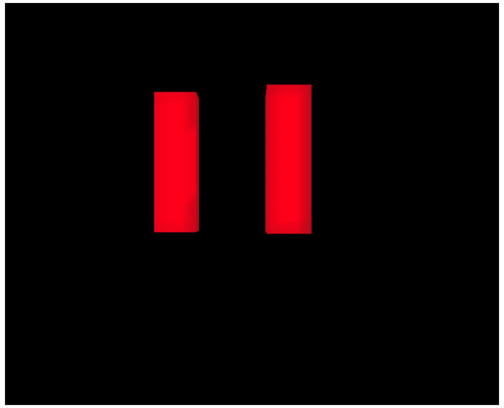
- composed by two main elements

A diagnostic reconstructor of the meteorological flow (**PSWIFT**)



A Lagrangian Particle Dispersion Model (**PSPRAY**)





- Independent parallelization of the two codes based on MPI paradigm:

  → reduce computational time

  → deal with "large" simulations (large areas and large time intervals)

Kernel Method

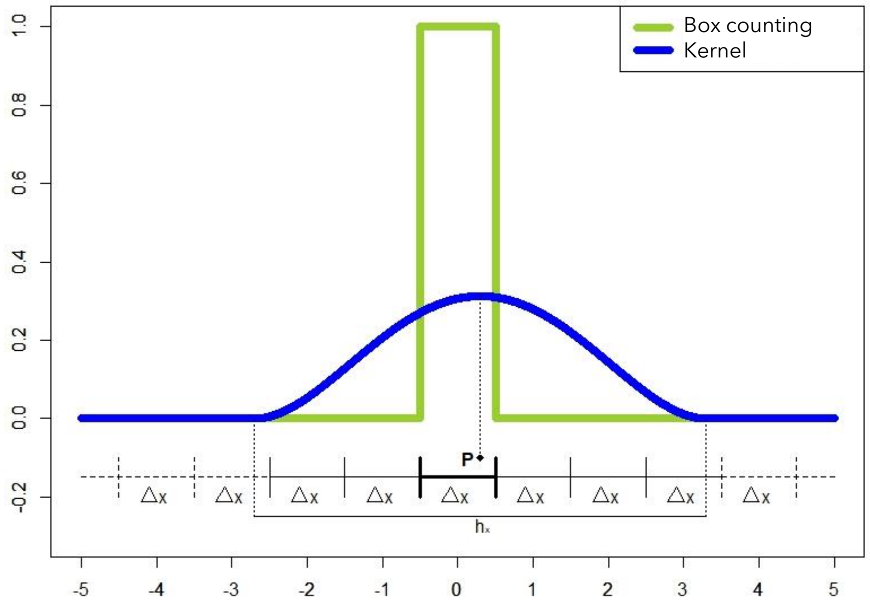
→ Alternative to the classic box-counting method to **compute 3D concentrations**

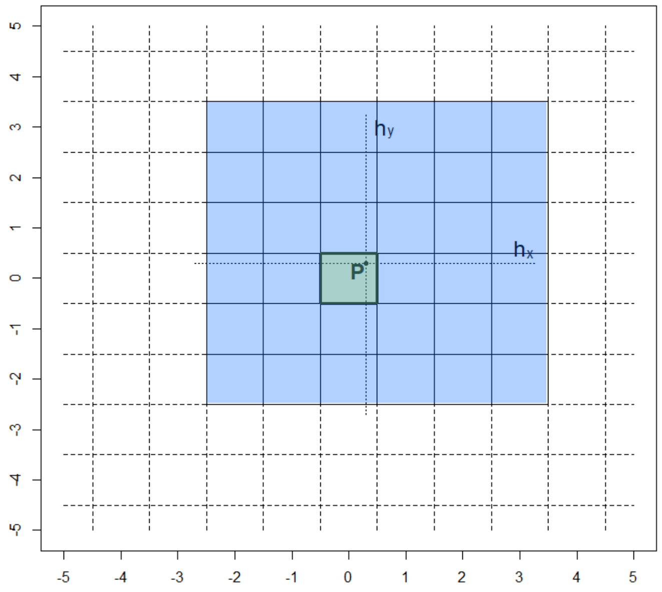
Box Counting Method

$$C_i = \frac{\sum_{j=1}^{N_{part,i}} m_j}{Volume_i} \quad \textit{with i=i-th cell}$$

Kernel Method

$$C(x,y,z;t) = \sum_{p=1}^{Ntot} \frac{m_p}{h_x h_y h_z} K\left(\frac{x_p - x}{h_x}\right) K\left(\frac{y_p - y}{h_y}\right) K\left(\frac{z_p - z}{h_z}\right)$$





Kernel Method in PMSS

→ Implemented in PMSS

- Bi-weight kernel function:

$$K(x) = \begin{cases} \frac{15}{16}\left[1 - \left(\frac{x_p - x}{h_x}\right)^2\right]^2 & \text{for } \left|\frac{x_p - x}{h_x}\right| \leq 1 \\ 0 & \text{for } \left|\frac{x_p - x}{h_x}\right| > 1 \end{cases}$$

$$K(x) \geq 0 \qquad \forall x \in Domain\ D$$

$$\int_D K(x)dx = 1$$

- Geometric formulation of bandwidths:

$$h_x = 3.5 * \Delta x$$

$$h_y = 3.5 * \Delta y$$

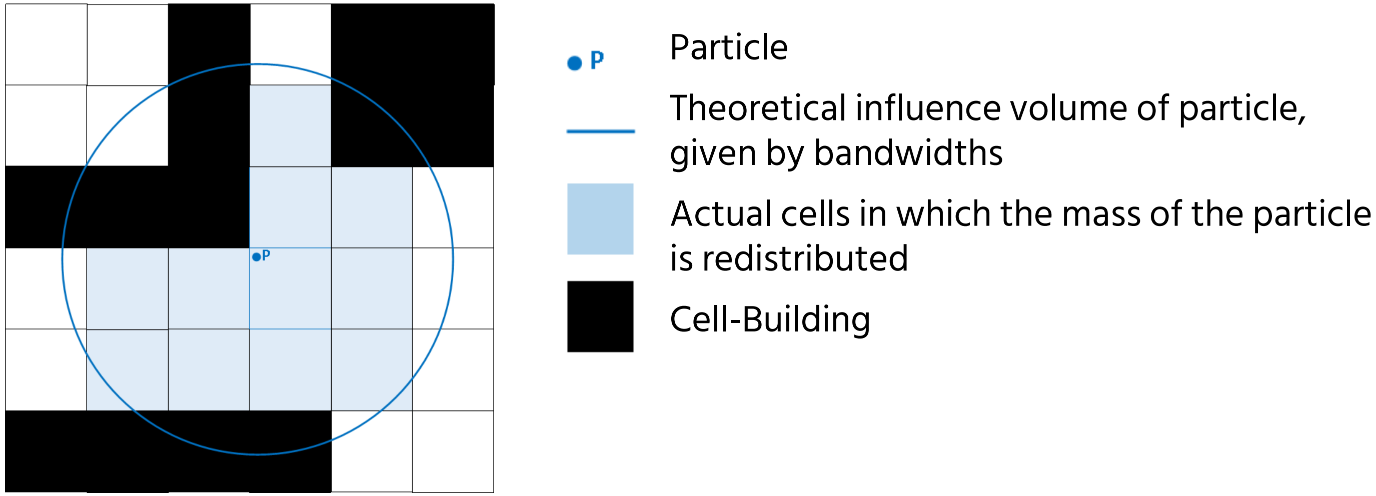
$h_z = 1.2 * h_0$ (h_0=height of ground level concentration)

Kernel Method in PMSS

1. Impermeable boundaries
    - Ground

      Reflection term $K(z) = K\left(\frac{z_p - z}{h_z}\right) + K\left(\frac{z_p + z}{h_z}\right)$
    - Obstacles

      Modification of the volume of influence

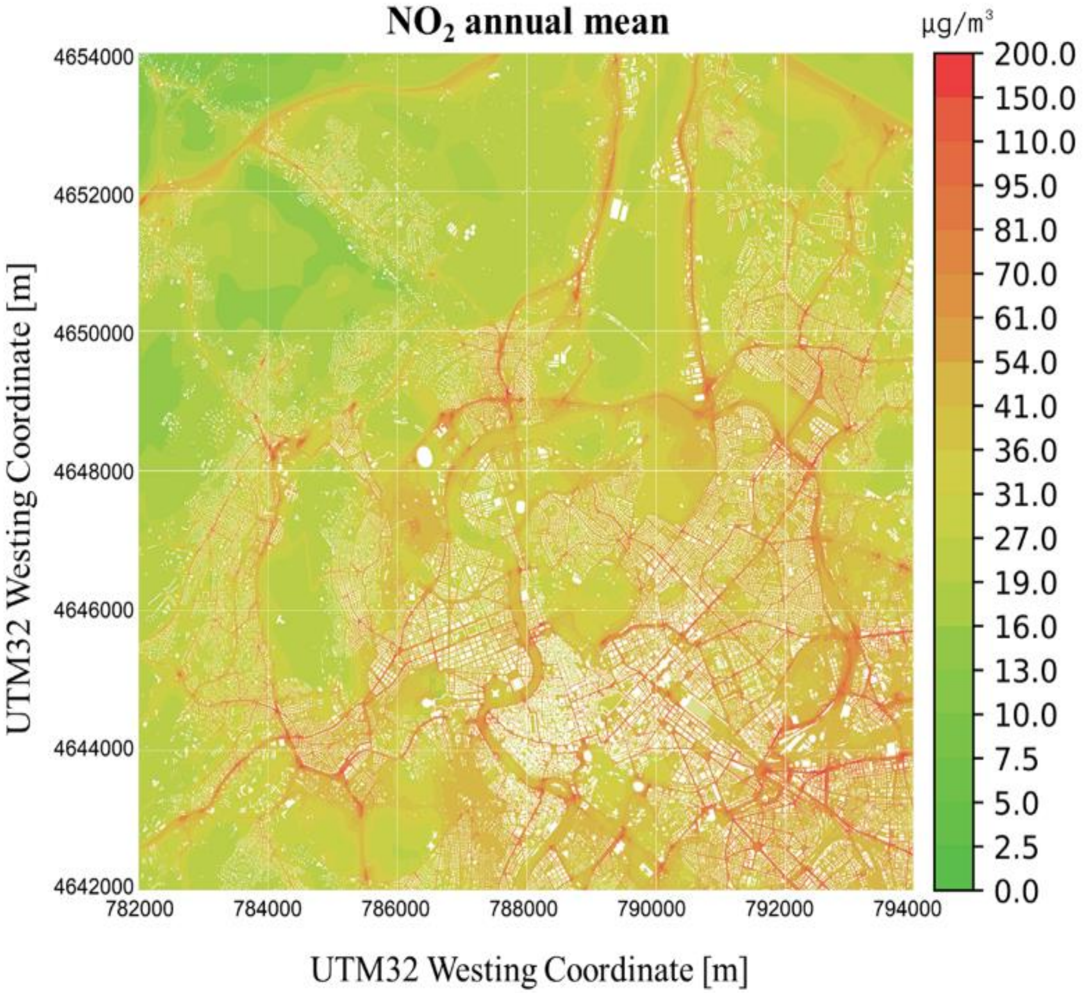


2. **Integration of deposition**

3. **Nested and tiled configuration**

Kernel method in PMSS

→ Already tested for traffic gases emissions



Index	Gas concentration
Particles reduction [%]	95%
Time reduction [%]	80%
Index of agreement	0.98

Test cases

Test case 1

- 1 punctual source
- Emission of gas

- Domain configuration
  - Microscale (1 m horizontal resolution)
  - Obstacles
  - Tiled configuration

- Averaging time interval: 1 hour

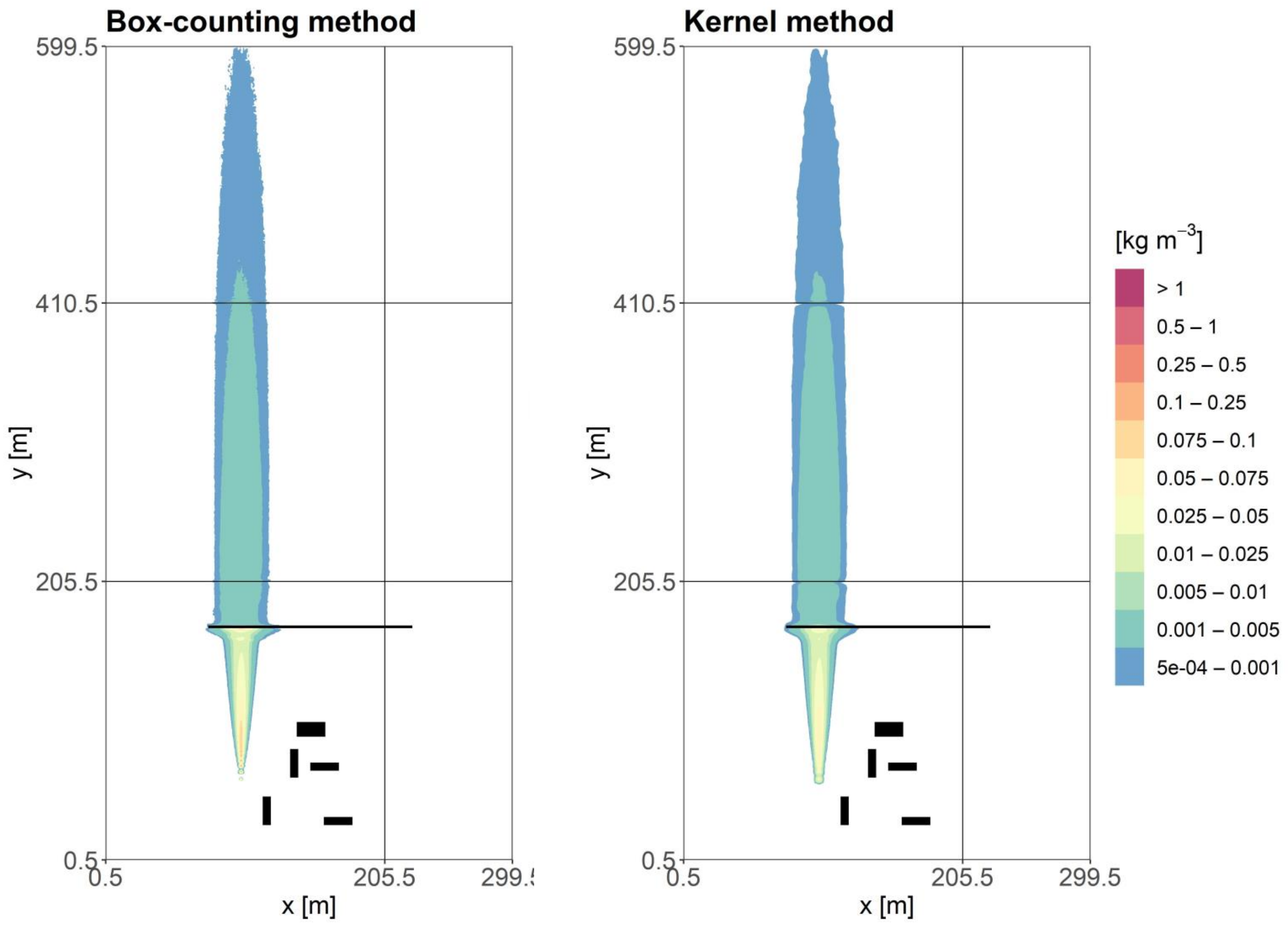
Test case 2

- 1 punctual source
- Emission of gas and particles
- Deposition

- Domain configuration
  - Microscale (1-2 m horizontal resolution)
  - Obstacles
  - Nested configuration

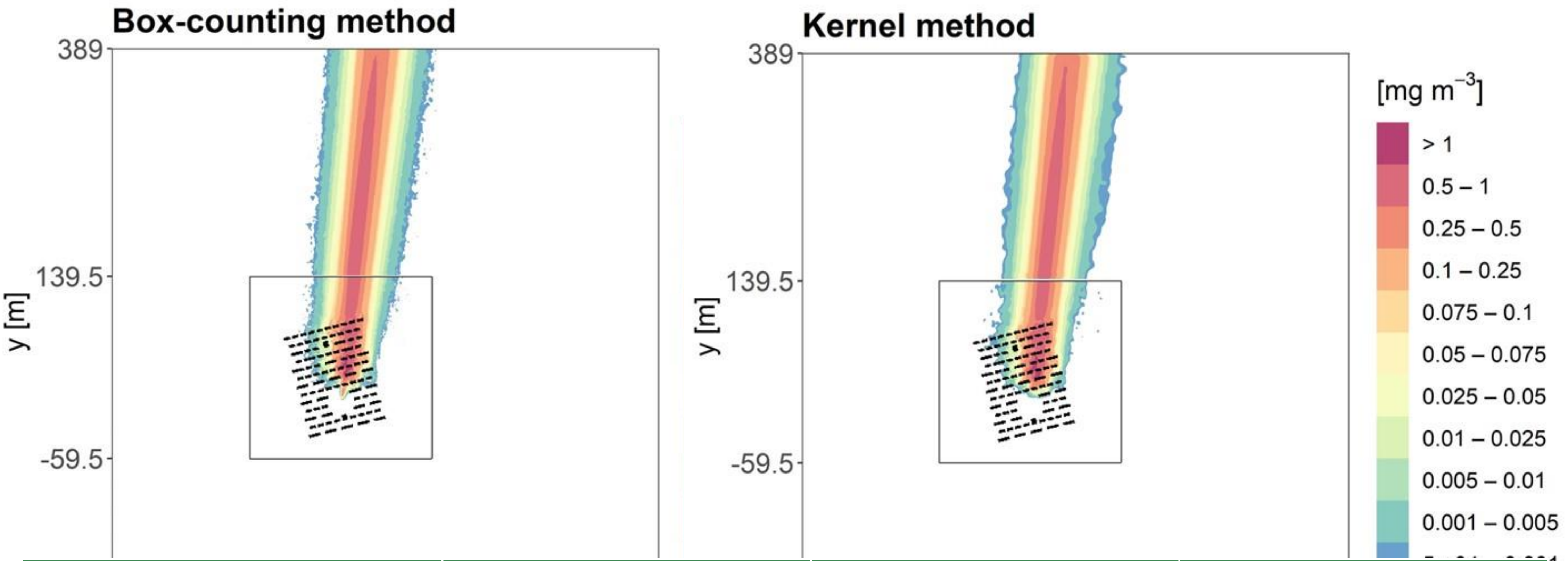
- Averaging time interval: 1 hour

Results – Test case 1



Index	Gas concentration
Particles reduction [%]	80%
Time reduction [%]	68%
FAC2	0.95
Correlation	0.94
Index of agreement	0.96

Results – Test case 2



	Gas Concentration	Particulate Concentration	Particulate Deposition
Particles reduction [%]	80%		
Time reduction [%]	80%		
FAC2	0.98	0.98	0.95
Correlation	0.94	0.95	0.90
Index of agreement	0.97	0.97	0.95

Conclusion

Kernel method successfully tested in PMSS for:

- Linear and point sources
- Emission of gaseous and particulate pollutant
- Deposition of particulate pollutant
- Tiled and nested domain configuration

→ Results are consistent for all configurations and show:

- with a **reduction of 80% of emitted computational particles**
- an **overall reduction of time between 60-80%**
- obtaining **hourly ground concentration fields** with an **IA of at least 0.95**