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The use of hybrid models to integrate the main dynamic characteristics of the physical phenomena

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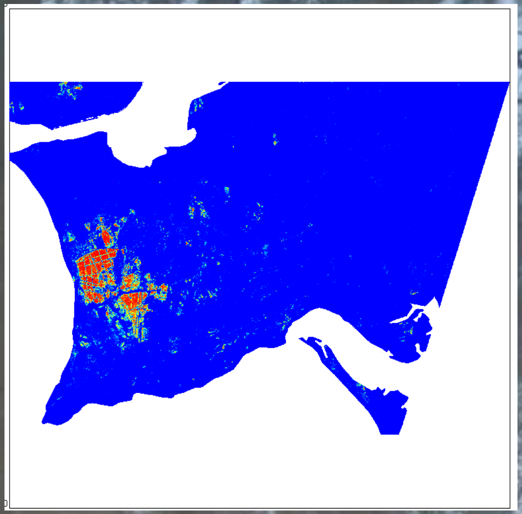
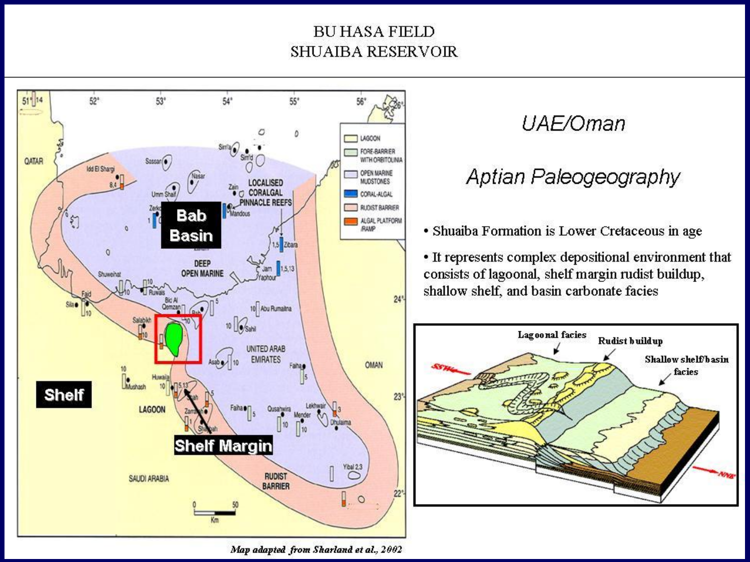


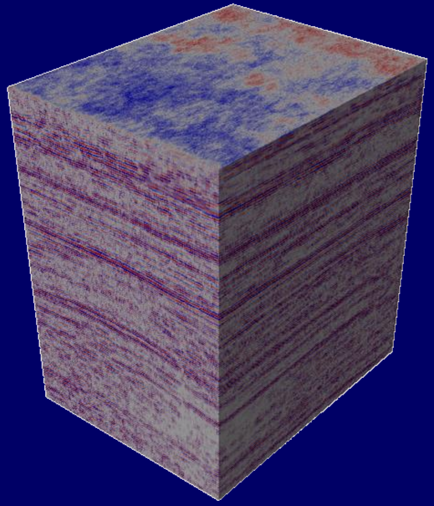
Integration of Different Data and Information

Integration of Different Data and Information to characterize geological phenomena

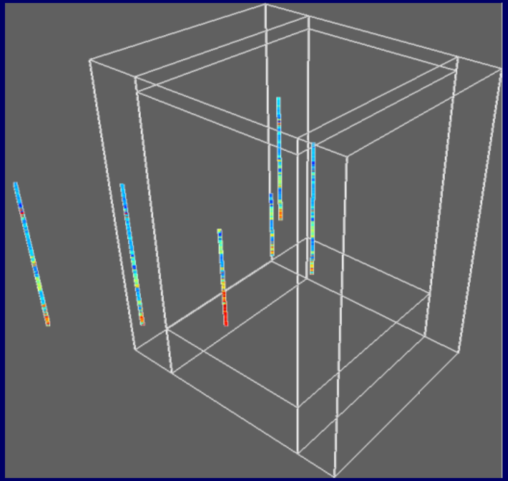
Geology

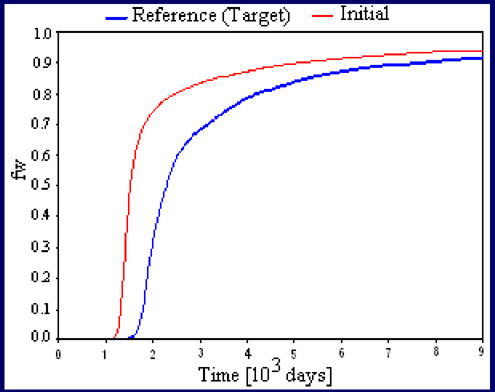


Geophysics



Well Data





Production Data

"A good model is the one that starts to be not bad and , at the end, gives good results..."

Deterministic (dispersion) models mime the main dynamic characteristics of the physical phenomena

Stochastic models (geostatistics) characterize the static components of the process (polutant concentration, petrophysic properties, etc..)

Motivation: integrate deterministic dispersion models in stochastic charaterization of the resource by adding the (predictive) temporal dimension, obtaining high resolution

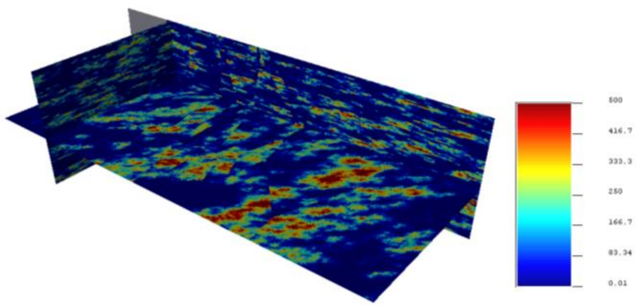
Motivation: integrate deterministic dispersion models in stochastic charaterization of natural resources by adding the (predictive) temporal dimension, obtaining high resolution images of the main characteristics and the uncertainty attached

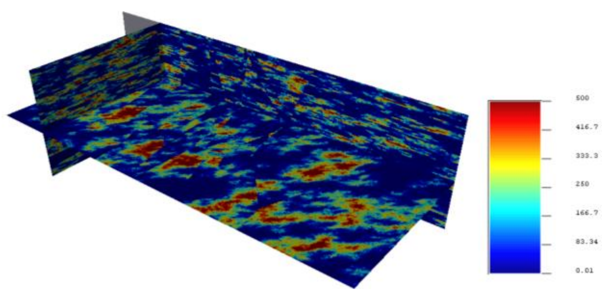
Hydrogeology and Petroleum applications

In hydrogeology and petroleum applications deterministic models, that mime the dynamic of physical phenomena, are integrated a posteriori, through inverse models.

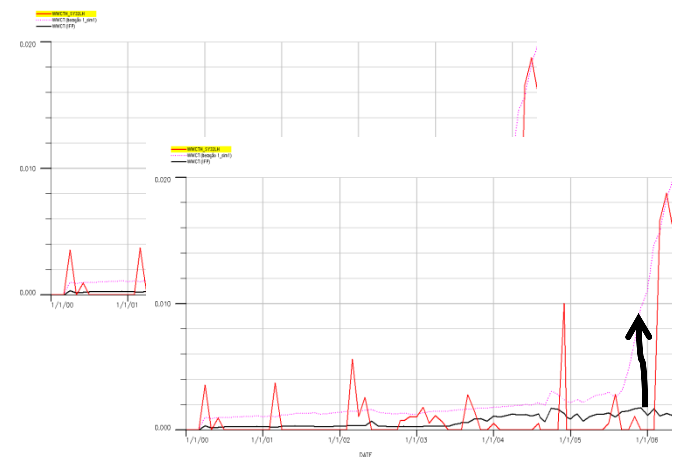
The idea is to calibrate/update the aquifer or reservoir parameters – internal properties, petrophysical properties, .. – with the dynamic data.

Stochastic Simulation of petrophysical parameters





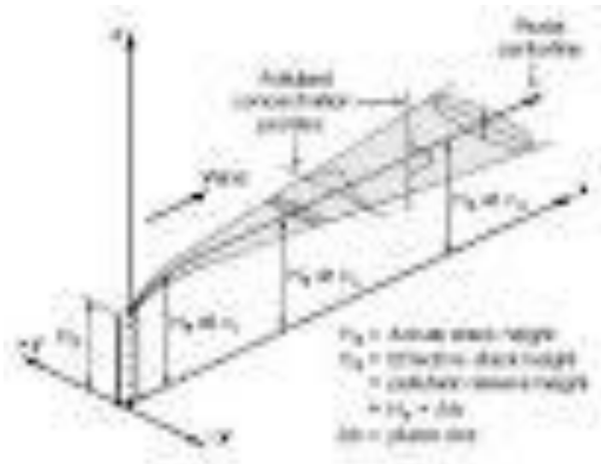
Obtain responses from dynamic simulator

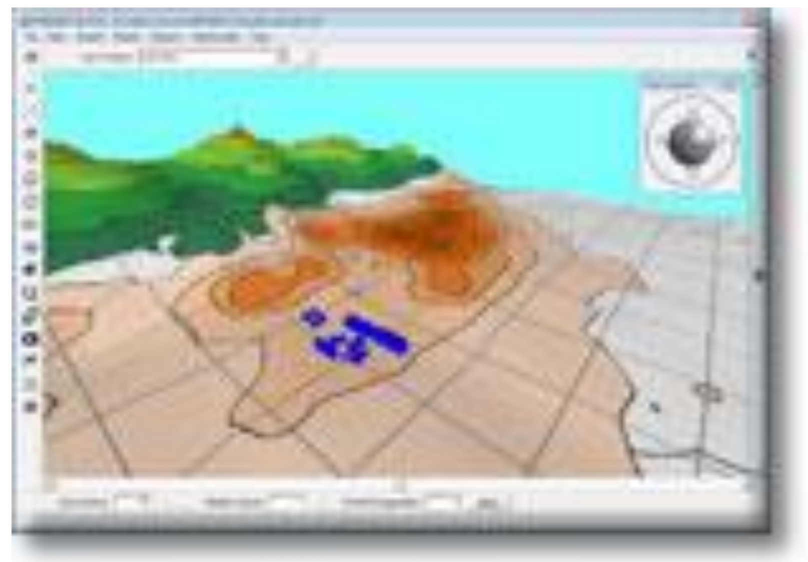


Perturbation/Optimization/.. of initial parameters until the desired match is obtained

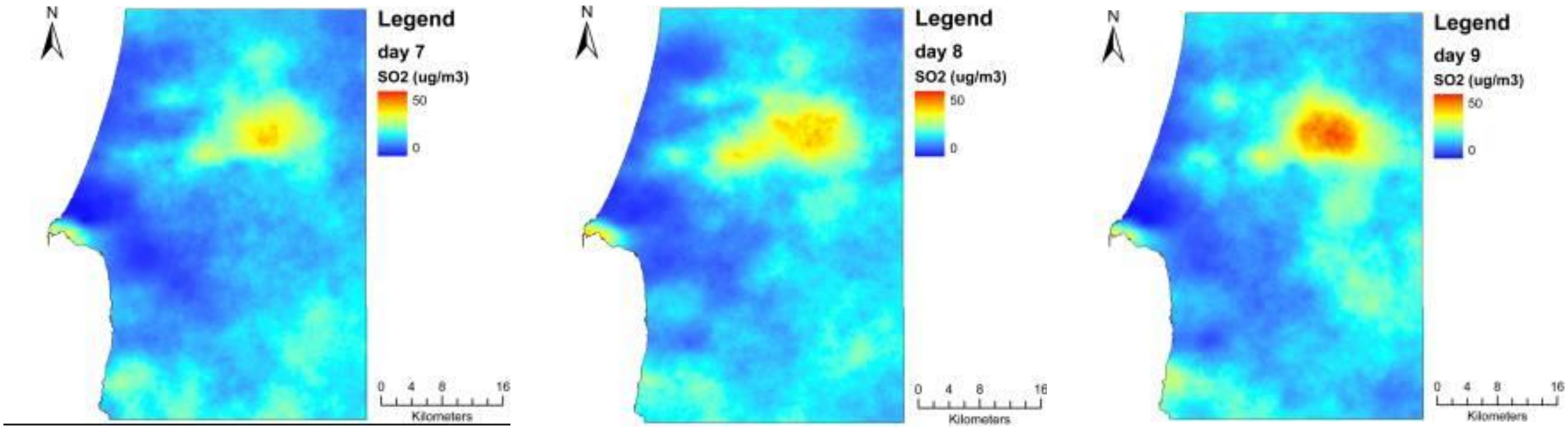
Air Quality Modelling

The most of deterministic dispersion models applied for air quality modelling faces, in general, two main limitations : the spatial scale/resolution and the calibration with experimental data values





Stochastic models (Geostatistics) produce high resolution models, honour the experimental data but are unable to predict in time domain



Stochastic Simulation of SO2 in space-time domain

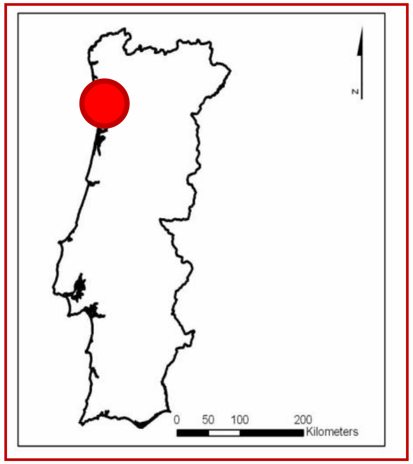
Example #1 – Case study of a Costal lagoon with contaminated sediments

Objective:

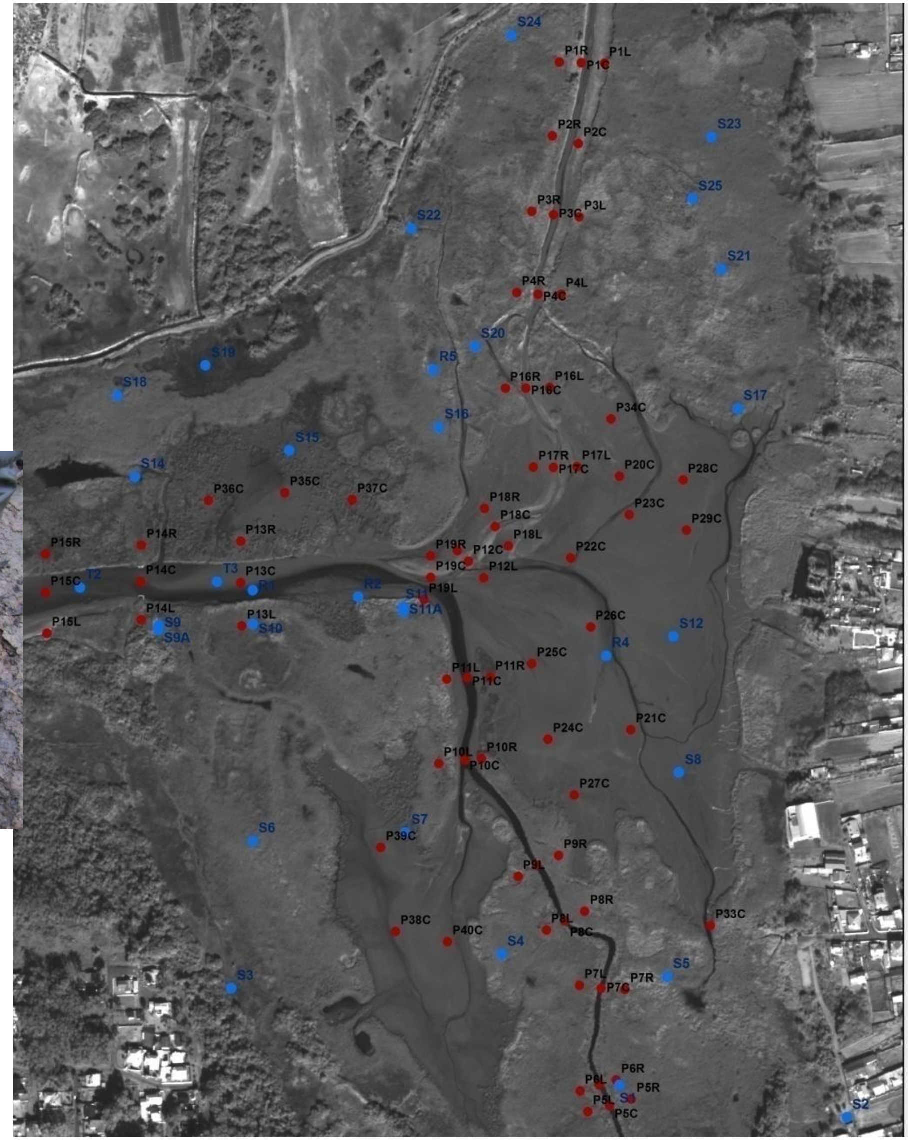
i- The use of hybrid models to integrate the main dynamic characteristics of the phenomenon

ii- Integration of uncertainty of different conceptual models of sediment depositional dynamics at the early stages of risk analysis of a contaminated site

Case study: Barrinha de Esmoriz, coastal lagoon with contaminated sediments



Available data: two sampling campaigns



2001– 30 samples

2008 – 69 samples

Conceptual depositional model: contaminated sediments are driven by the fluid flow

•Morphology of meanders structure are extracted by EO –Earth Oservation data.
•Main flow characteristics (direction, velocity) are taken by a dynamic simulator

Proposed Methodology: Stochastic simulation of a continuous variable with local anisotropies (Horta et al, 2009)

Continuous variable Z(x) with a distributions function Fz(z) = prob {Z(x) ≤ z}

Dss with local anisotropies

i) Define the random path over the entire grid of nodes x_u, u=1, Ns, to be simulated

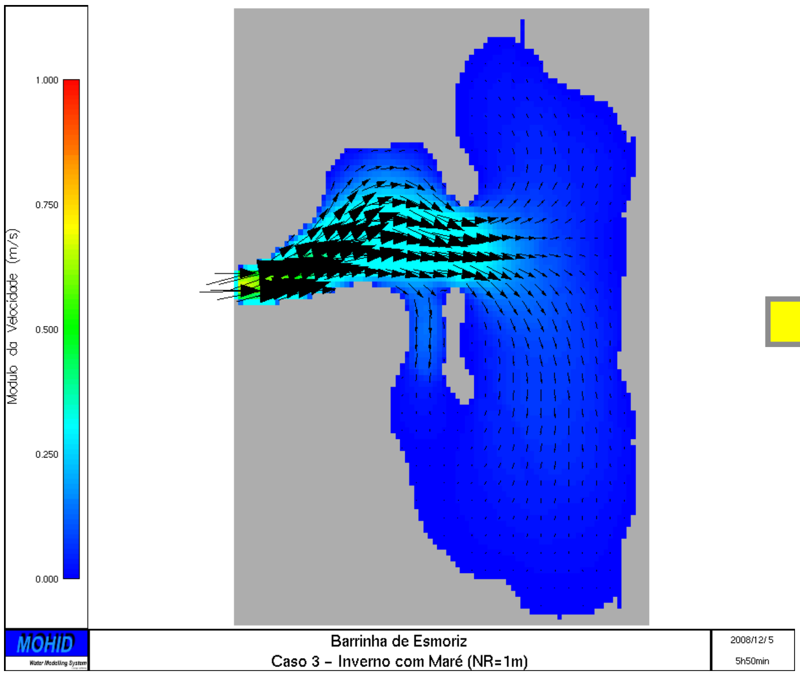
ii) Estimate the local mean (simple kriging estimate $z(x_u)^*$) and variance (estimation variance $\sigma^2_{sk}(x_u)$) conditioned to local models of covariance anisotropy.

iii) Define the interval of $F_z(z)$ interval to be sampled (defined by the local mean and variance of z(x))

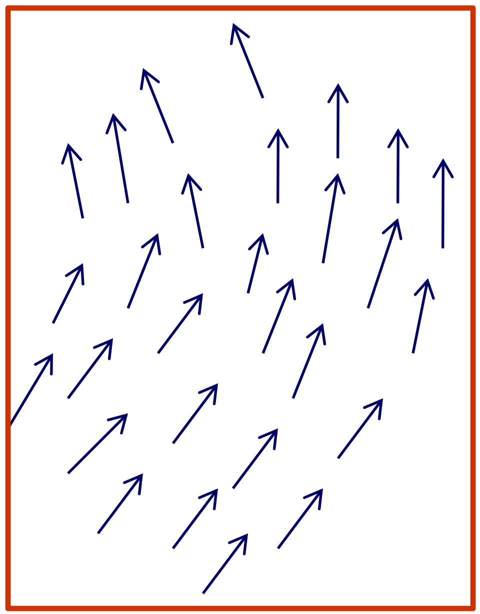
iv) Draw the value $z^s(x_0)$ from the cdf $F_z(z)$

v) Loop until all Ns nodes have been visited and simulated

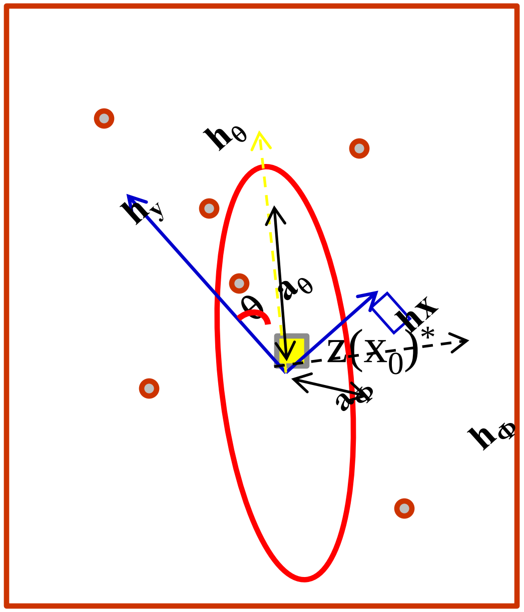
Idea: to convert the output of dynamic simulator – directions and velocities of flow – in local anisotropy ratios and main directions



The main directions and local anisotropy ratios, are accounted in the simple kriging system to estimate local means and variances at a given location x0,



local models of $C_\theta(h)$ are defined in a regular grid node



Simple kriging with local models of $C_\theta(h)$

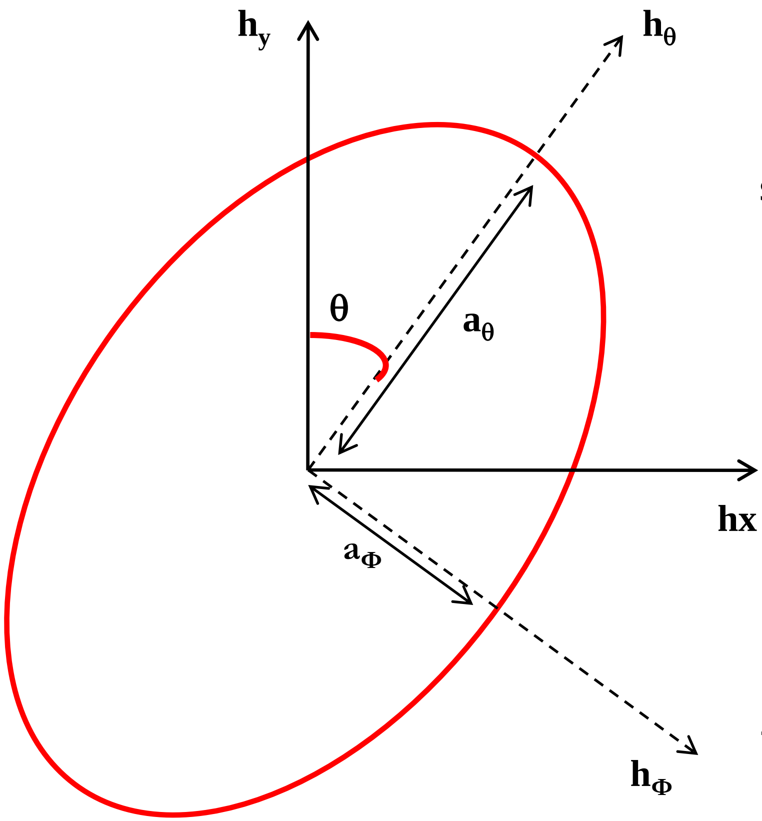
$$z(x_0)^* = \sum_\alpha \lambda_\alpha c_\theta(x_0, x_\alpha)$$

Simple kriging system

$$\lambda_{sk}(u) = K_{sk}^{-1} \cdot k_{sk}$$

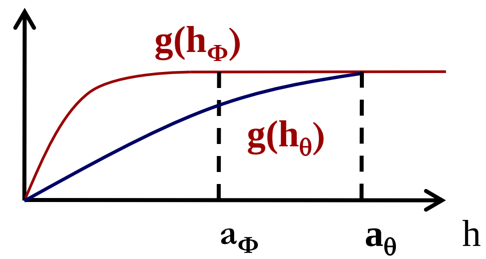
$$[\lambda] = \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \cdots \\ \lambda_n \end{bmatrix} \qquad [K] = \begin{bmatrix} C_{(1,1)} & C_{(1,2)} & \cdots & C_{(1,n)} \\ C_{(2,1)} & C_{(2,2)} & \cdots & C_{(2,n)} \\ \cdots & \cdots & \cdots & \cdots \\ C_{(n,1)} & C_{(n,2)} & \cdots & C_{(n,n)} \end{bmatrix} \qquad [k] = \begin{bmatrix} C_{(x_1,x_0)} \\ C_{(x_2,x_0)} \\ \cdots \\ C_{(x_n,x_0)} \end{bmatrix}$$

Vector of simple kriging weights **Matrix of data covariances** **Vector of data-to-unknown covariances**



Data search assuming geometric anisotropy:

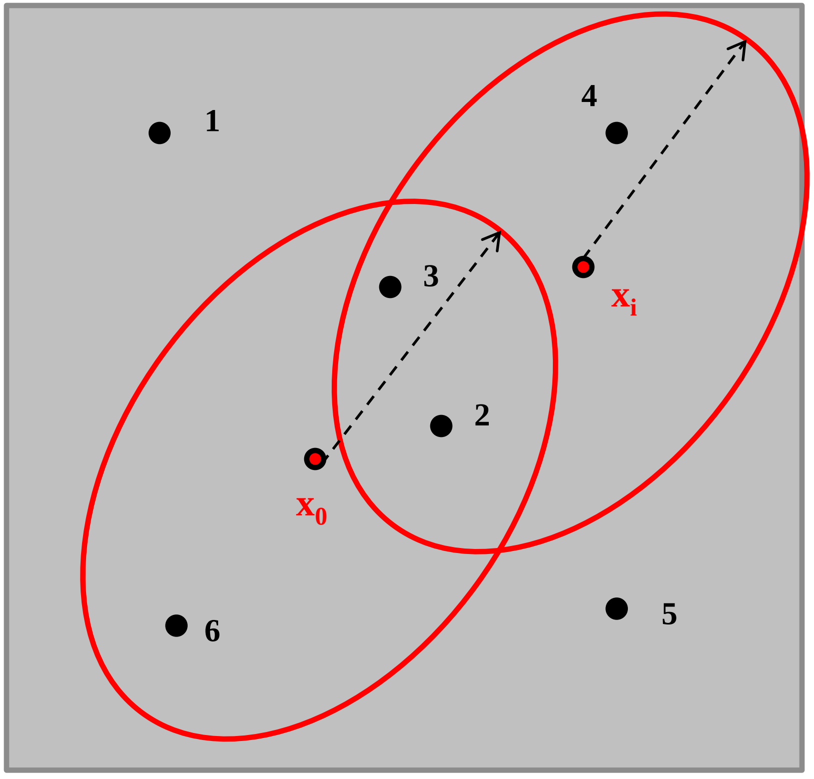
Pattern of spatial variability given by the sample variogram



Elliptical diagram of ranges:

- Direction of maximum continuity (azimuth θ)
- Range of maximum continuity (major axis a_θ)
- $AnisotropyRatio = \frac{a_\theta}{a_\phi}$

DSS



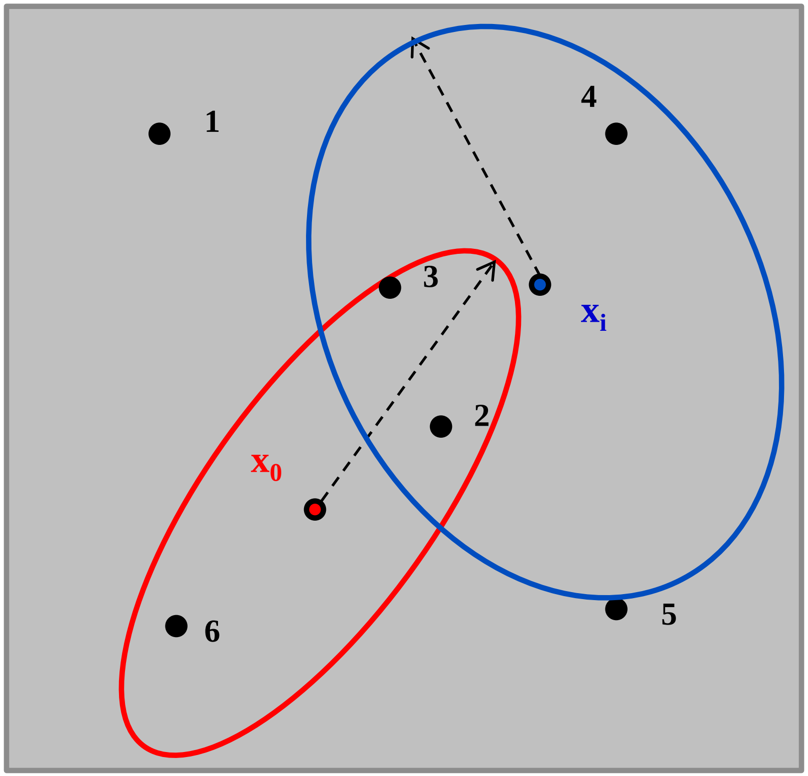
$$\theta_{DSS_{x_0}} = \theta_{DSS_{x_i}}$$

$$\begin{cases} a_{\theta\,DSS_{x_0}} = a_{\theta\,DSS_{x_i}} \\ a_{\Phi\,DSS_{x_0}} = a_{\Phi\,DSS_{x_i}} \end{cases}$$

$$\Downarrow$$

$$\text{Ratio}_{\,DSS_{x_0}} = \text{Ratio}_{\,DSS_{x_i}}$$

DSS with local anisotropy



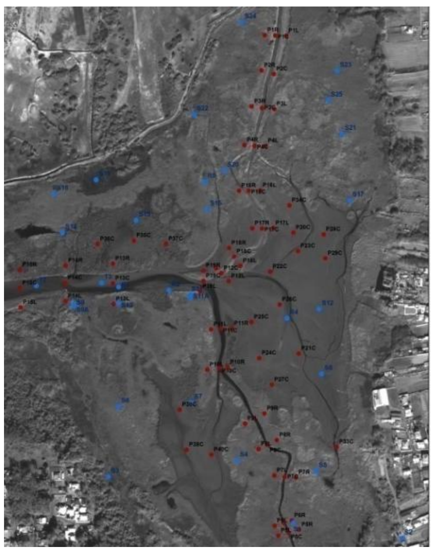
$$\theta_{DSS_{x_0}} \neq \theta_{DSS_{x_i}}$$

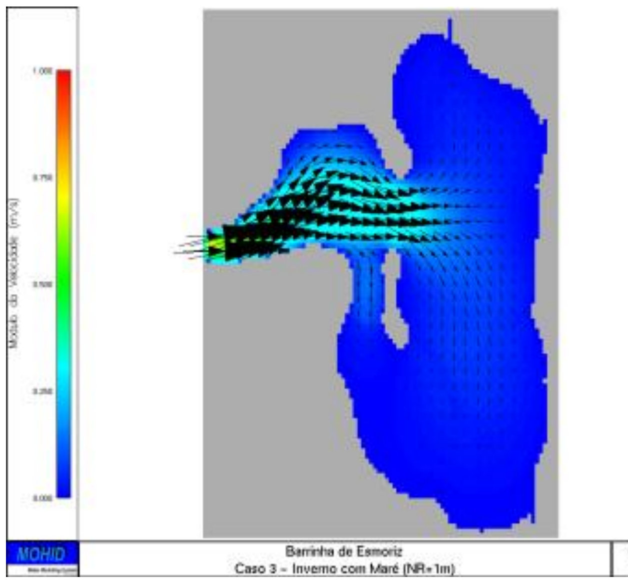
$$\begin{cases} a_{\theta\ DSS_{x_0}} = a_{\theta\ DSS_{x_i}} \\ a_{\Phi\ DSS_{x_0}} \neq a_{\Phi DSS_{x_i}} \end{cases}$$

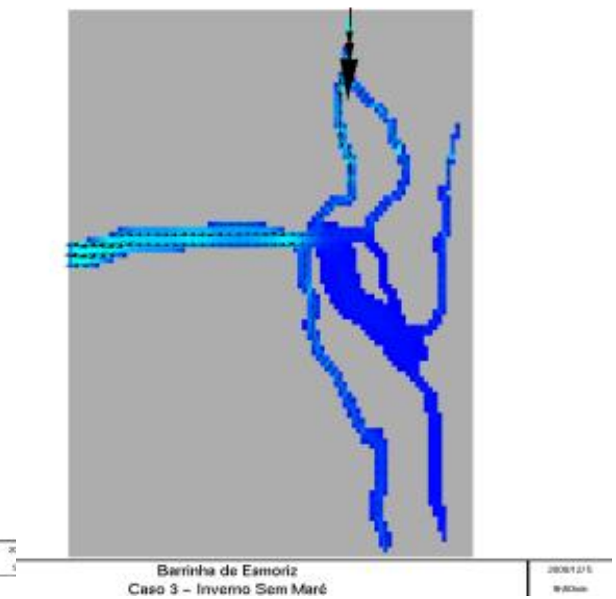
$$\Downarrow$$

$$\text{Ratio}_{\ DSS_{x_0}} \neq \text{Ratio}_{\ DSS_{x_i}}$$

Depositional models of Barrinha contaminated sediments generated by a fluid flow simulator

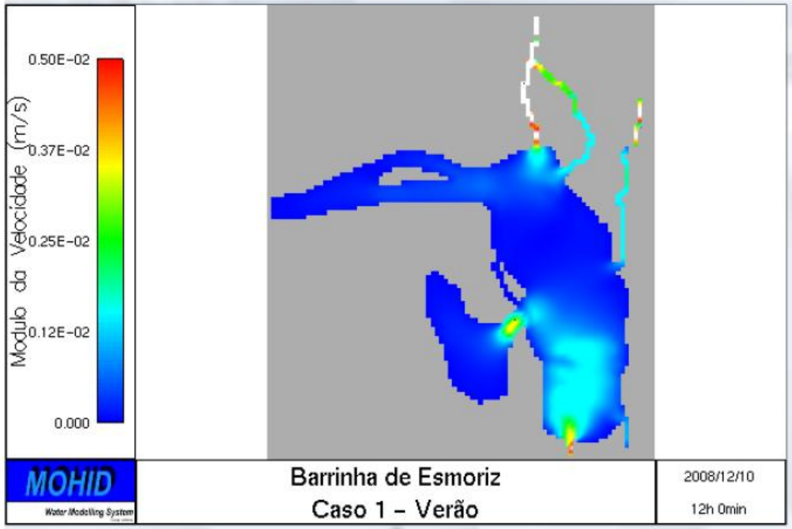






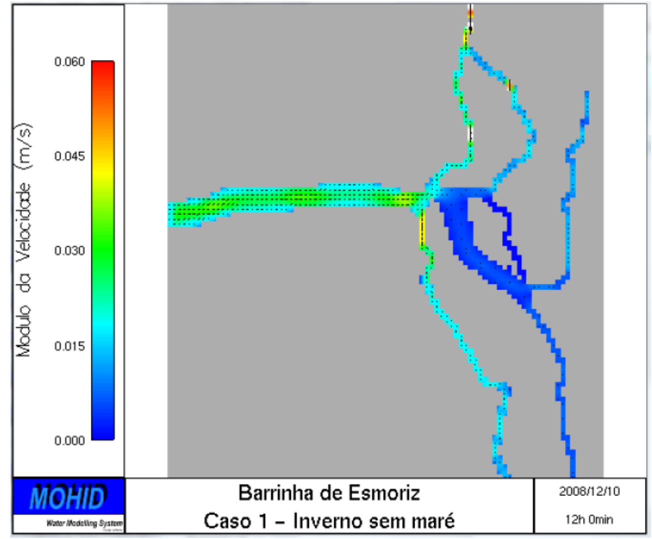
Winter with tide   Winter without tide

summer



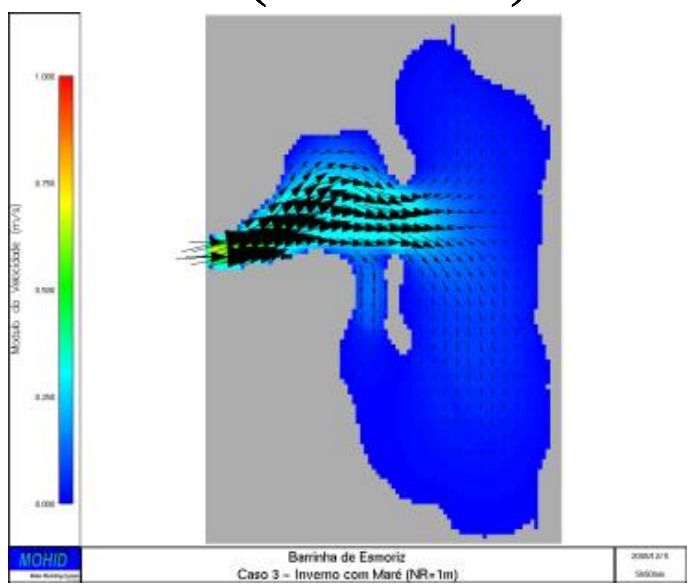
(b)

Winter (no tide)



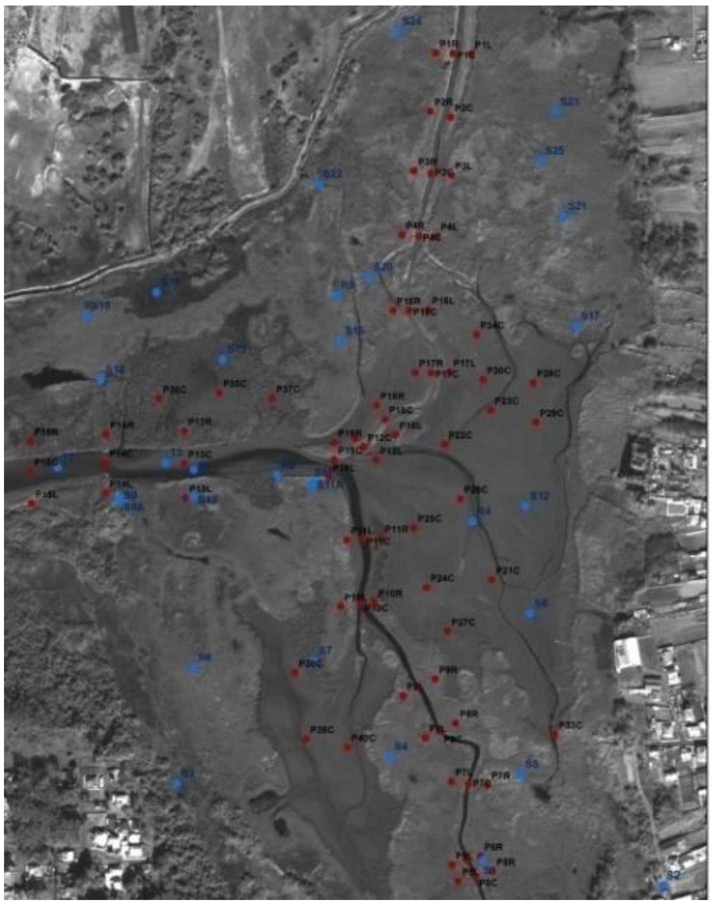
(b)

Winter (with tide)

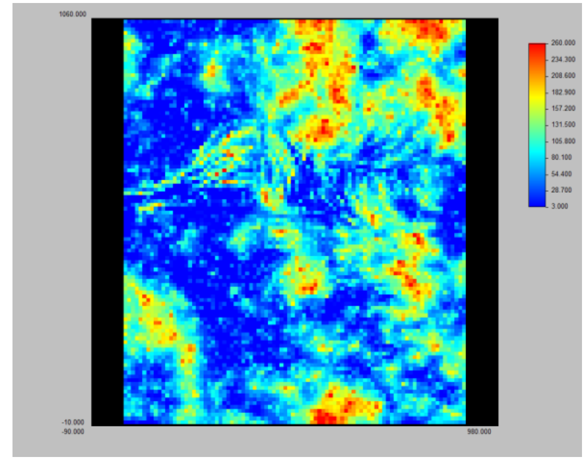


Results

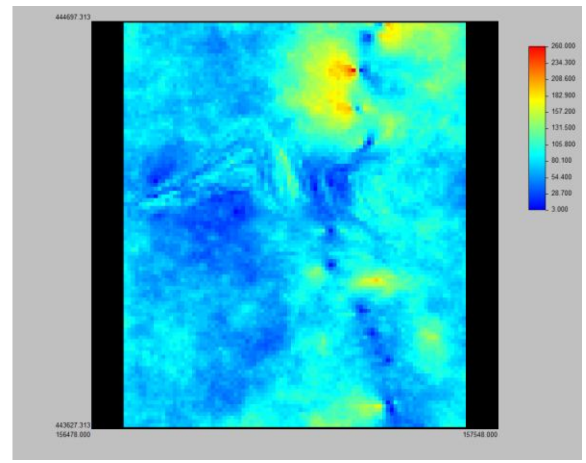
Input MOHID, Cu



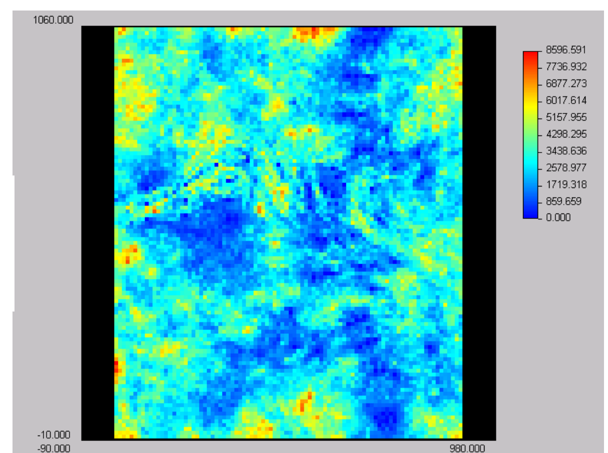
Simulated image



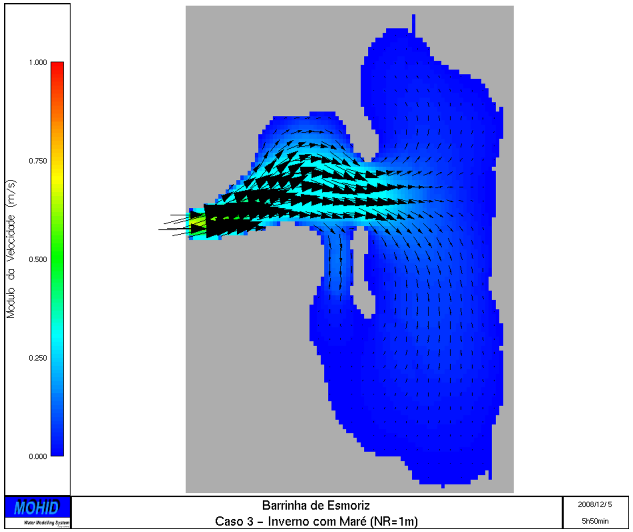
Average



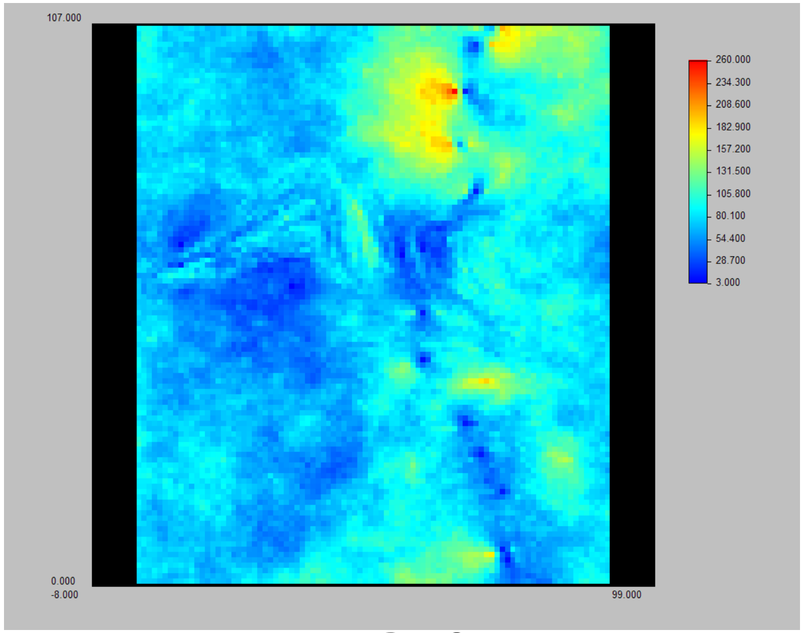
Spatial uncertainty



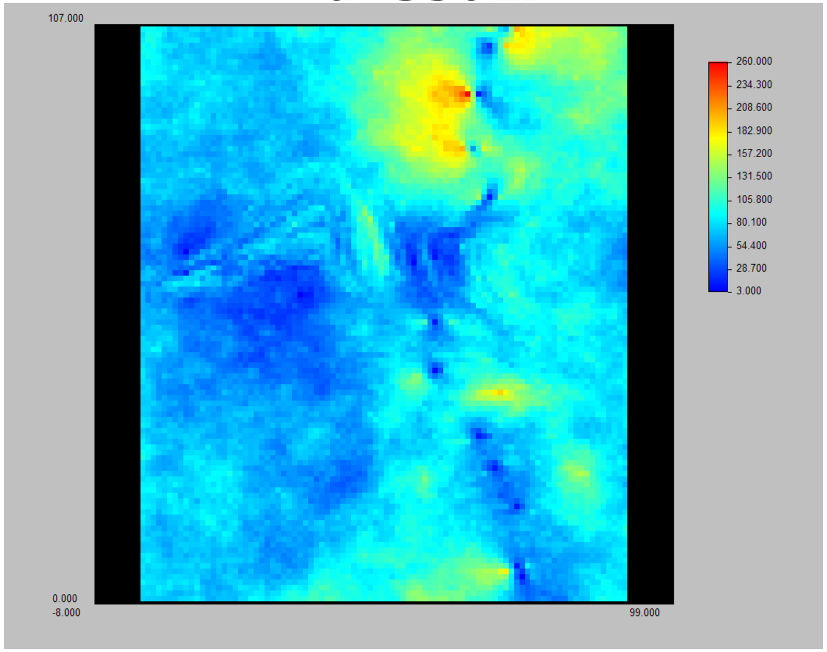
Cu – Scenario A



Average images

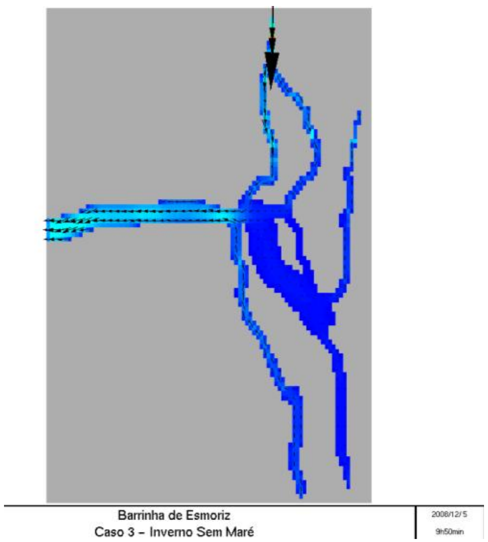


a=350m

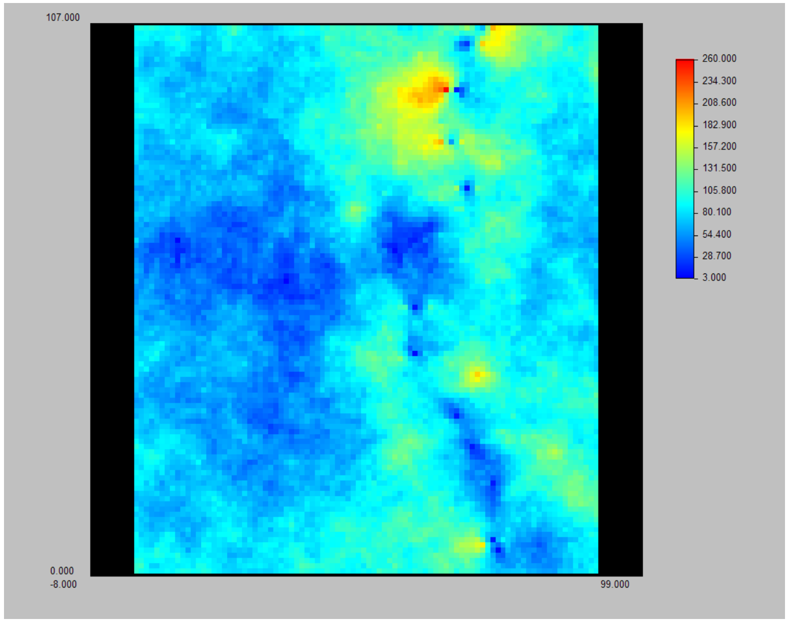


a=500m

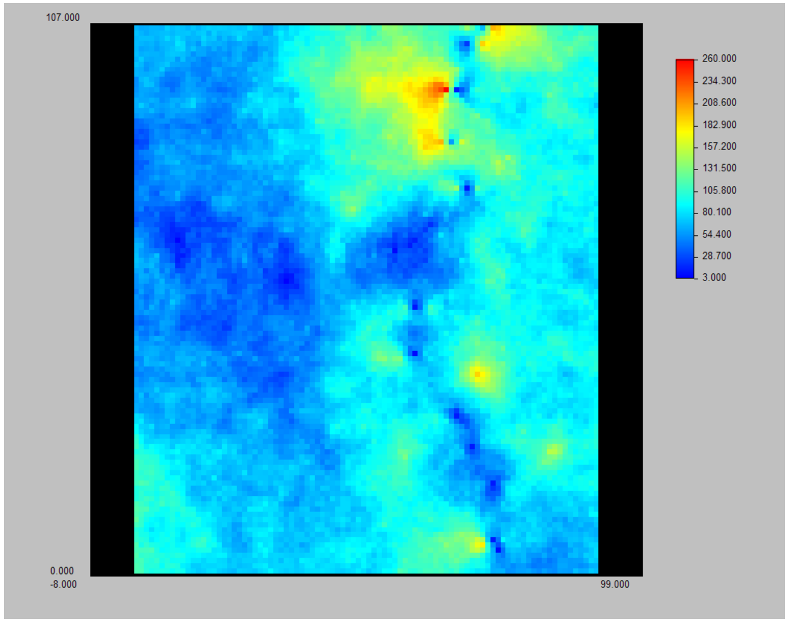
Cu – Scenario B



Average images



a=350m



a=500m

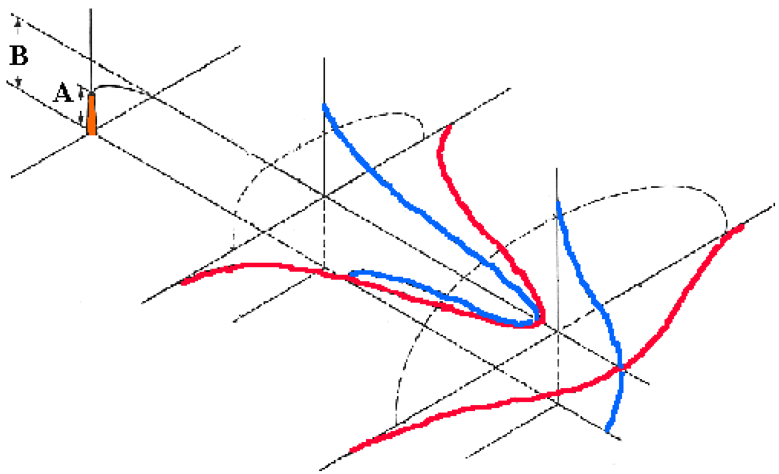
Example #2 - Downscaling of air quality dispersion models: an hybrid multi-scale model

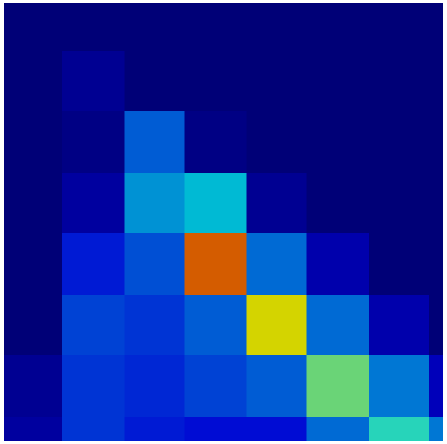
Objective:

. Hybrid multi-scale approach as a methodology for predicting air quality

- Downscaling and calibration (with experimental point data) of images obtained by deterministic dispersion models

Air quality deterministic dispersion models





Advantages

- Incorporate meteorological factors
- Incorporate atmospheric photochemical reactions
- It is able to predict scenarios

Disadvantages

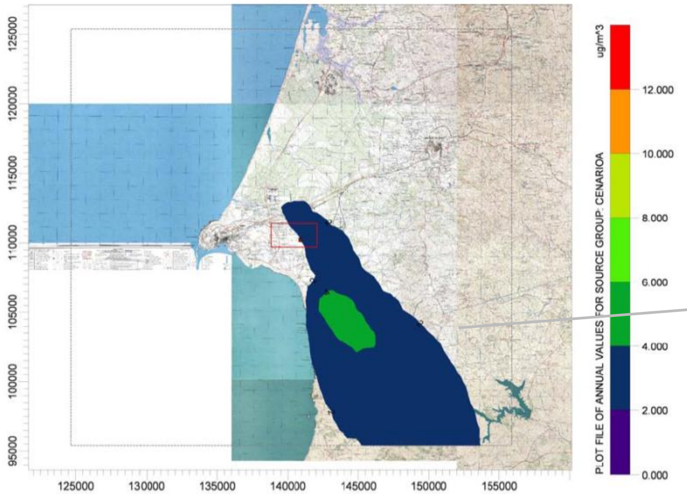
- A large number of input variables
- Difficult to calibrate for fine grid scales

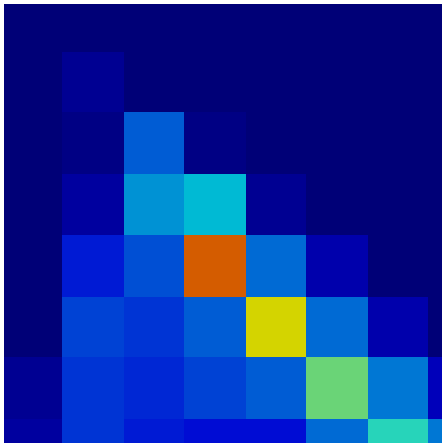
Geostatistical stochastic simulation

- Prediction of pollutant dispersion in space and time (past) at fine scales reproducing the mean variability of data

- The ability of predicting pollutant dispersion in time is limited: the models do not directly incorporate meteorological data

Uncertainty and Support





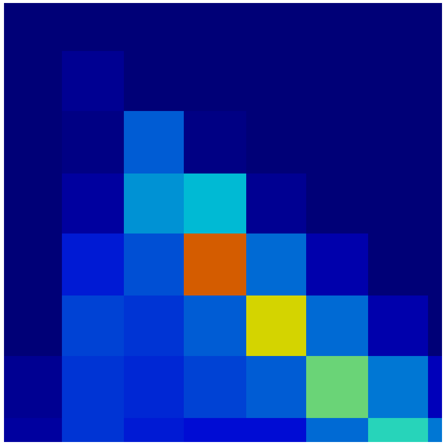
results from the air pollution dispersion models can be assumed as real values of atmospheric pollutant concentration in support v , but with associated uncertainty

Rationale – Hybrid model (proposal)

1st Step – transformation of i input hard data in a image of air quality

Input data:
- Meteorological variables
- Emissions

Air quality dispersion model



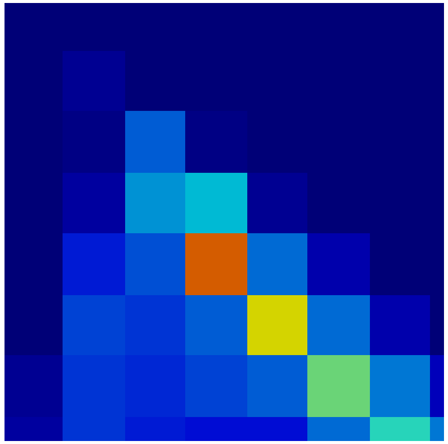
Block data

Air Quality Dispersion Model transforms the real meteorological data (wind directions, pressure,.., emissions) in a coarse image of a pollutant concentration – the Block data

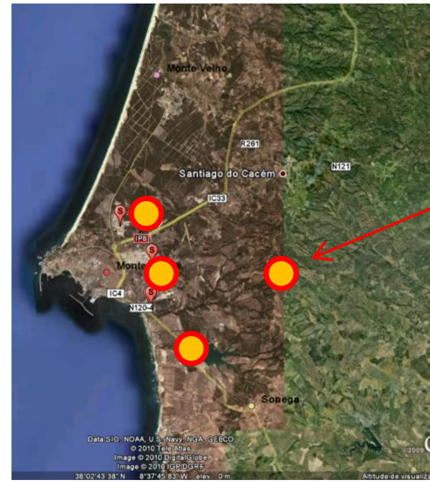
This transformation implies an error that must be accounted in the simulation process

Rationale – Hybrid model (proposal)

2nd Step

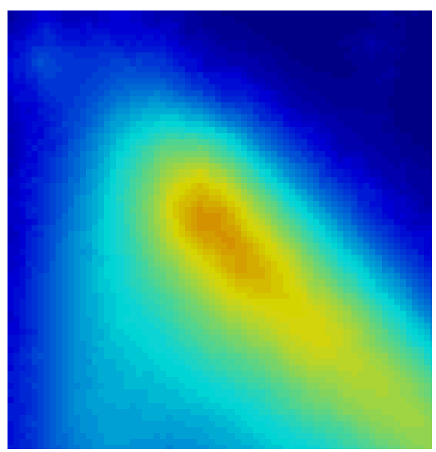


Block data



Point data

• pollutant atmospheric concentration measurements



Geostatistical stochastic simulation

Block Sequential Simulation (BSSIM)

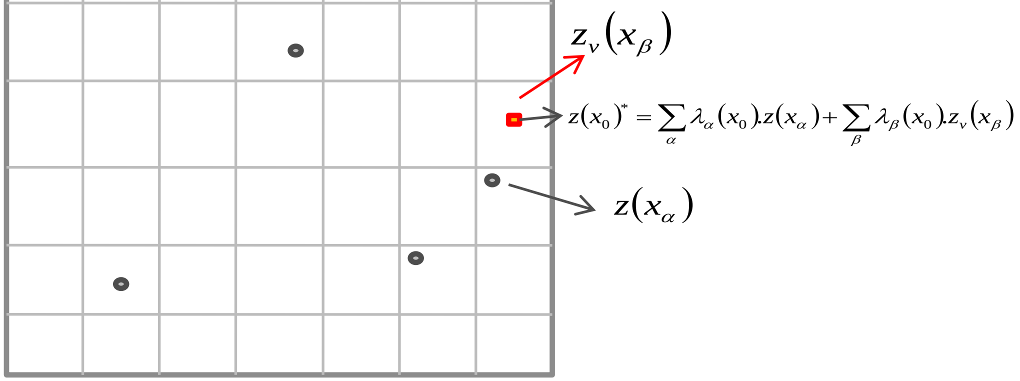
Simulation of point values conditioned to block and point data

Objective: to characterize high resolution images of pollutant concentration based on block and point data

Block Direct Simulation

i. In the node x_0 of a random path of a regular grid, the following means and variances are calculated by block co-kriging:

$$z(x_0)^* = \sum_\alpha \lambda_\alpha(x_0).z(x_\alpha) + \sum_\beta \lambda_\beta(x_0).z_v(x_\beta)$$



Note that the kriging system requires the knowledge of spatial convariaces point-point , point-block and block-block : C(.,.) , C(.,v) e C(v,v)

ii. Simulation of a "point" value $z^s(x_0)$ by re-sampling the global cdf global of Z(x) (Direct Sequential Simulation Approach).

Block Kriging

Data taken at different scales, both on block-support and on point-support are considered in the kriging system

block data is a linear average of point values

$$B(\mathbf{v}_\alpha) = \frac{1}{|\mathbf{v}_\alpha|}\int_{\mathbf{v}_\alpha} L_\alpha(Z(\mathbf{u}'))d\mathbf{u}' \quad \forall\alpha$$

Block Kriging

$$Z^*_{SK}(\mathbf{u}) - m = \Lambda^t \mathbf{D} = \sum_{\alpha=1}^{n(\mathbf{u})} \lambda_\alpha(\mathbf{u})\left[D(\mathbf{u}_\alpha) - m\right]$$

$\Lambda^t = [\lambda_P \lambda_B]$ - Kriging weights

$\mathbf{D}^t = [\mathbf{PB}]$ - data value vector

$D(\mathbf{u}_\alpha)$ - specific datum at location $\mathbf{u}_\alpha$

$n(\mathbf{u})$ - number of data

Kriging system:

$$\mathbf{K}\Lambda = \mathbf{k} \qquad \mathbf{K} = \begin{bmatrix} \mathbf{C}_{PP} & \overline{\mathbf{C}}_{PB} \\ \overline{\mathbf{C}}^T_{PB} & \overline{\overline{\mathbf{C}}}_{BB} \end{bmatrix} \qquad \mathbf{k} = \begin{bmatrix} \mathbf{C}_{PP_0} \\ \overline{\mathbf{C}}_{BP_0} \end{bmatrix}$$

Block-data error incorporation

Data D_B is equal to the "true" value B plus an error R

$$D_B(\mathbf{v}_\alpha) = B(\mathbf{v}_\alpha) + R(\mathbf{v}_\alpha)$$

Assuming that block errors are homoscedastic and not cross-correlated, with zero mean and known variance, then:

Error covariance $$C_R = Cov\left[R(\mathbf{v}_\alpha), R(\mathbf{v}_\beta)\right] = \begin{cases} \sigma_R^2(\mathbf{v}_\alpha) \ if \ \mathbf{v}_\alpha = \mathbf{v}_\beta \\ 0 \ if \ \mathbf{v}_\alpha \neq \mathbf{v}_\beta \end{cases}$$

Block-data error incorporation

If errors are independent of the signal, uncorrelated and with known variance

$$\bar{C}_{B_\alpha B_\beta} = \begin{cases} \bar{C}_B(0) + \sigma_R^2\left(\mathbf{v}_\alpha\right) \; if \; \mathbf{v}_\alpha = \mathbf{v}_\beta \\ \bar{C}_B\left(\mathbf{v}_\alpha, \mathbf{v}_\beta\right) if \; \mathbf{v}_\alpha \neq \mathbf{v}_\beta \end{cases}$$

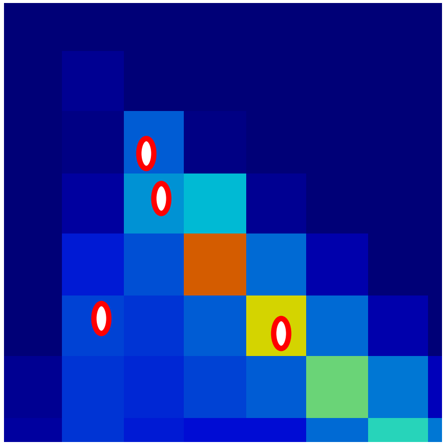
Block-data error incorporation

The error variance can be obtained by a priori calibration

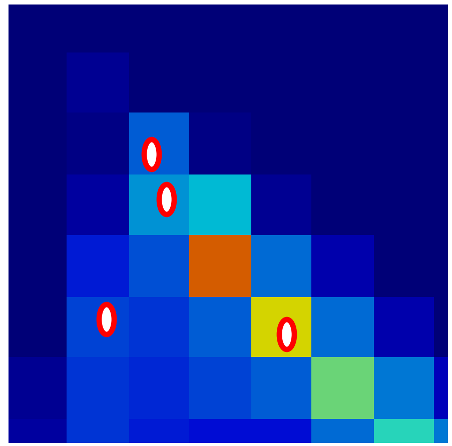
Error is the diference between the data D and the “true” value B :

$$R_B(\mathbf{v}_\alpha) = D(\mathbf{v}_\alpha) - B(\mathbf{v}_\alpha)$$

Choosing the blocks with point data

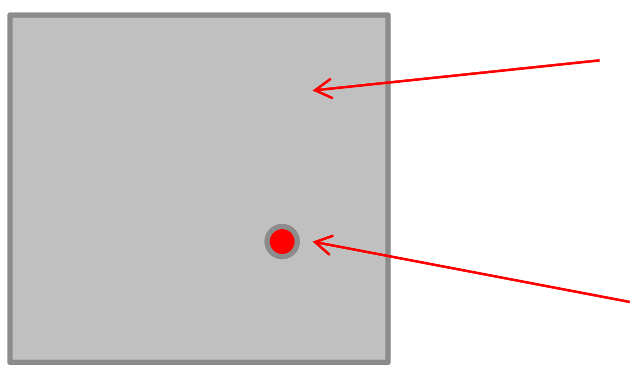


Choosing the blocks with point data



The "true" value can be replaced by the conditional simulated block data B^l

$$R_B(\mathbf{v}_\alpha) \approx D(\mathbf{v}_\alpha) - B^l(\mathbf{v}_\alpha)$$



$B^l(\mathbf{v}_\alpha)$

Conditional simulated block data

Conditioning point data: observation from a monitoring station

Block-data error incorporation

The variance of block error is obtained with the N_s realizations of B^l and the N_t time periods.

$$\sigma_R^2(\mathbf{v}_\alpha) = \frac{1}{N_t . N_s} \sum_{i=1}^{N_t} \sum_{l=1}^{N_s} \left(D(\mathbf{v}_\alpha, t_i) - B^l(\mathbf{v}_\alpha, t_i) \right)^2$$

The variance of block error can be parametrized for different meteorological conditions

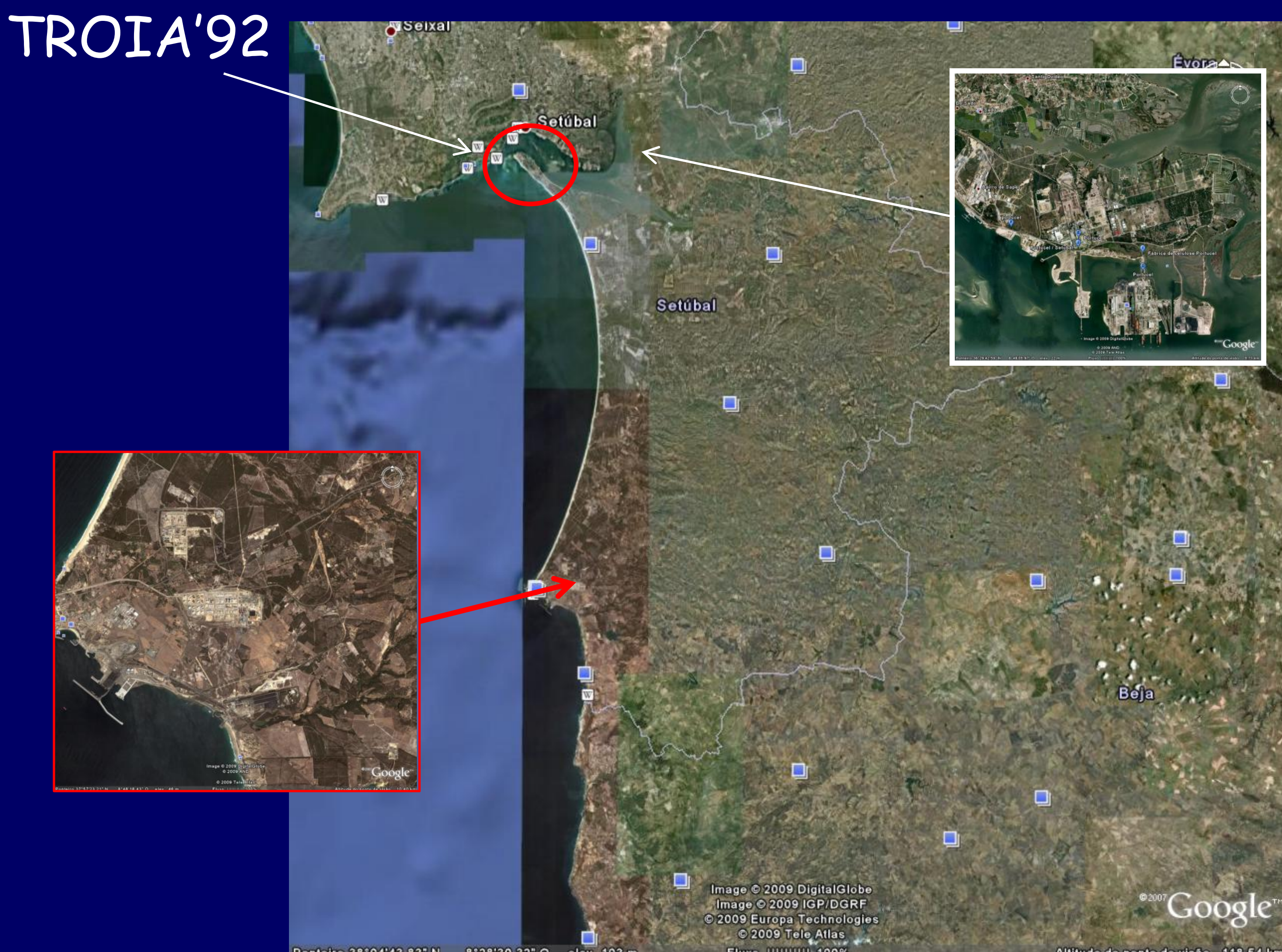
Block sequential simulation (BSSIM)

1. Define a random path visiting each node **u** of the grid. For each location **u** along the path:
2. Search conditioning data (point data, block data, previously simulated values)
3. Compute the local block-to-block, block-to-point, point-to-block and point-to-point covariances
4. Calculate local mean and variance by solving the mixed scale kringing system
5. Draw a value from the global cdf and add the simulated value to data set
6. Repeat (2-6) to generate another simulated realization

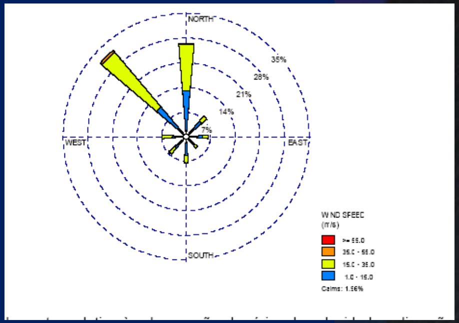
Air quality characterization at industrial area of Sines

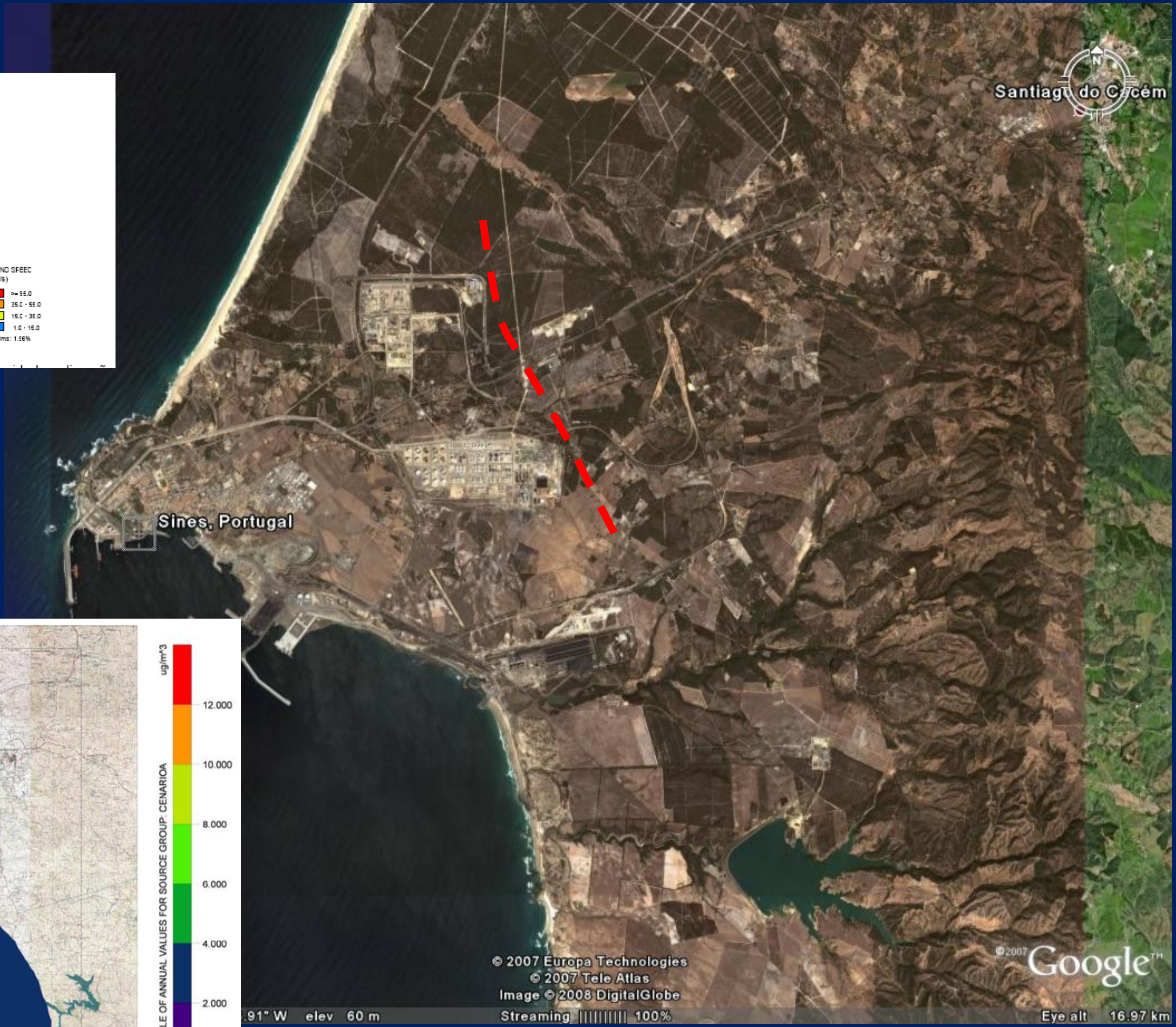


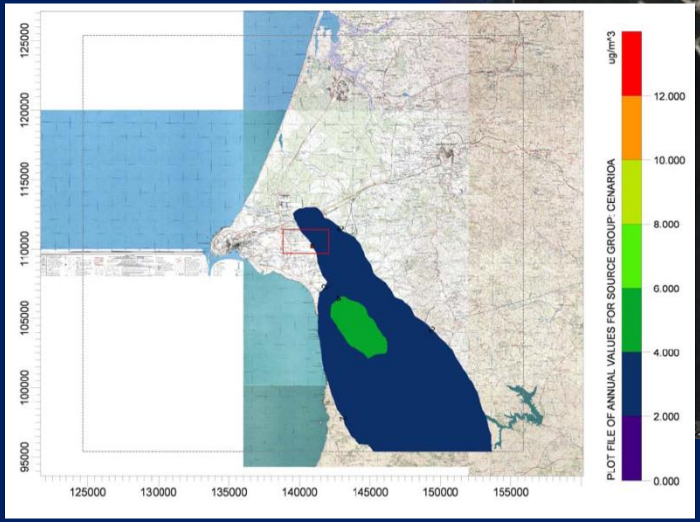

Sines Industrial Area



Emissions and Meteorological Conditions

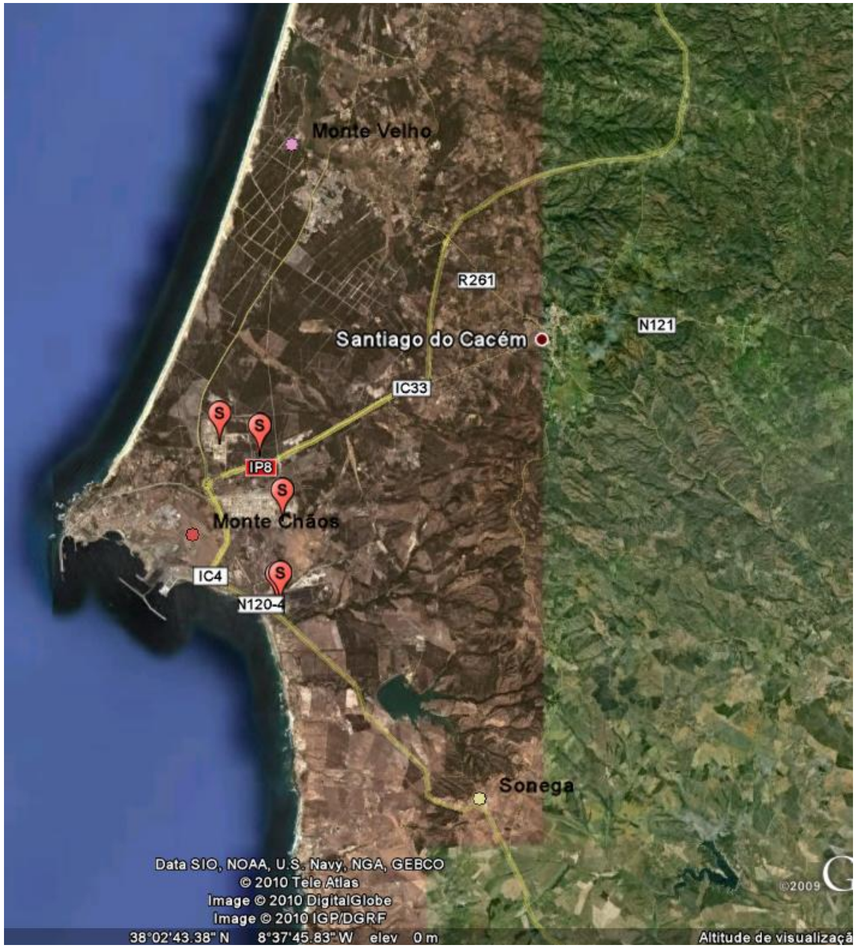






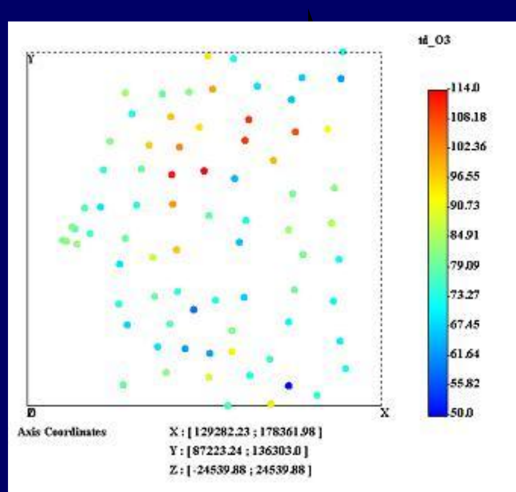
Sampling the Air Quality

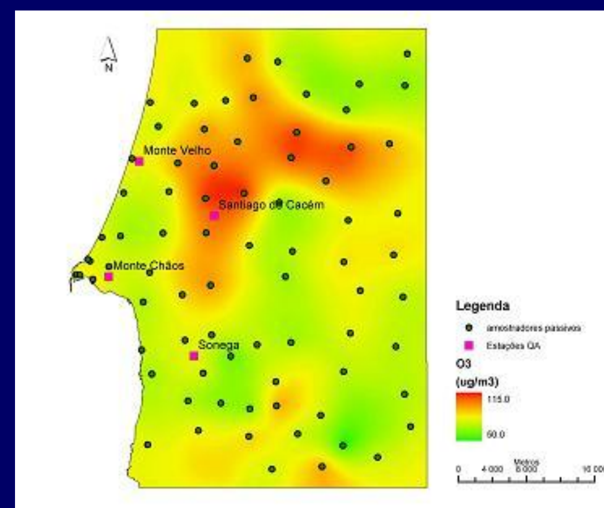
Case study



- SO_2 daily average atmospheric concentrations measurements (3 stations)
- SO_2 daily average emissions (5 stacks)
- Meteorological hourly data
- ICST3 (EPA)
- 24/07/2006 a 28/07/2006

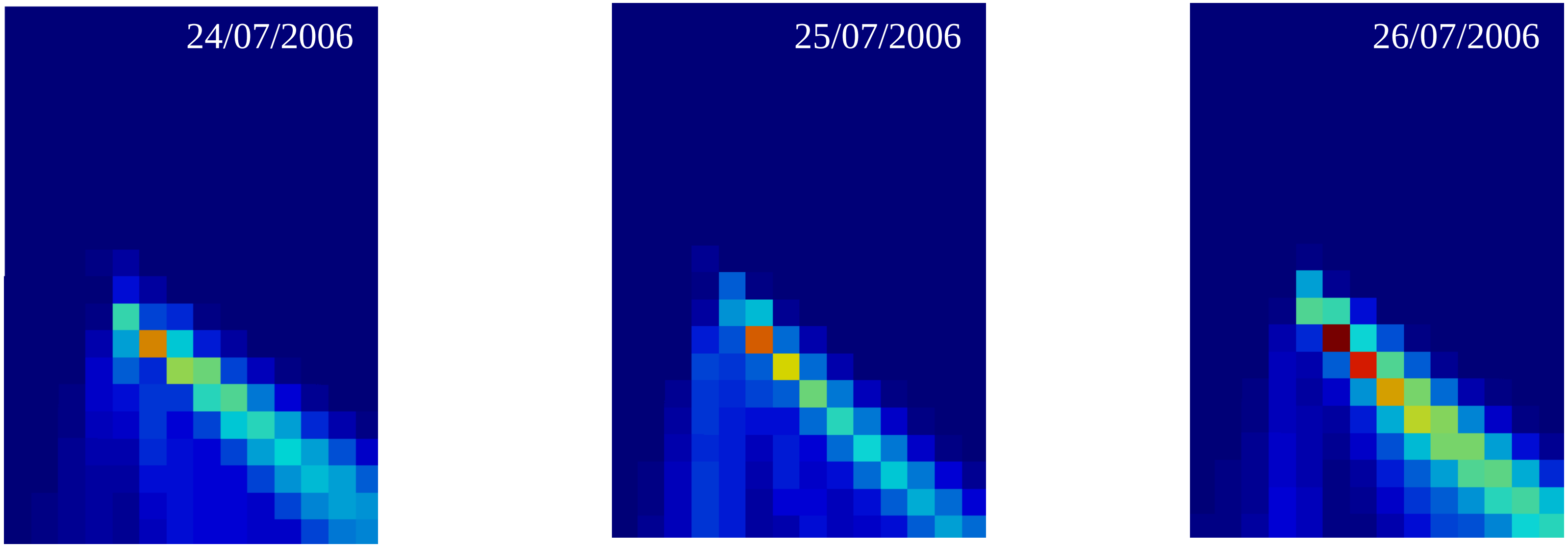
Difusive Tubes Campaign

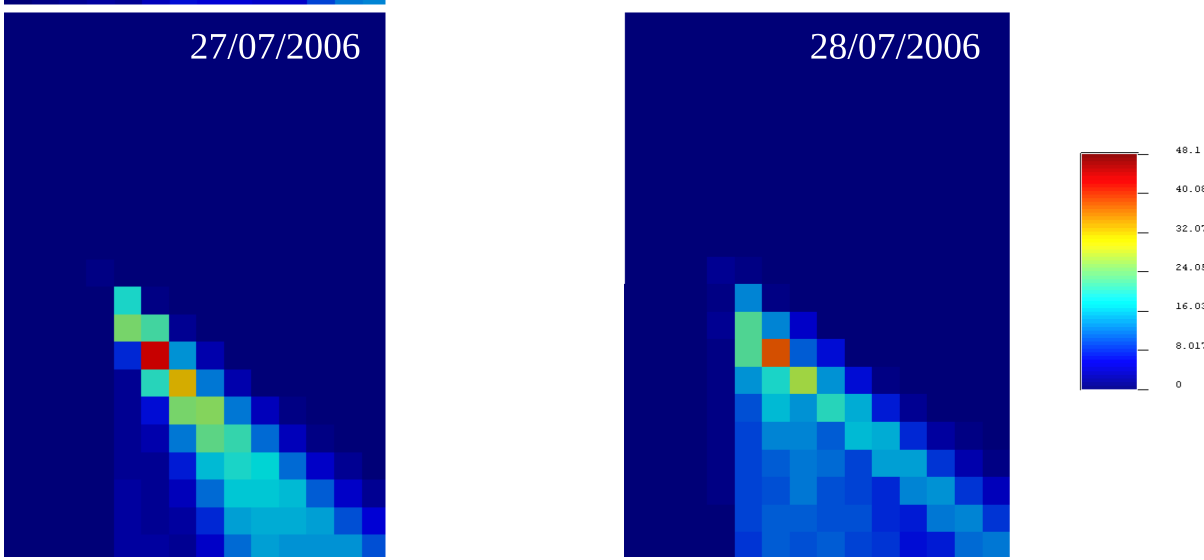




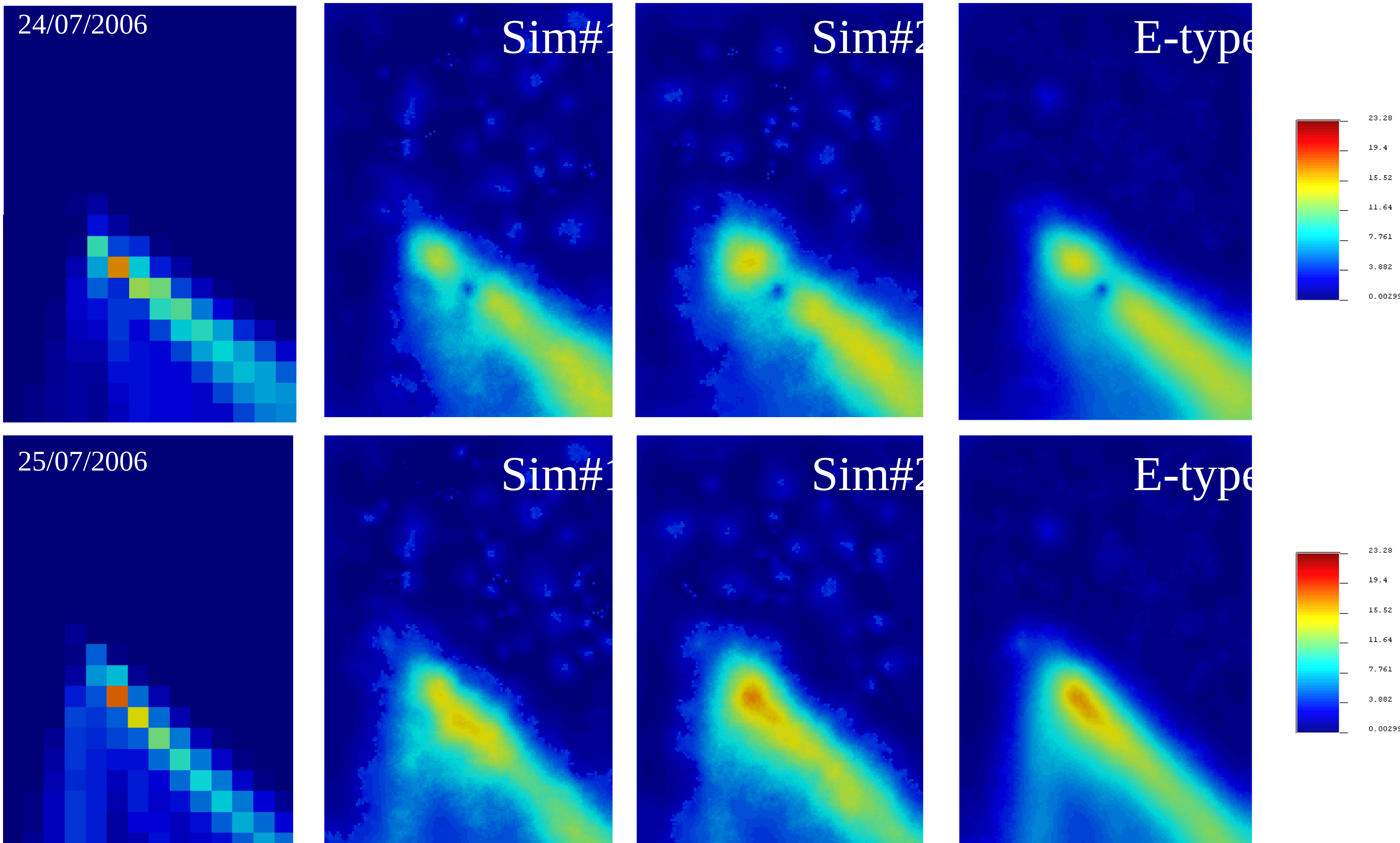
E.D. A nalysis ,Spatial variograms, calibration of Guassian Plume model

Gaussian Plume model : Block data

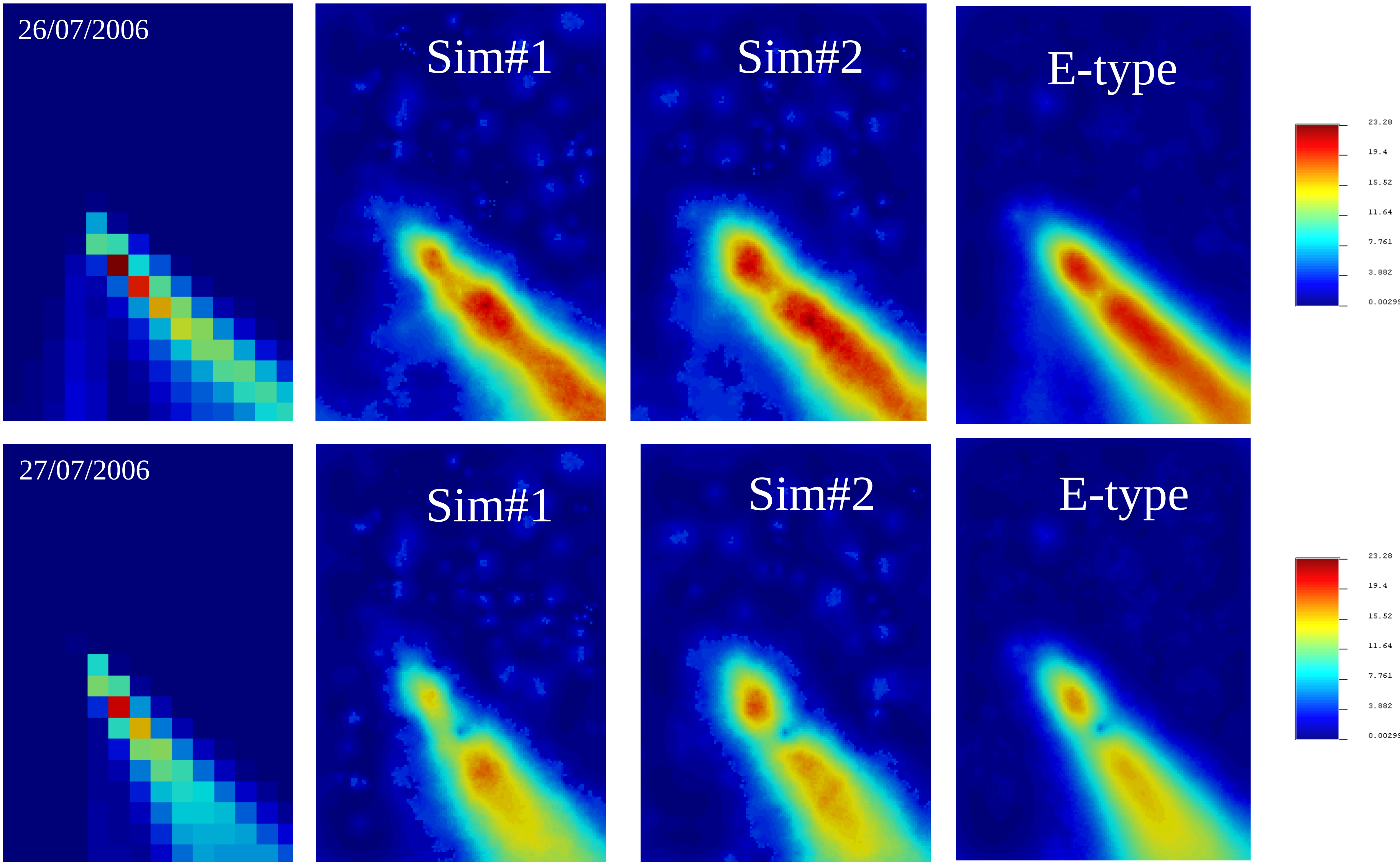




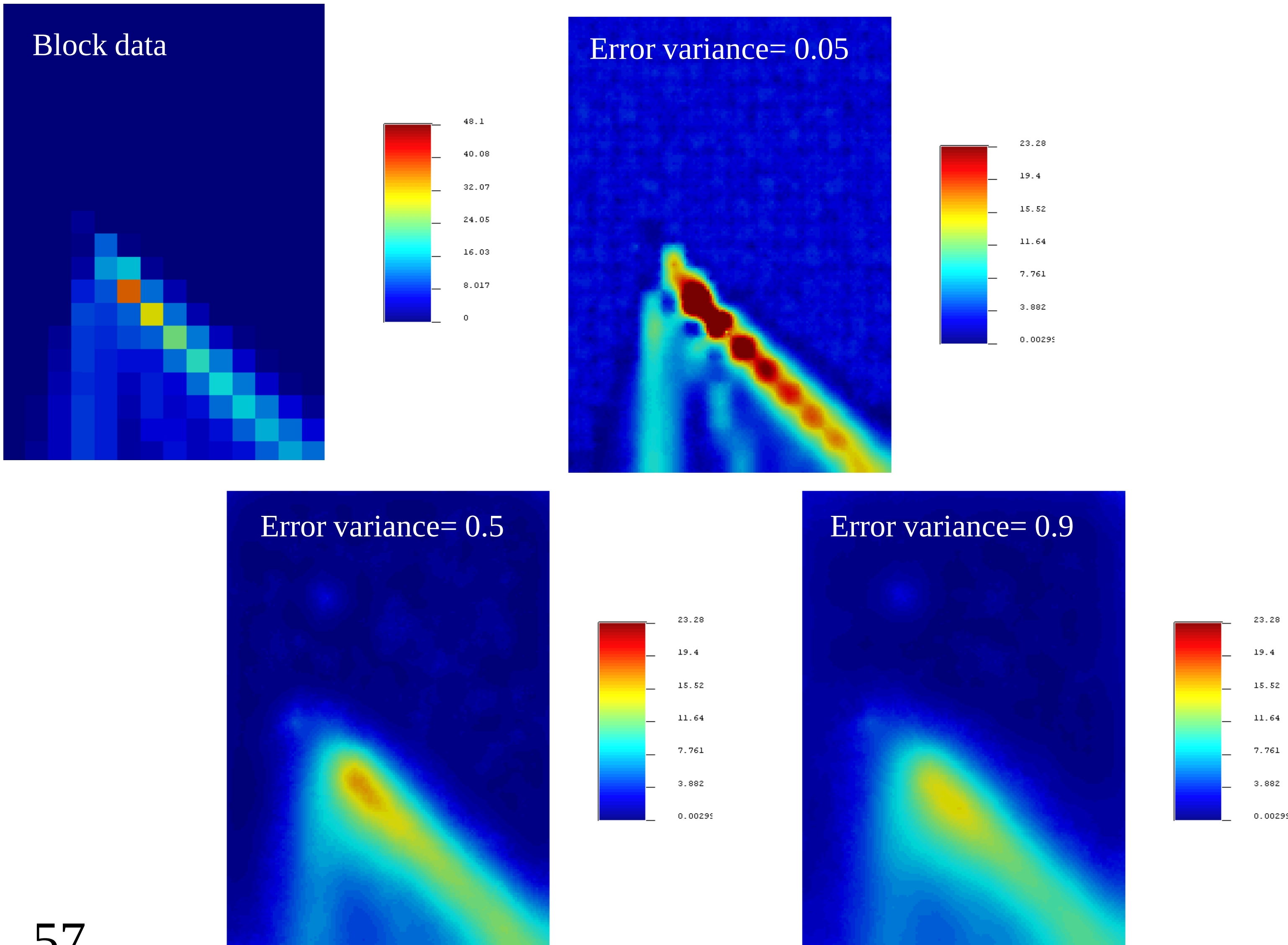
Number of blocks: 280
Block Size: 2500 m x 2500 m
Block Discretization: 3x3


24/07/2006
Sim#
Sim#
E-typ
23.28
19.4
15.52
11.64
7.761
3.882
25/07/2006
Sim#
Sim#
E-typ
23.28
19.4
15.52
11.64
7.761
3.882

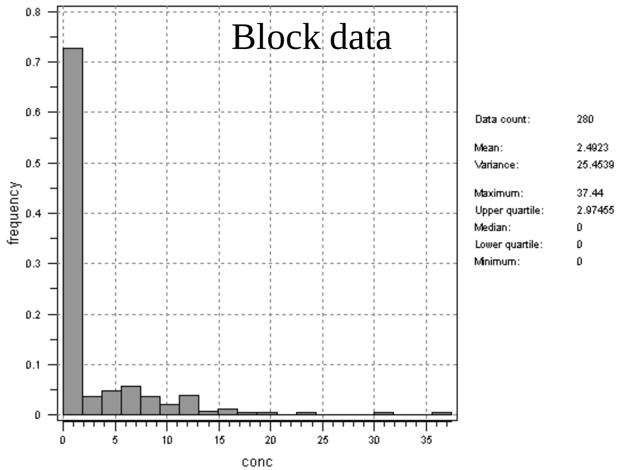
Results

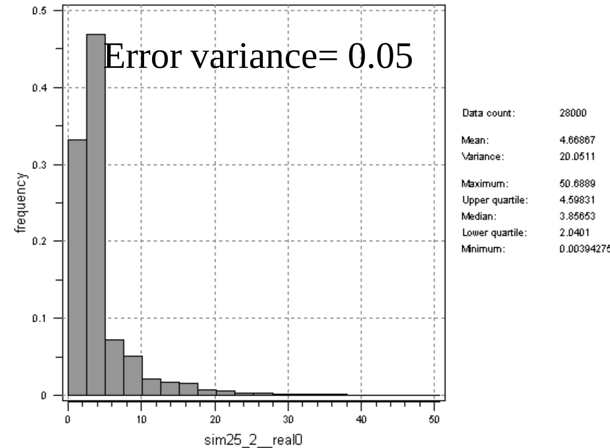

26/07/2006
Sim#1
Sim#2
E-type
27/07/2006
Sim#1
Sim#2
E-type
23.28
19.4
15.52
11.64
7.761
3.882
23.28
19.4
15.52
11.64
7.761
3.882

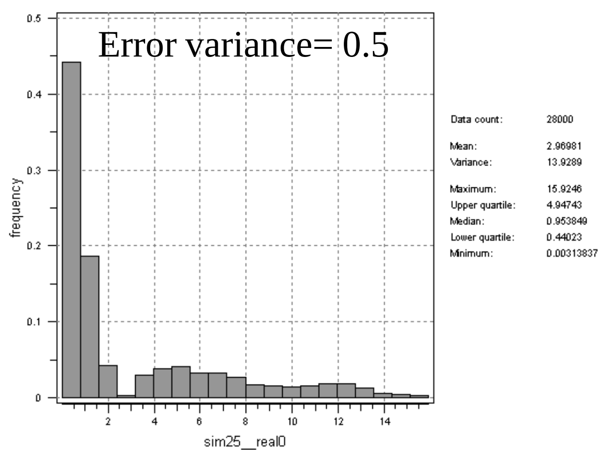
Block error effect

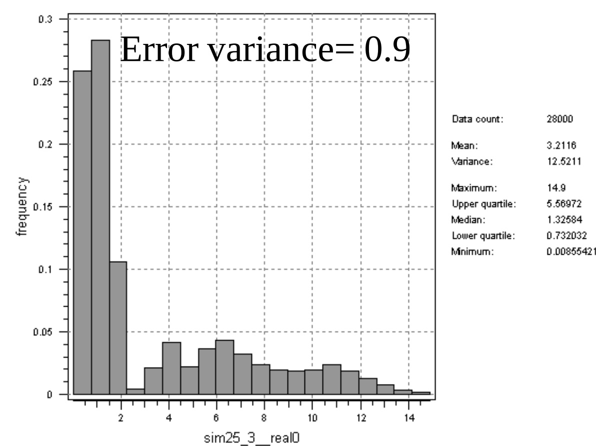


Block Error effect









Final remarks

- This hybrid multi-scale approach is a valuable methodology for predicting air quality

- Downscaling and calibration (with experimental point data) of maps obtained by deterministic dispersion models is achieved by the proposed method

Thank you