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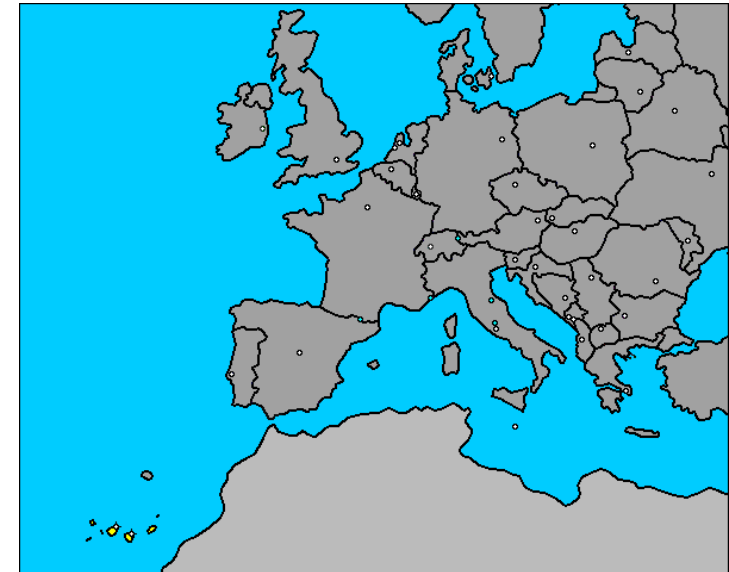
Application of genetic algorithms for the calibration of an air quality model and its validation using pollutant measures from the surroundings of an electric power plant

J. Ramírez ⁽¹⁾, A. Oliver ⁽¹⁾, E. Rodríguez ⁽¹⁾

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Motivation

- Validation of the framework proposed by the authors (Oliver et al. 2013, Energy) through experimental data from an electric power plant
- Gran Canaria island (Canary Islands)



- Two different stages: Modeling and Calibration – Two kinds of data are needed:
 - 1) Wind data
 - 2) Pollutant concentration data

- WIND DATA: For modeling and calibration
 - Wind data from 1 station close to power plant
 - Wind data from forecasting model
 - 3 consecutive days of wind data (hourly)
 - Calibration of mode through genetic algorithms



Motivation

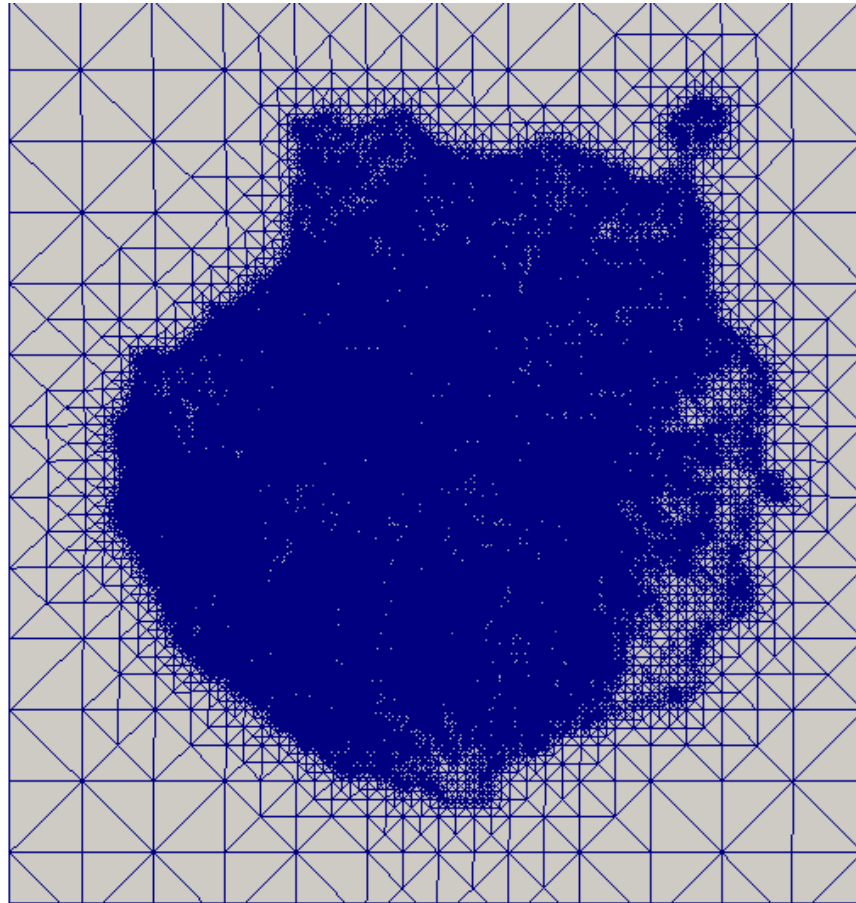
- Pollutants data: Some data for modeling and other for calibrating
 - One emission stack (Electric power plant) (modeling)
 - 3 immission stations (calibration)
 - 1 inmission station (validation)
 - 3 consecutive days of emission and immission data (hourly)
 - Calibration of model variables attending experimental data from **immission**



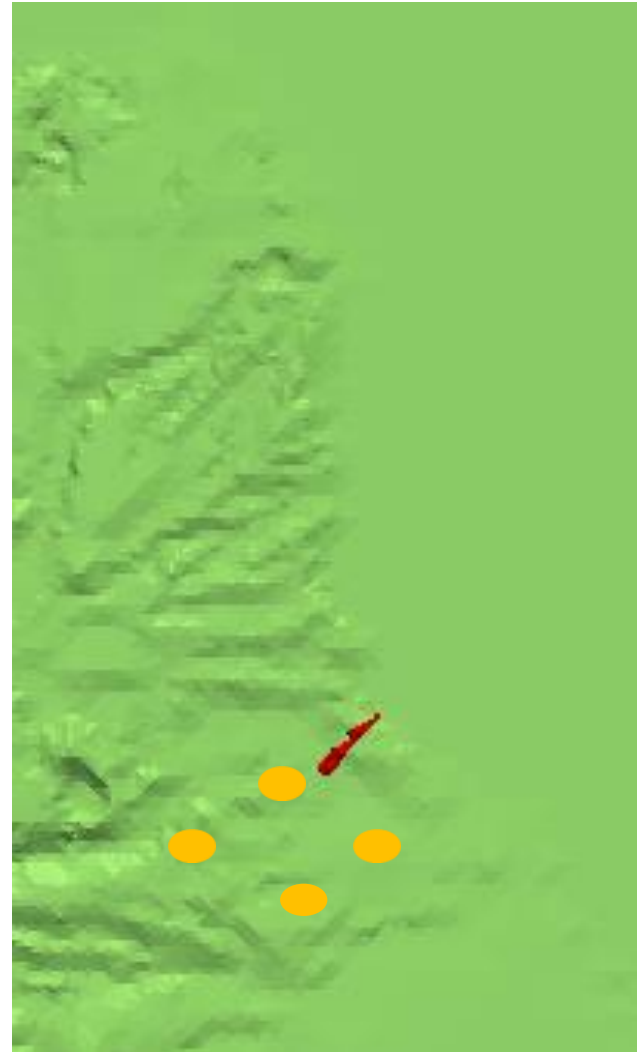
Adaptive Finite Element Model

- Construction of a tetrahedral mesh adapted to the terrain
- Wind field modeling from experimental and meteorological data
- Pollutant dispersion modeling

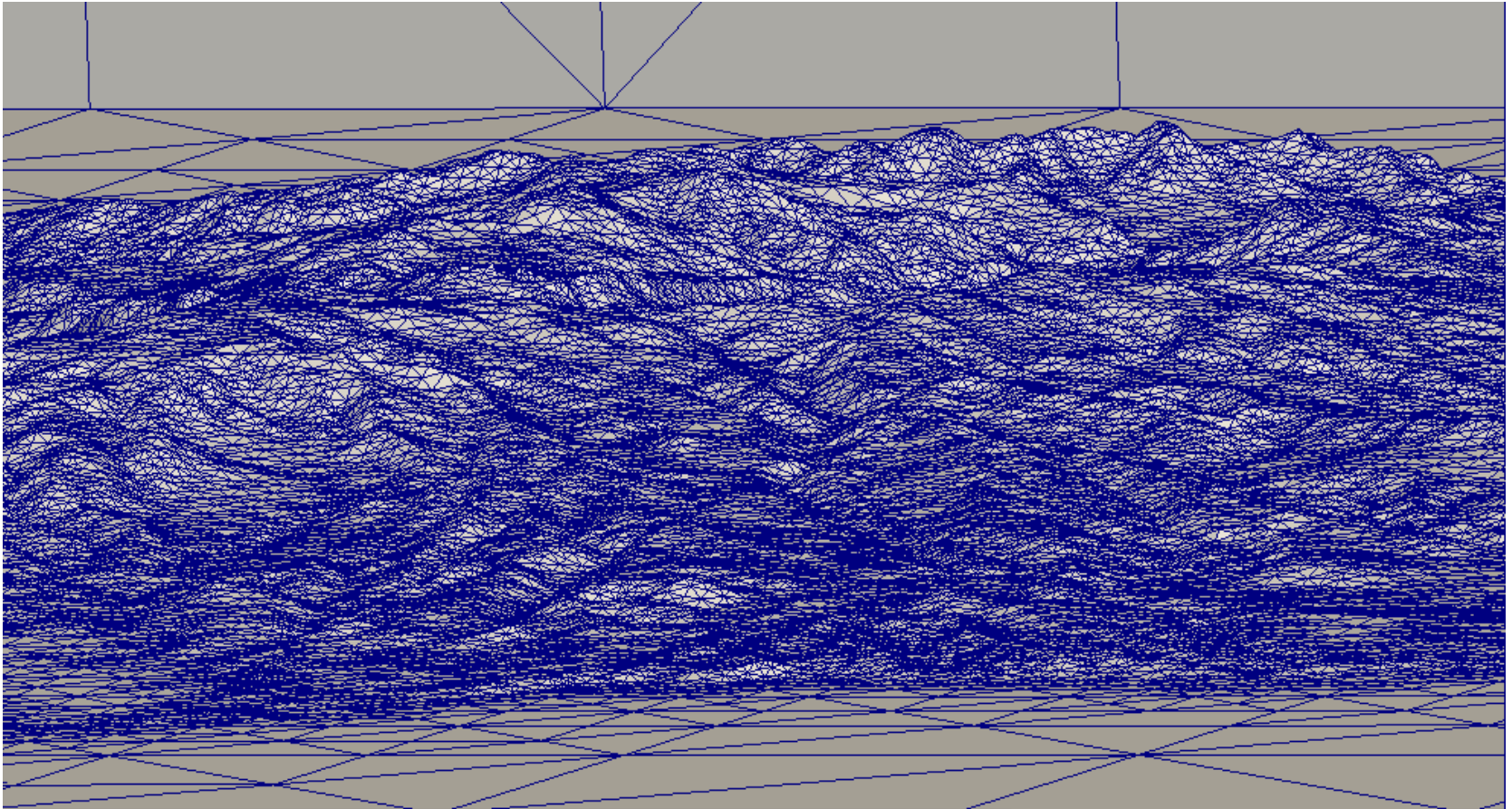
Gran Canaria Mesh



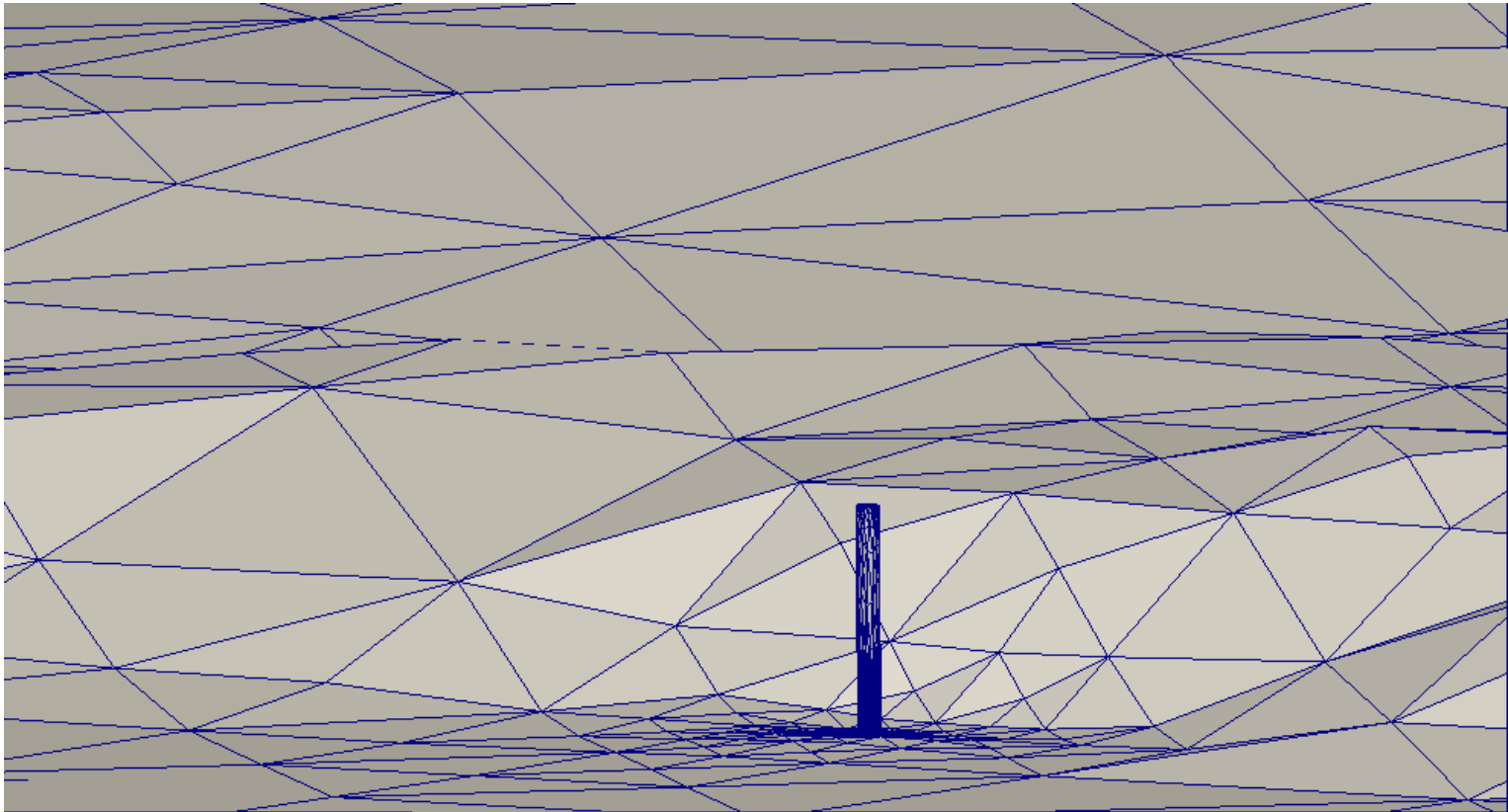
Gran Canaria Mesh (II)



Gran Canaria Mesh



Gran Canaria Mesh

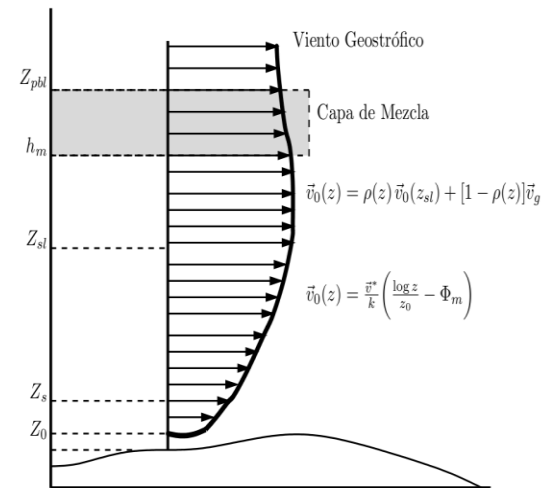


Wind field modeling

- Experimental data from 1 station (power plant)
- Use Harmonie model

- Horizontal interpolation
 - Weighting inverse to the squared distance and inverse height differences
- Vertical interpolation
 - Log-linear wind profile

$$\tilde{\mathbf{v}}_0(z_m) = \varepsilon \frac{\sum_{n=1}^N \frac{\tilde{\mathbf{v}}_n}{d_n^2}}{\sum_{n=1}^N \frac{1}{d_n^2}} + (1 - \varepsilon) \frac{\sum_{n=1}^N \frac{\tilde{\mathbf{v}}_n}{|\Delta h_n|}}{\sum_{n=1}^N \frac{1}{|\Delta h_n|}}$$



Wind field modeling

- The resulting mass-consistent wind field \mathbf{u} verifies:

$$\begin{aligned}\nabla \cdot \mathbf{u} &= 0 && \text{in } \Omega \\ \mathbf{n} \cdot \mathbf{u} &= 0 && \text{on } \Gamma_a\end{aligned}$$

and minimizes the adjusting functional

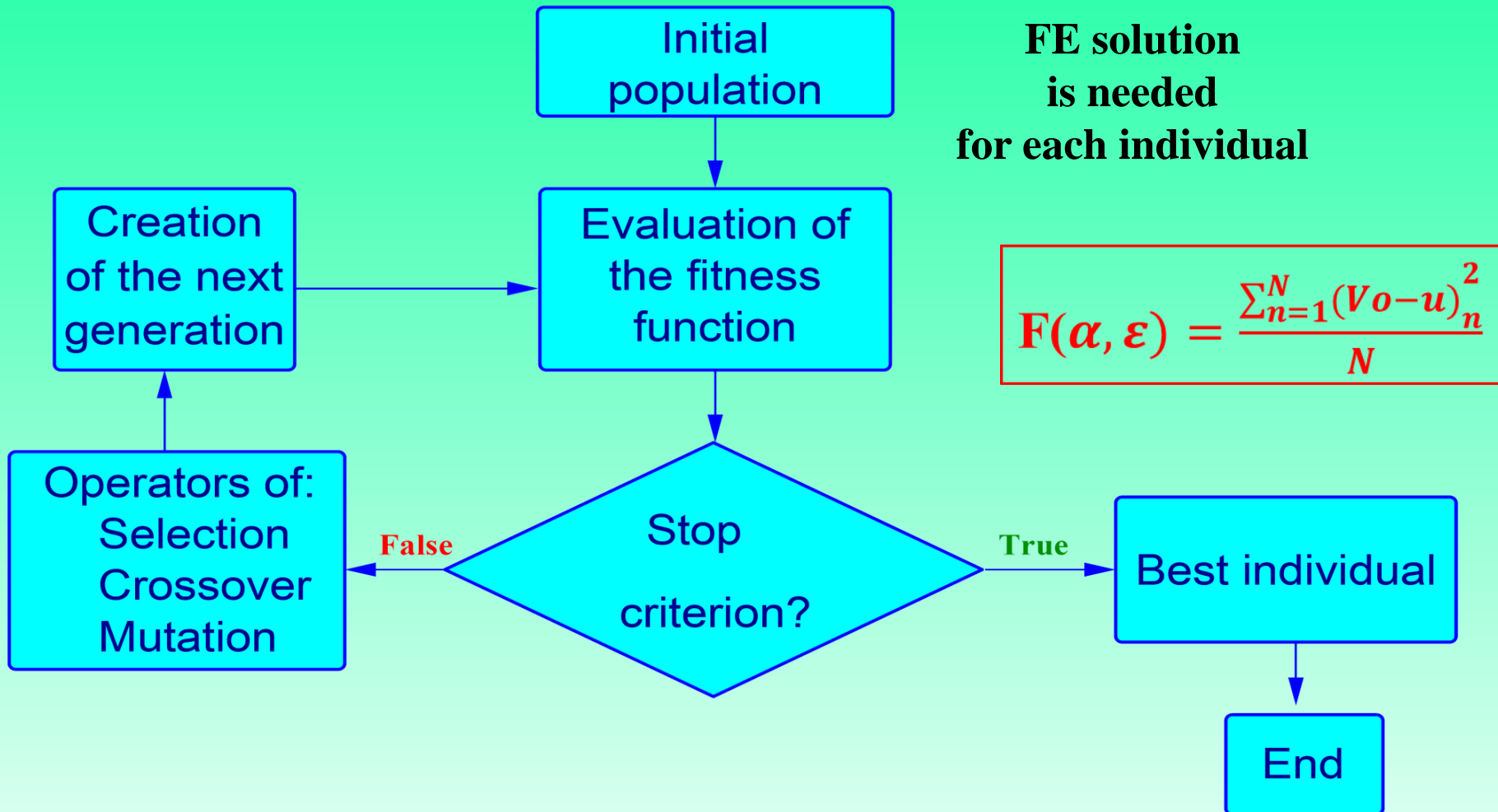
$$E(\mathbf{v}) = \frac{1}{2} \int_{\Omega} (\mathbf{v} - \mathbf{u}_0)^t \mathbf{P} (\mathbf{v} - \mathbf{u}_0) d\Omega$$

- Introducing a Lagrange multiplier and solving an elliptic problem

- Calibration
 - ε (Horizontal interpolation weight)
 - T_v T_h (Mass consistent factors, $\alpha = \frac{T_h}{T_v}$)

- Genetic algorithms
 - *G. Montero, E. Rodriguez, R. Montenegro, J.M. Escobar, J.M. Gonzalez-Yuste, **Genetic algorithms for na improved parameter estimation with local refinement of tetrahedral meshes in a wind model**, Advances in Engineering Software, Volume 36, Issue 1, January 2005, Pages 3-10, ISSN 0965-9978, [DOI:10.1016/j.advengsoft.2004.03.011]*

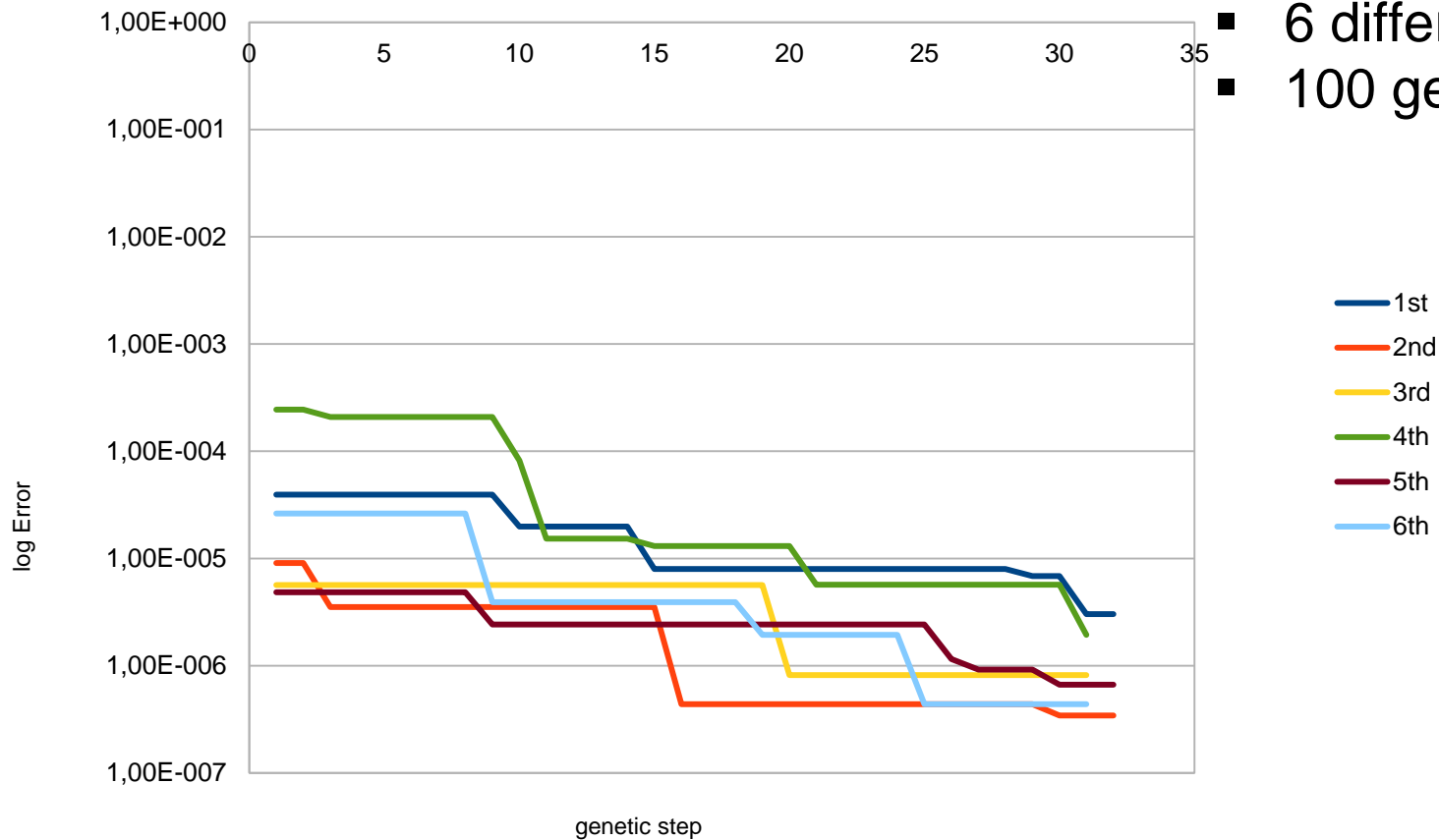
Wind field Calibration



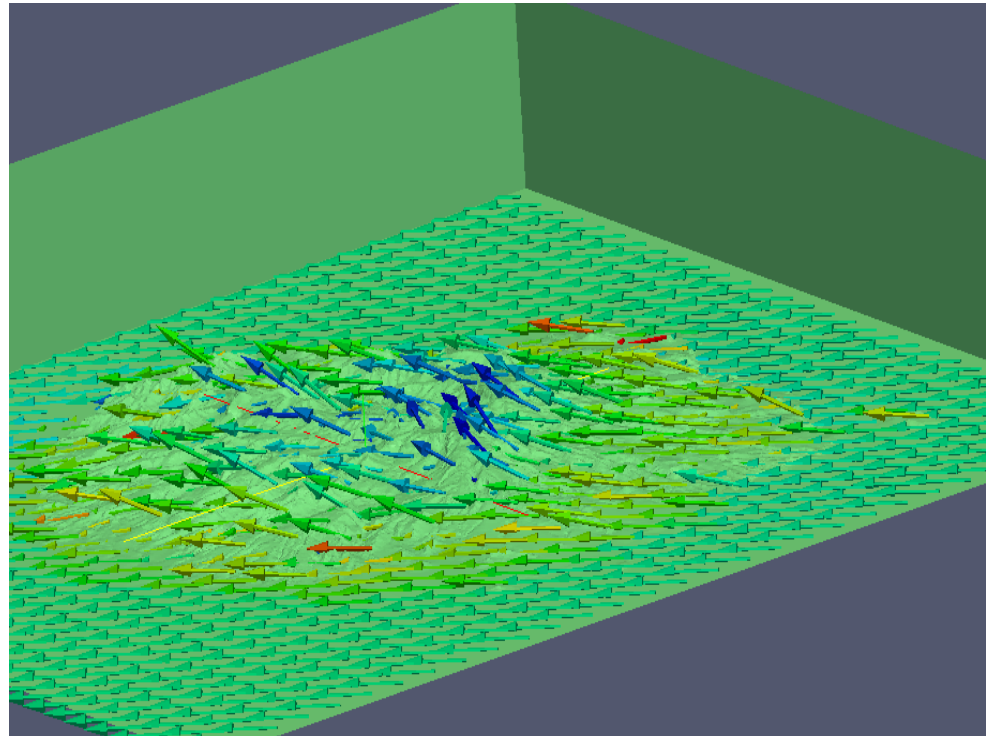
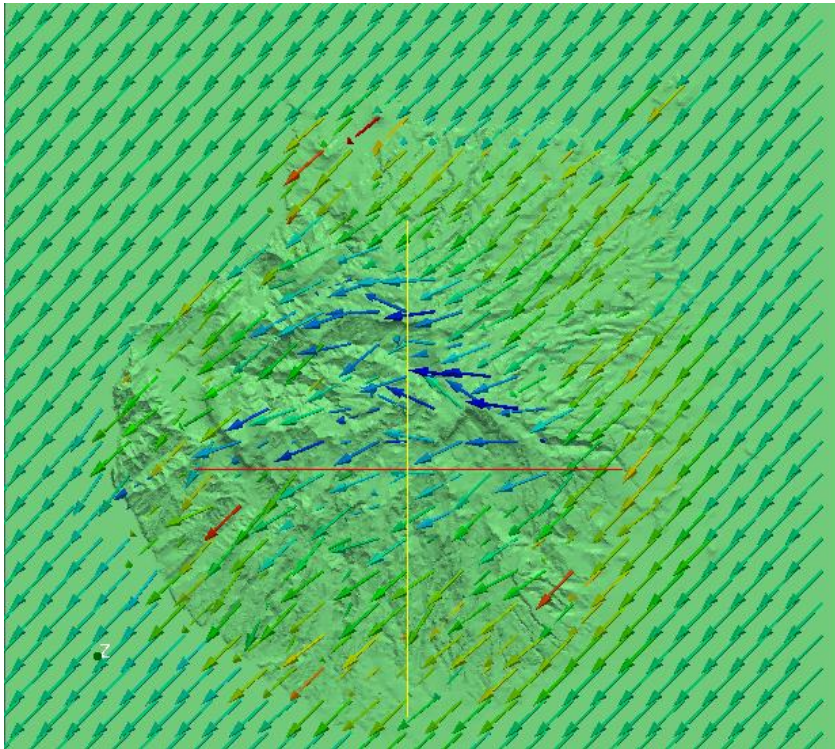
Wind field Calibration

Genetic Algorithm evolution

- Initial population 1000
- 6 different episodes
- 100 genetic iterations



Wind field results



Air quality modeling

Find concentration $\mathbf{c}(\mathbf{x}, t)$ for $(\mathbf{x}, t) \in \Omega \times (0, t^{end}]$

$$\frac{\partial \mathbf{c}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{c} = \nabla \cdot (\mathbf{K} \nabla \mathbf{c}) + \mathbf{e} + \mathbf{s}(\mathbf{c})$$

$$c(x, t) = c^{emi} \quad \text{Stack outflow}$$

$$c(x, t) = c^{amb} \quad \text{Inlet wind boundaries}$$

$$n \cdot \nabla c = 0 \quad \text{Outlet wind boundaries}$$

$$c(x, 0) = c^{ini} \quad \text{Initial condition}$$

$$n \cdot k \nabla c = -V^d c \quad \text{Terrain condition} \quad (\text{Vd is the deposition diagonal matrix})$$

- Temporal discretization: Cranck-Nicolson
- Spatial discretization: Least Squares FEM
- System solver: Conjugate gradient preconditioned with an Incomplete Cholesky Factorization
- Matrix storage: sparse MCS (matrix column storage)

- Calibration
 - Diffusion (K), minimization of F(k):

$$F(k) = RMSE = \sqrt{\frac{\sum_{n=1}^N (c - c_t)^2}{N}}$$

K = diffusion parameter

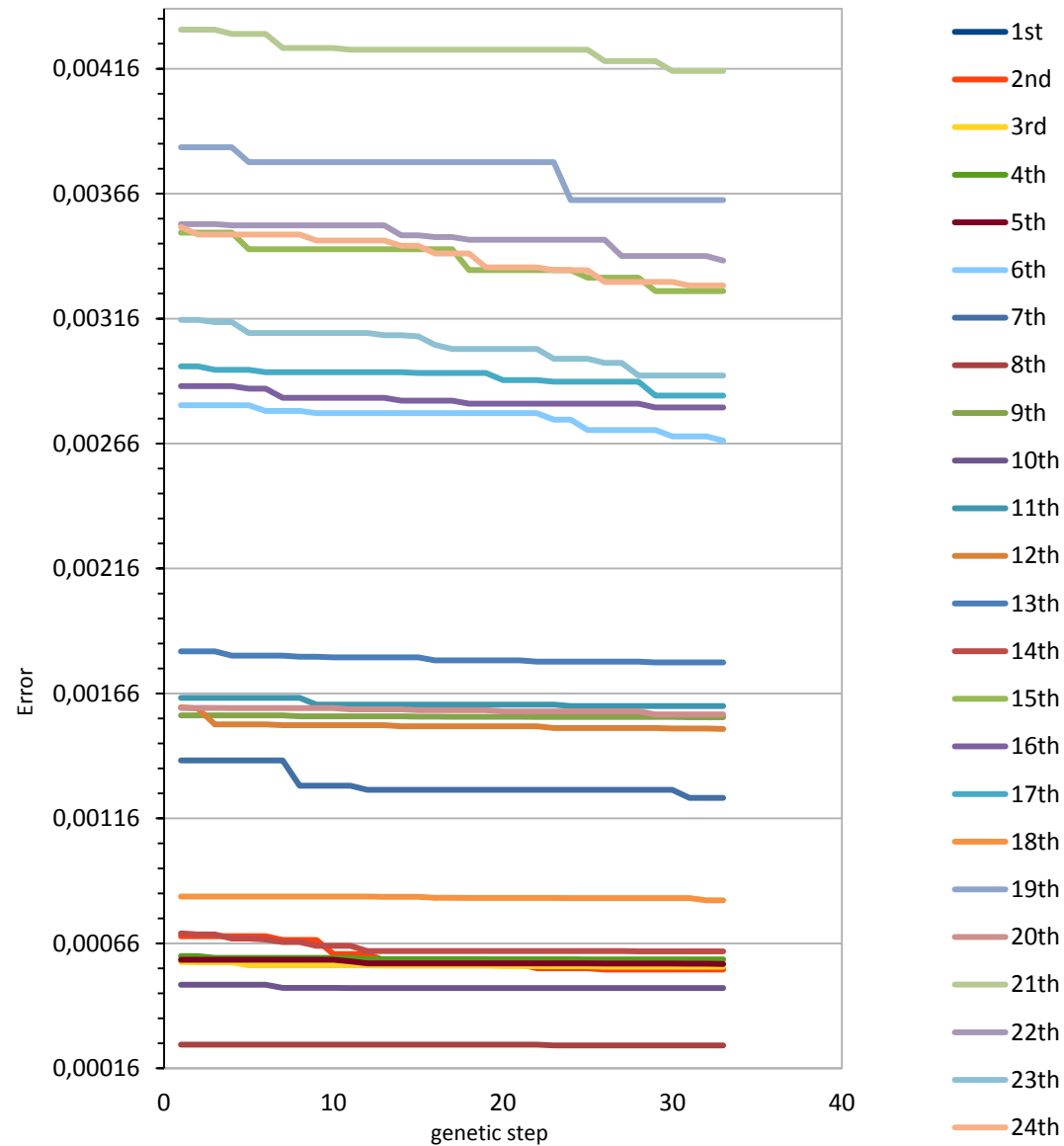
N = number of stations

C = measured concentration in the station

C_t = Calculated concentration

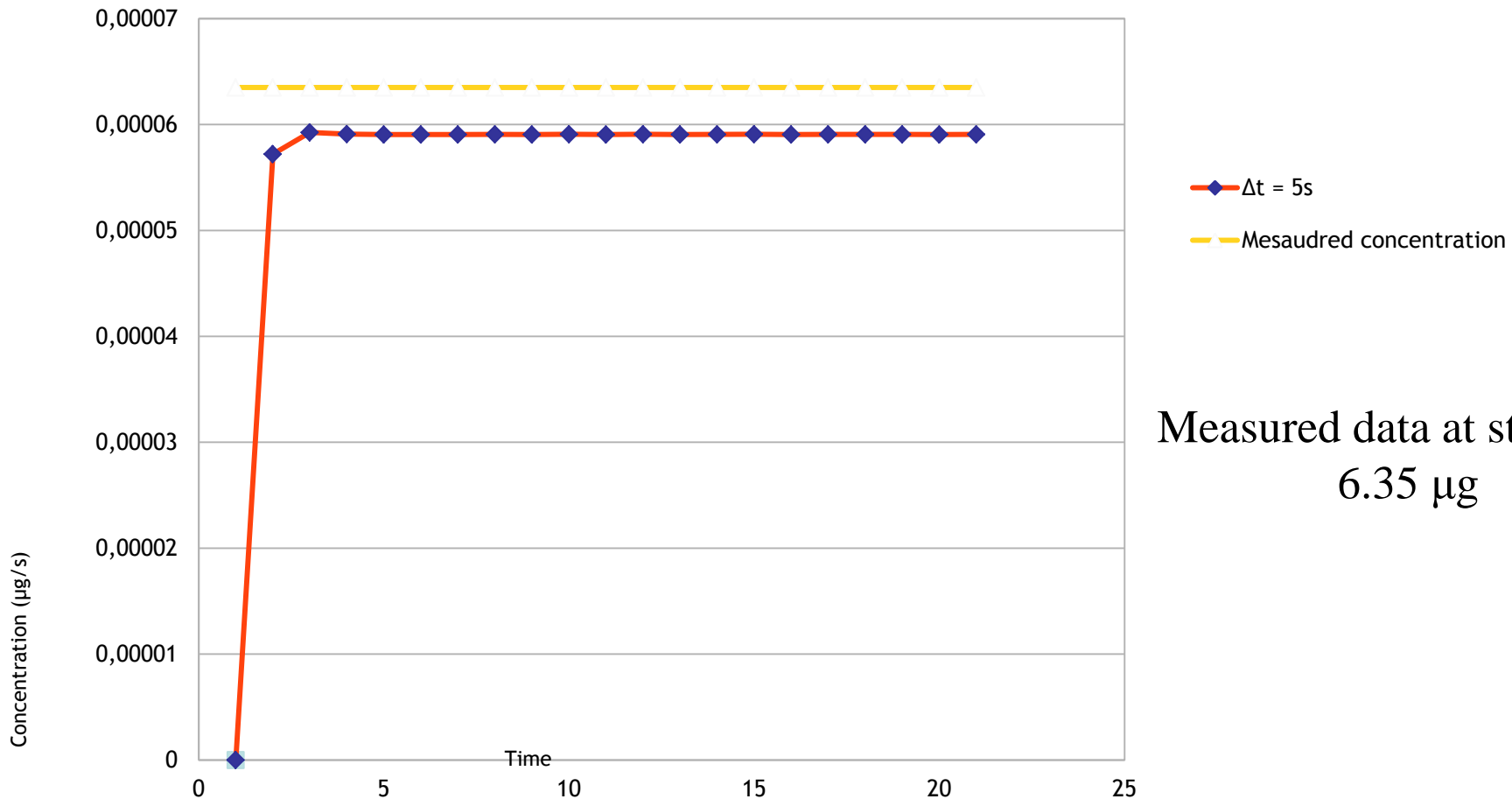
Air quality Calibration

- Genetic algorithm evolution
- 24 hours simulation
- 64 individual population
- 32 genetic steps
- Based on 3 stations data



Air quality Validation

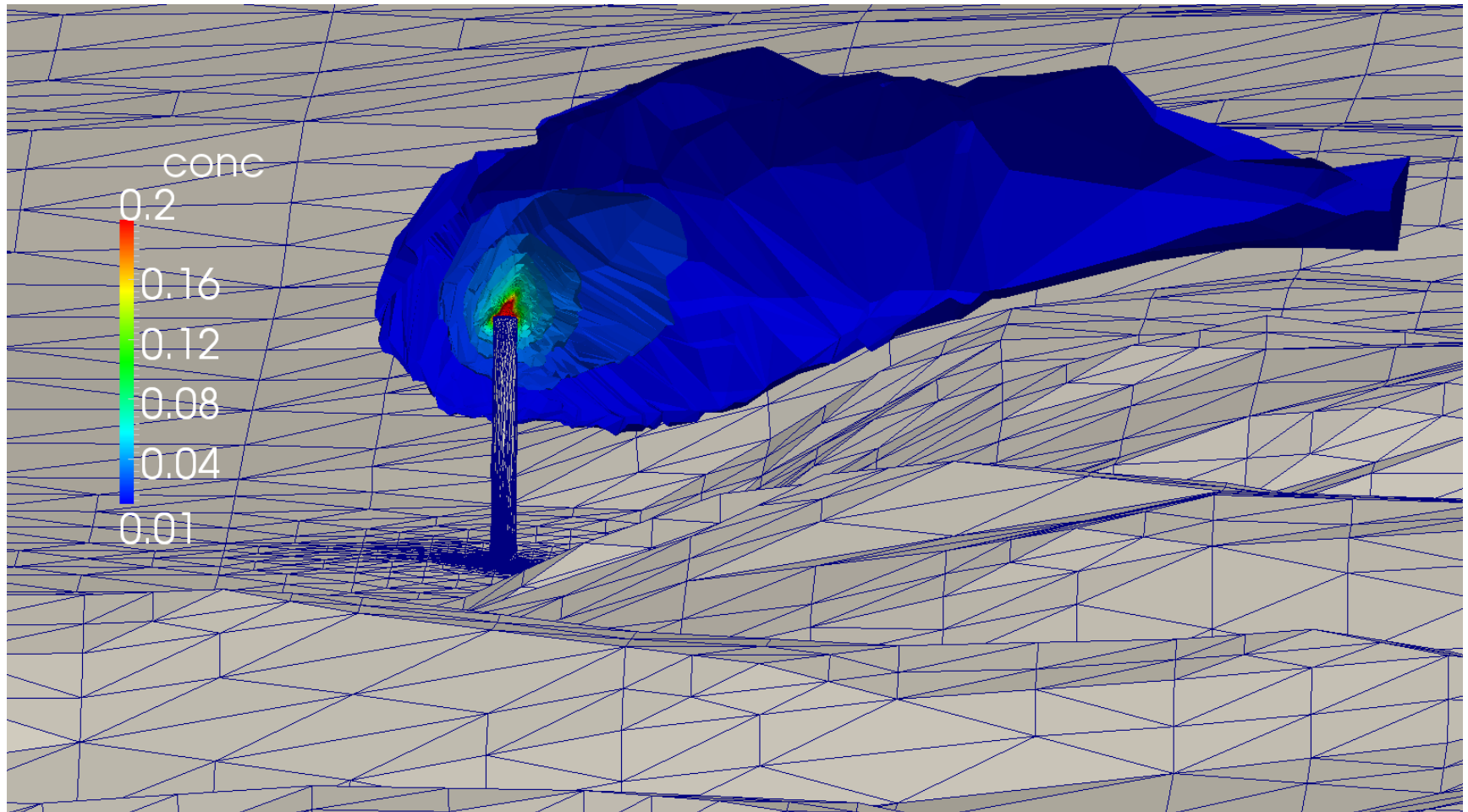
Validation



Measured data at station 1:
6.35 μg

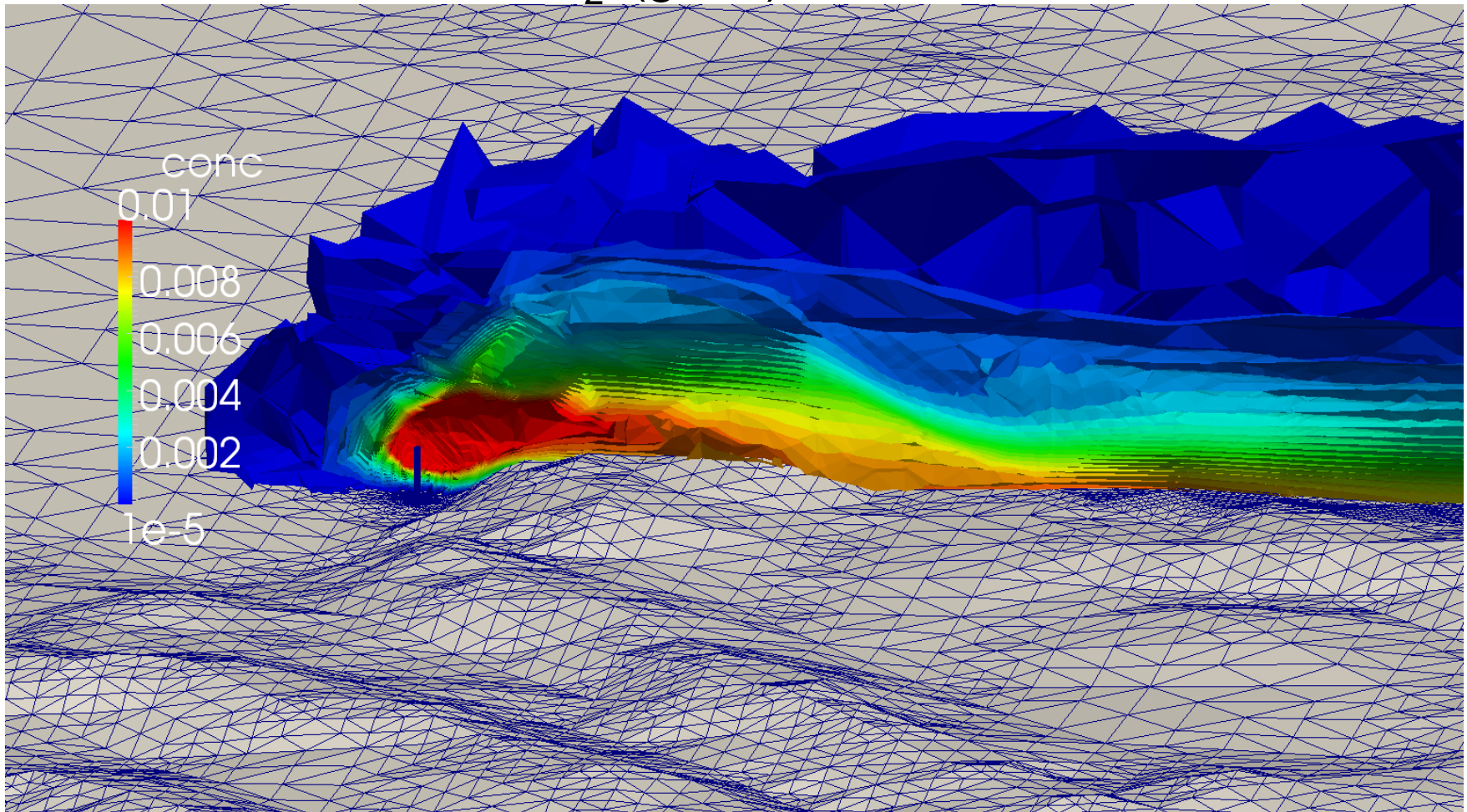
Air quality Results

Concentration SO_2 (g/m^3) after 1000 seconds



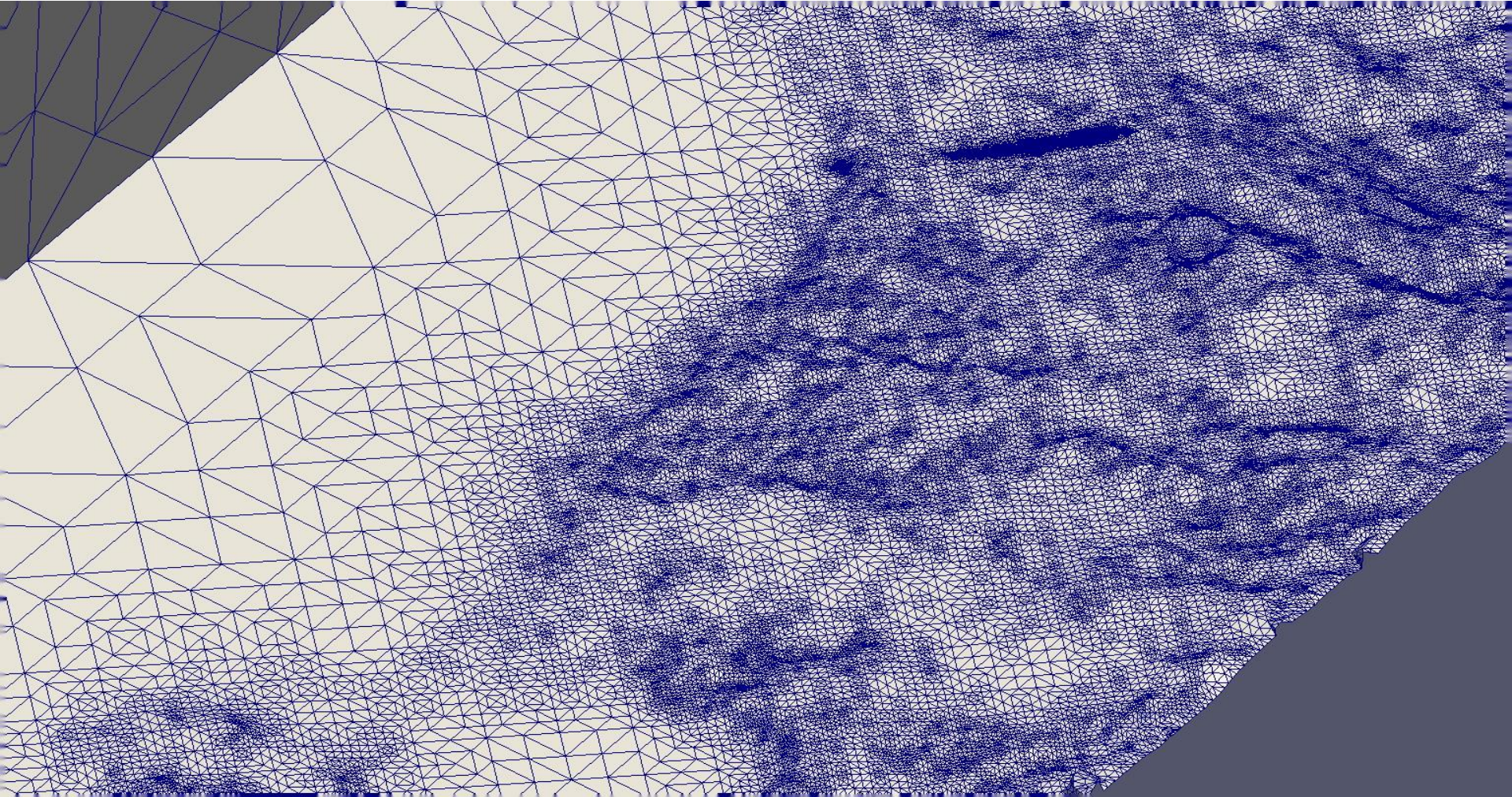
Air quality Results

Concentration SO_2 (g/m^3) after 1000 seconds



Air quality Results

Isosurface evolution $1 \mu\text{g}/\text{m}^3$



- Suitable approach for modeling air transport and reaction over complex terrains
 - A. Oliver, G. Montero, R. Montenegro, E. Rodríguez, J.M. Escobar, A. Pérez-Foguet, **Adaptive finite element simulation of stack pollutant emissions over complex terrains**, Energy, Volume 49, 1 January 2013, Pages 47-60, ISSN 0360-5442, <http://dx.doi.org/10.1016/j.energy.2012.10.051>.
- Genetic algorithms useful for calibration
- Validation comparing model outcomes with experimental data



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