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Calibration and validation of an air quality finite element model around an electric power plant in Gran Canaria island

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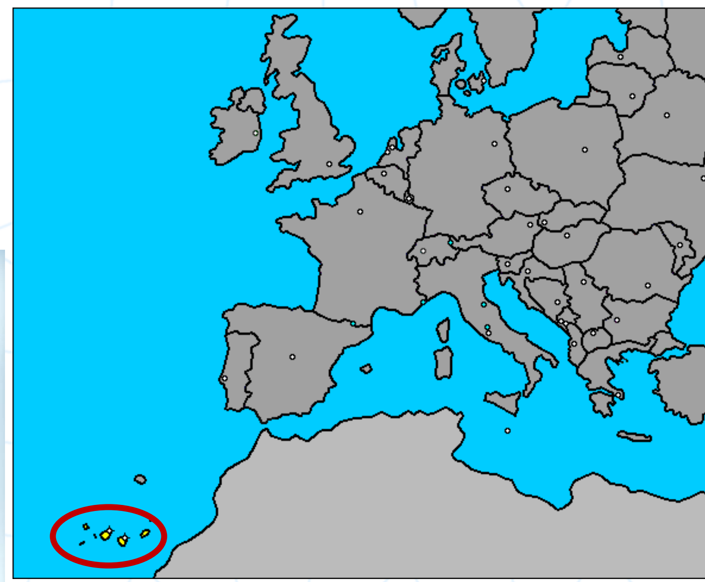
Motivation

- 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)



Motivation

- Two different stages: Modeling and Calibration – Two kinds of data are needed:

1) Wind data
2) Pollutant concentration data

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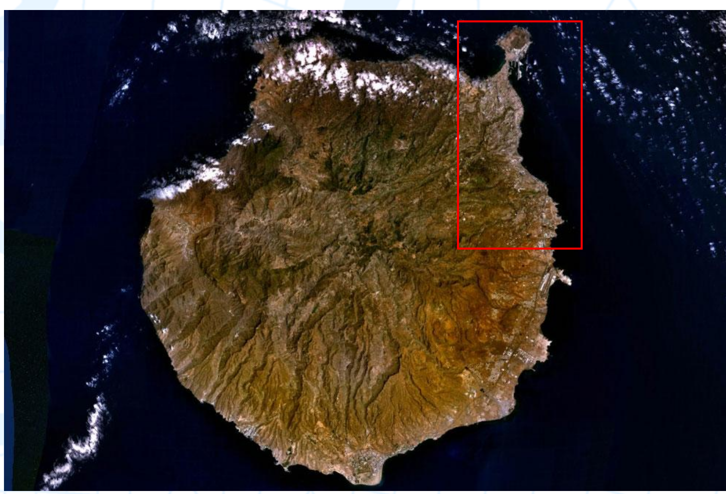
Motivation

- 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)
  - 4 immission stations (calibration)
  - 3 consecutive days of emission and immission data (hourly)
  - Calibration of model variables attending experimental data from **immission**



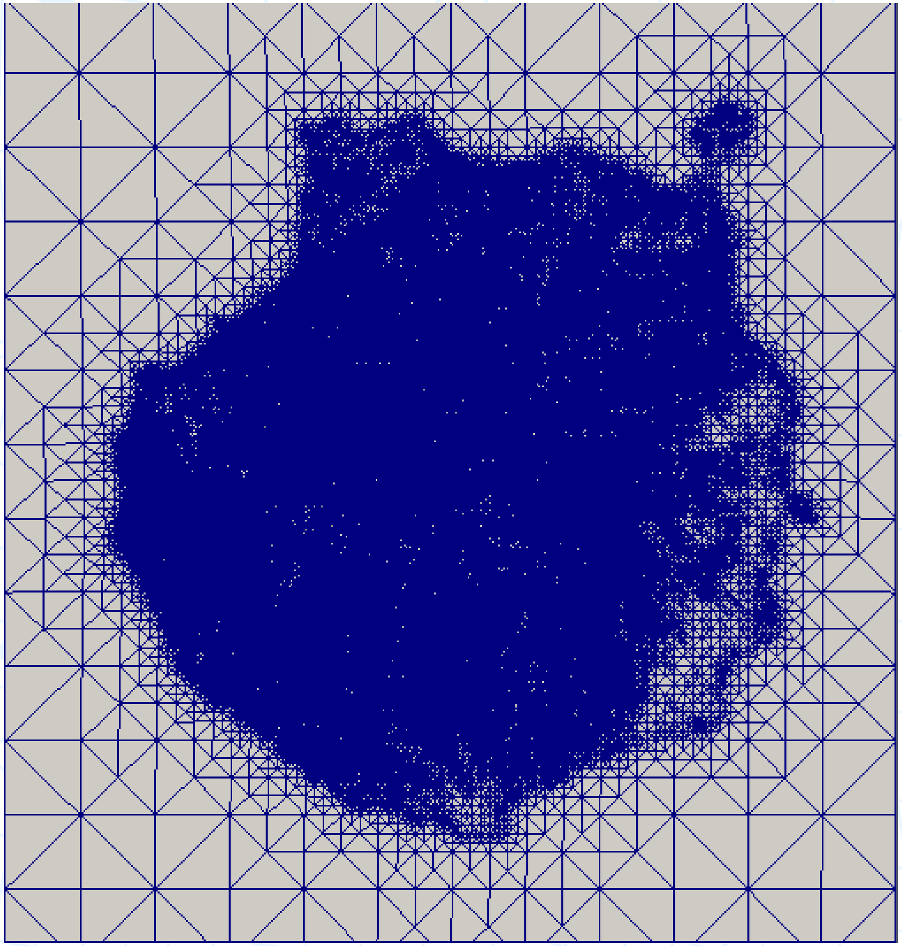
Algorithm

Adaptive Finite Element Model

- Construction of a tetrahedral mesh adapted to the terrain with the Meccano method
- Wind field modeling from experimental and meteorological data
  - Horizontal and vertical interpolation from HARMONIE data and experimental wind data from station
  - Mass consistent computation
  - Calibration of wind parameters
- Pollutant dispersion modeling
  - Wind field plume rise perturbation
  - Transport and reaction pollutant simulation
  - Calibration of transport parameters

Mesh construction

Gran Canaria Mesh



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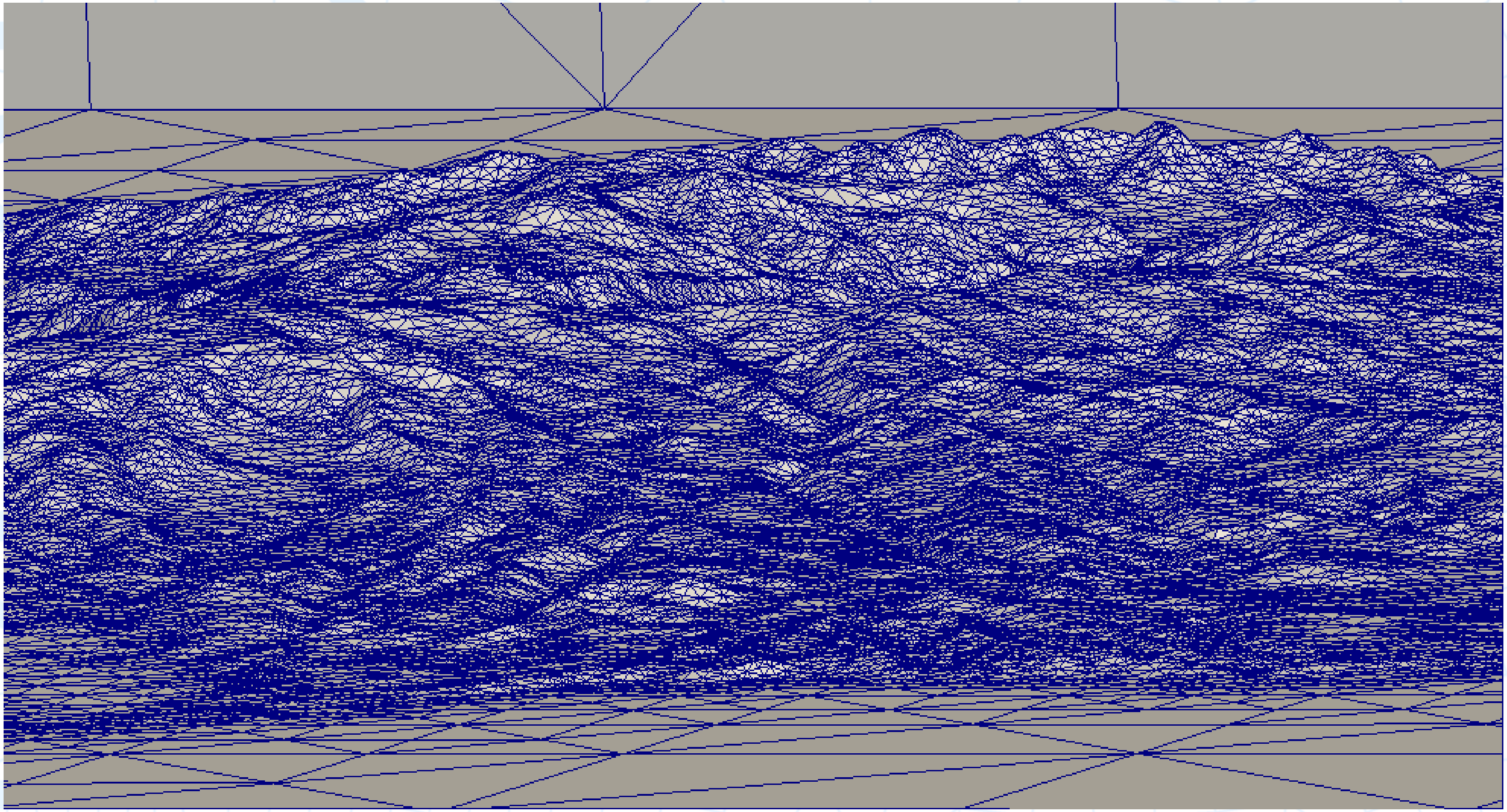
Mesh construction

Gran Canaria Mesh (II)

Mesh construction

Gran Canaria Mesh



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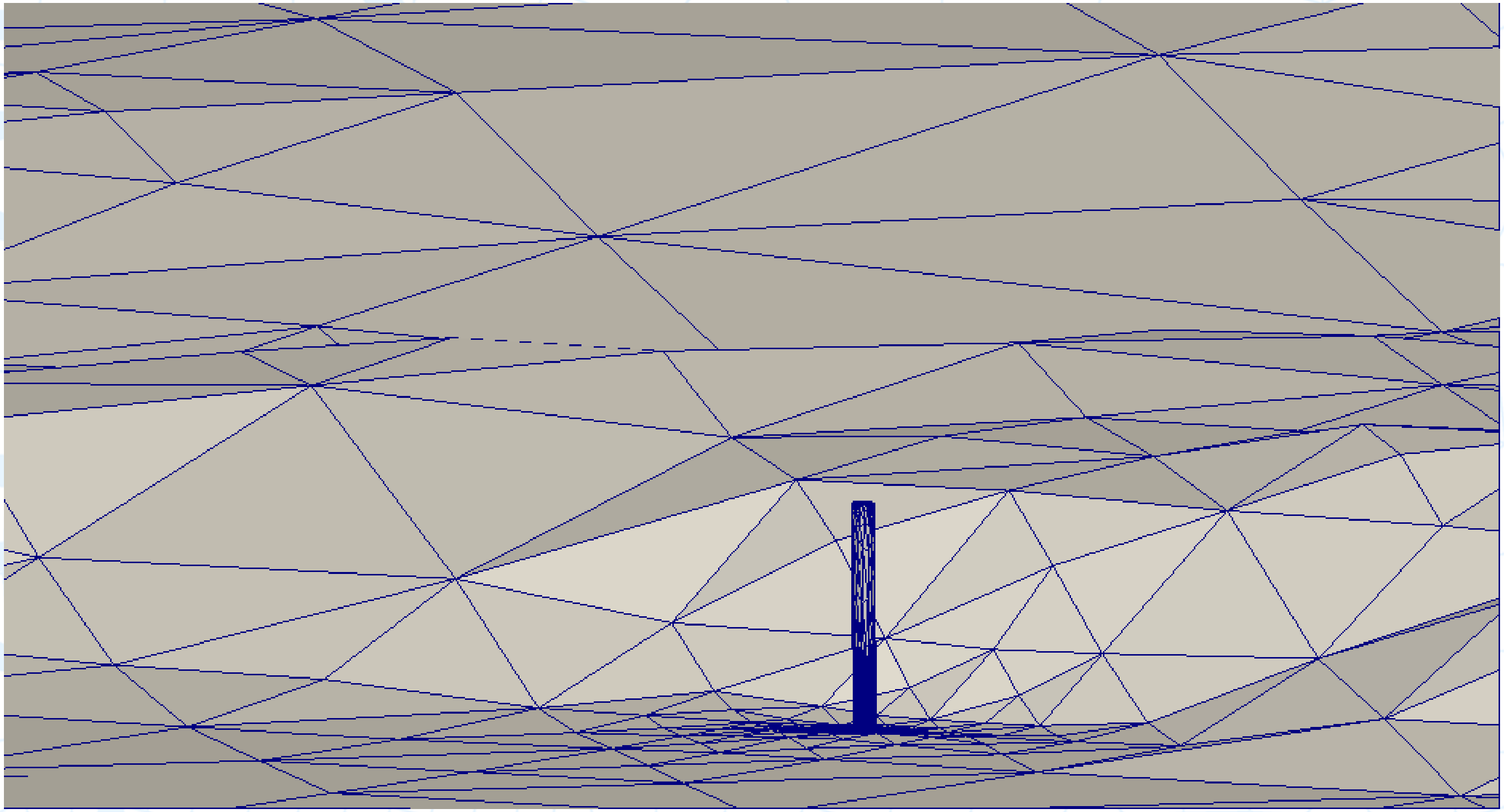
Adaptative Mesh

Gran Canaria Mesh



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Wind field modeling

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

- Harmonie is a non-hidrostatic weather forecasting model
- U_{10} and V_{10} data at grid points from Harmonie has been used as measure stations data
- Geostrophic wind from Harmonie

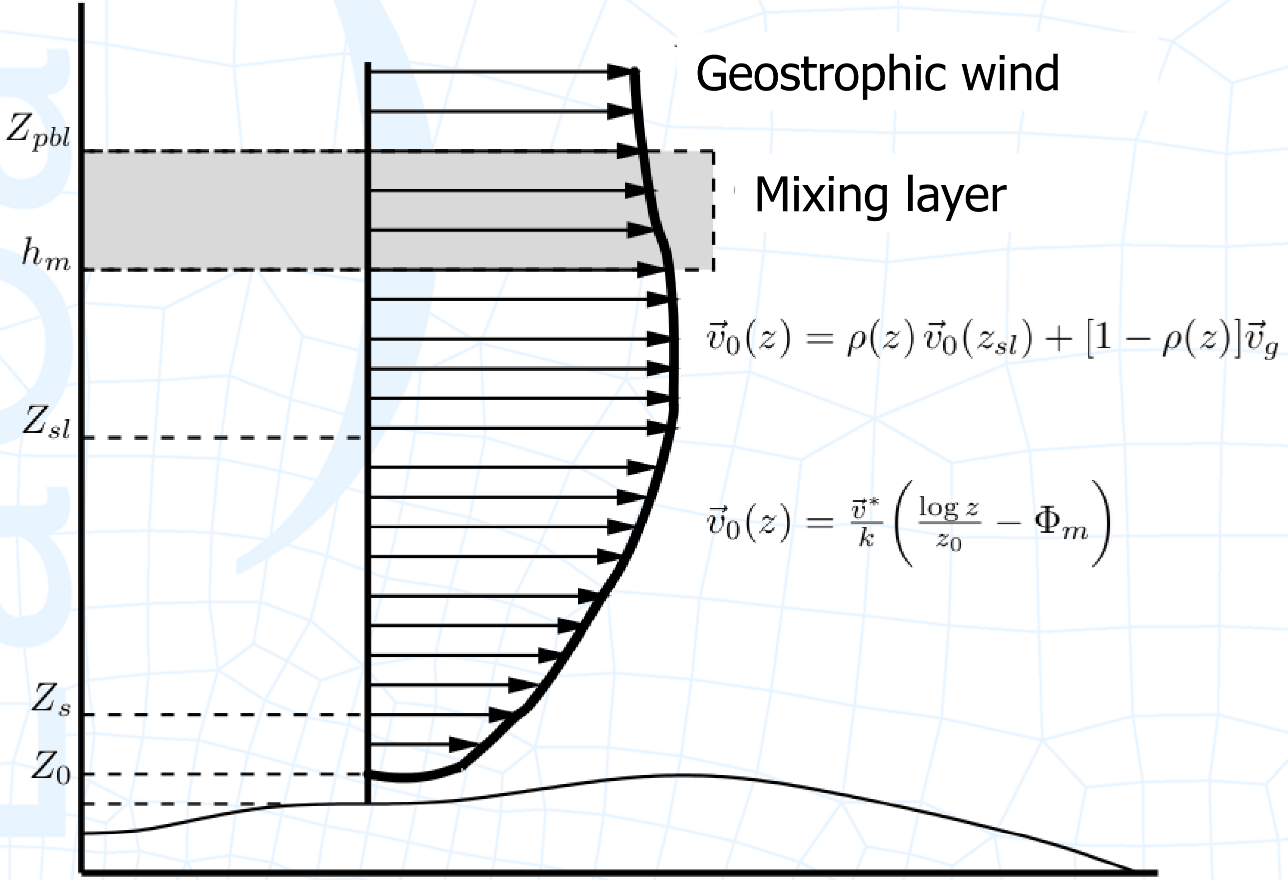
Wind field modeling

- Horizontal interpolation
  - Weighting inverse to the squared distance and inverse height differences

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

Wind field modeling

- Vertical interpolation
  - Log-linear wind profile



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Wind field modeling

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

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

and minimizes the adjusting functional

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

Wind field modeling

- Introducing a Lagrange multiplier ϕ

$$u = u_0 + T_h \frac{\partial \phi}{\partial x}, \quad v = v_0 + T_h \frac{\partial \phi}{\partial y}, \quad w = w_0 + T_v \frac{\partial \phi}{\partial z},$$

- Such that it verifies an elliptic problem in Ω

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{T_v}{T_h} \frac{\partial^2 \phi}{\partial z^2} = -\frac{1}{T_h} \left(\frac{\partial u_0}{\partial x} + \frac{\partial v_0}{\partial y} + \frac{\partial w_0}{\partial z} \right) \quad \text{in } \Omega$$

$$\phi = 0 \quad \text{on } \Gamma_a$$

$$\vec{n} \cdot T \vec{\nabla} \mu = -\vec{n} \cdot \vec{v}_0 \quad \text{on } \Gamma_b$$

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Wind field Calibration

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

- 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]*

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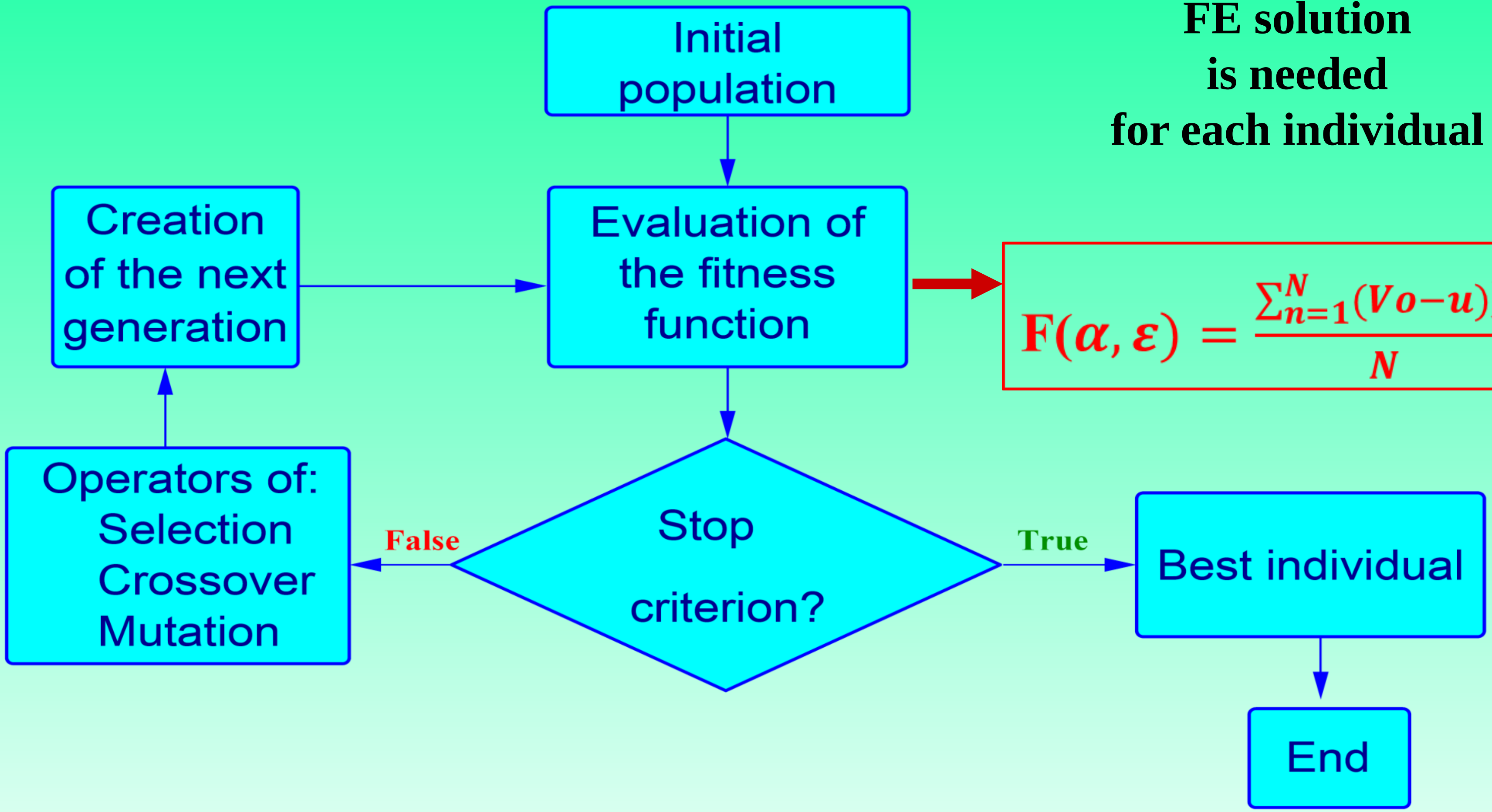
Wind field Calibration

FE solution is needed for each individual



$$F(\alpha, \varepsilon) = \frac{\sum_{n=1}^{N} (Vo-u)_n^2}{N}$$

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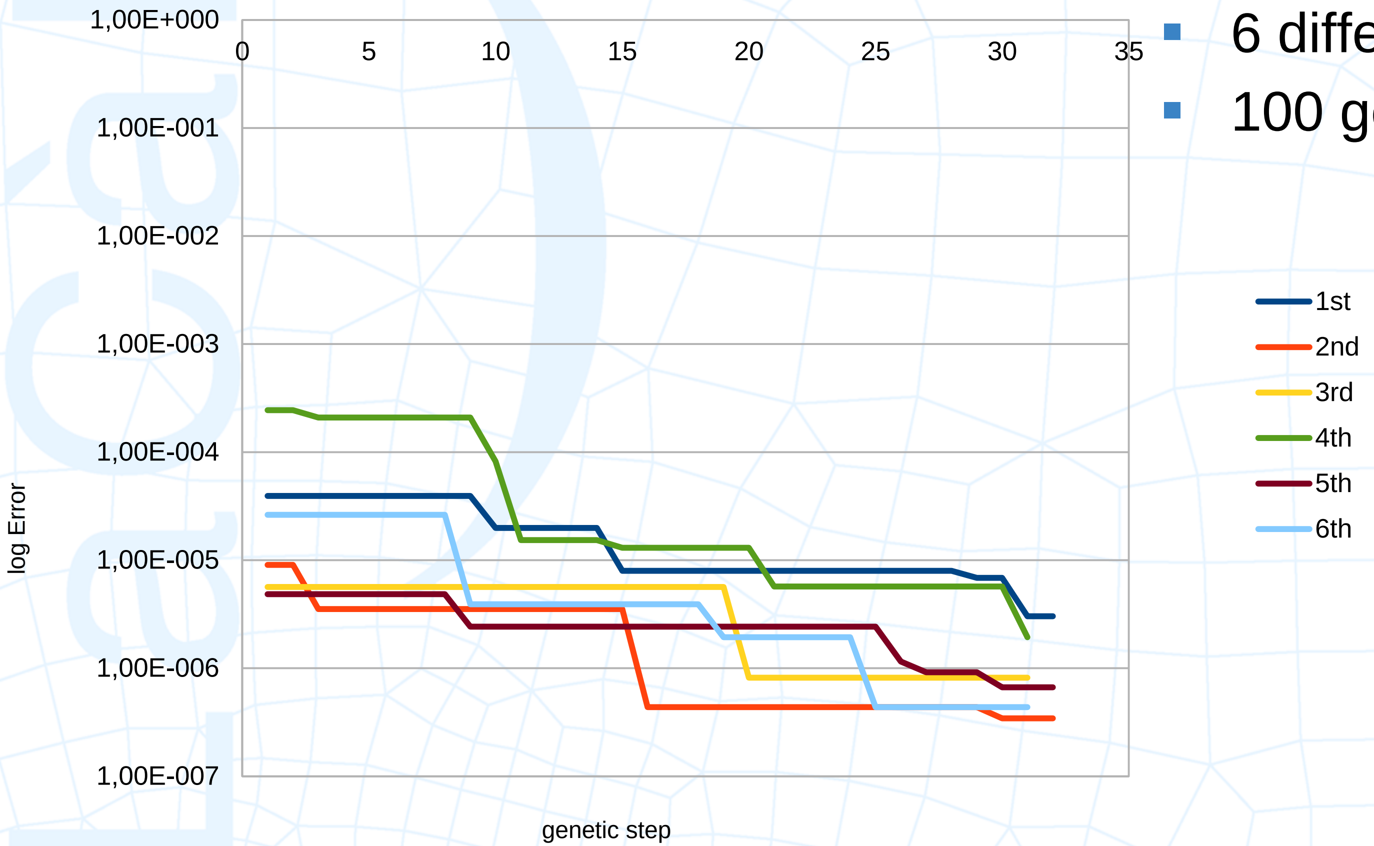
Wind field Calibration

- Genetic Algorithm evolution



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

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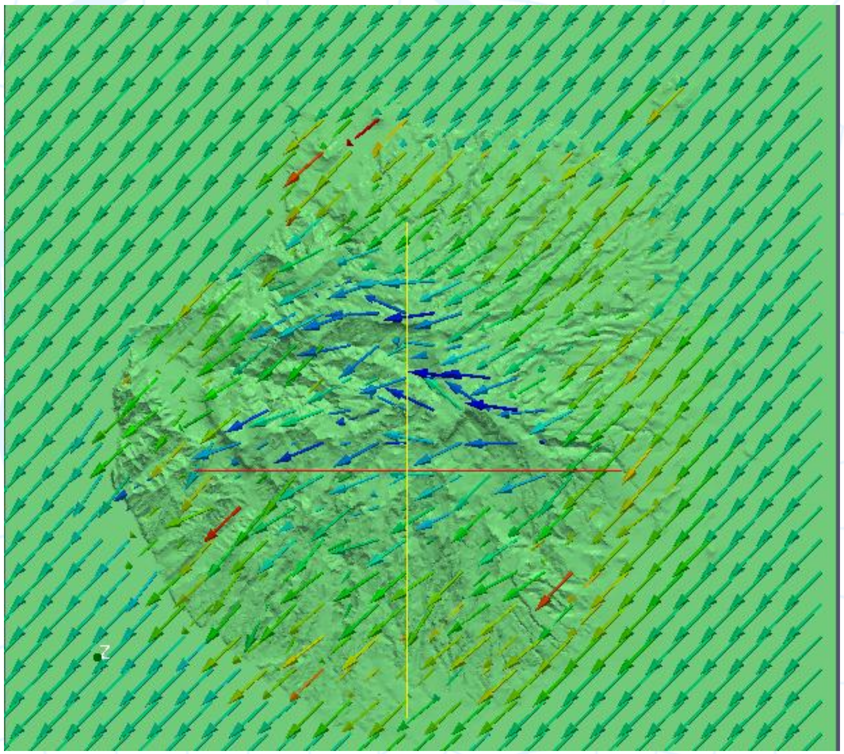
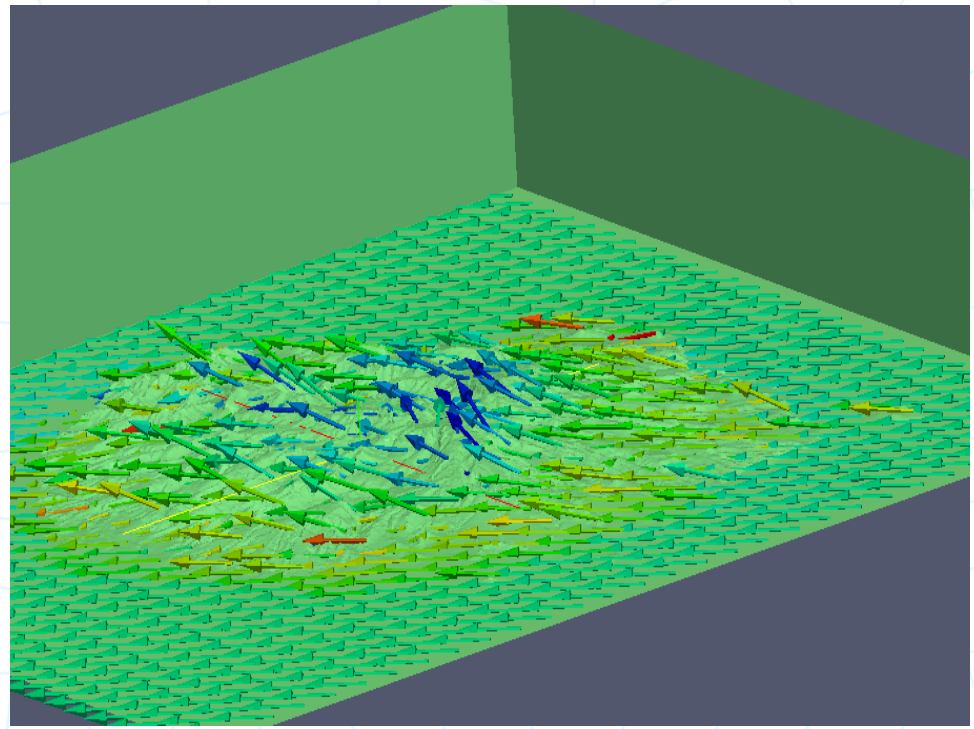
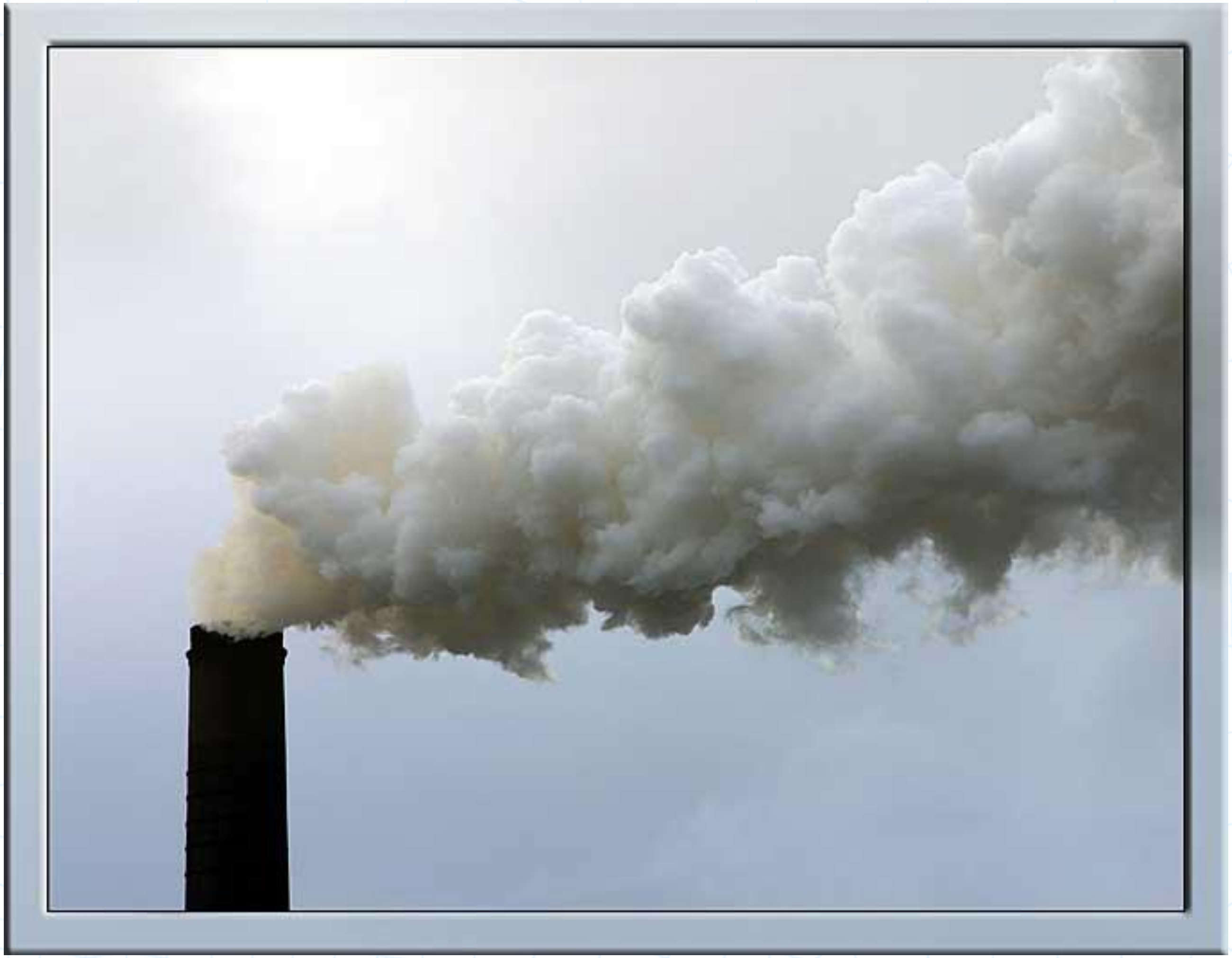
Wind field results





20 m

Plume rise modeling



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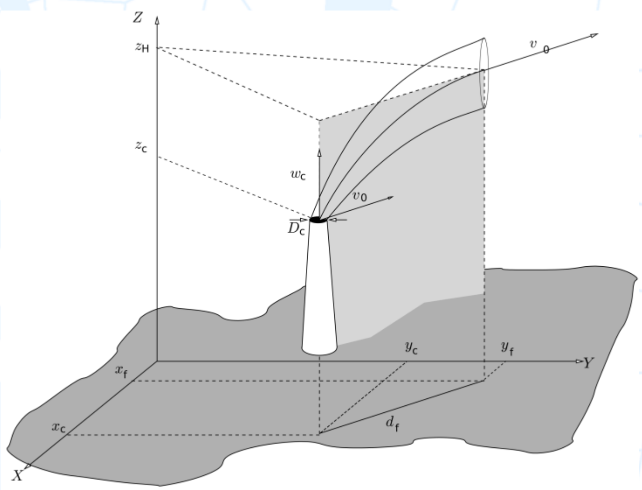
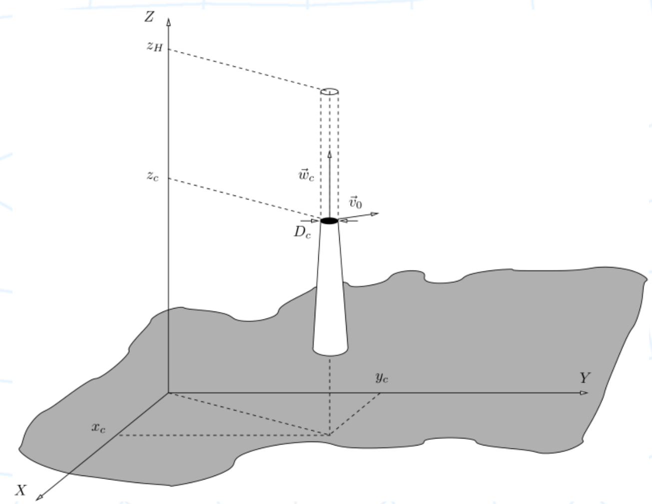
Plume rise modeling

- Briggs formula
  - Buoyant (wc < 4Vo)
    - Driving-force: gas temperature difference
    - Curved trajectory
  - Momentum (wc > 4Vo)
    - Driving-force: Gas velocity
    - Vertical straight trajectory





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Air quality modeling

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

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

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

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

$$\mathbf{n} \cdot \mathbf{K} \nabla u = 0$$ Outlet wind boundaries

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

Air quality modeling

RIVAD reactive model (4 species)

$$\mathbf{s}_1(\mathbf{c}) = -\alpha_1(\mathbf{c})\mathbf{c}_1 = -\mathbf{s}_2(\mathbf{c})$$
$$\mathbf{s}_3(\mathbf{c}) = -\alpha_3(\mathbf{c})\mathbf{c}_3 = -\mathbf{s}_4(\mathbf{c})$$

$$\alpha_1(\mathbf{c}) = \gamma_1/(\mathbf{c}_1 + \delta_1\mathbf{c}_3)$$
$$\alpha_3(\mathbf{c}) = \gamma_3/(\mathbf{c}_1 + \delta_3\mathbf{c}_3)$$

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Air quality modeling

Splitting (Strang Splitting)

$$\begin{cases} \dfrac{\partial \mathbf{c}^*}{\partial t} = \mathbf{s}(\mathbf{c}^*) & [0, \Delta t/2], \quad \mathbf{c}^*(\mathbf{x}, 0) = \mathbf{c}^n(\mathbf{x}) \\ \dfrac{\partial \mathbf{c}^{**}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{c}^{**} = \nabla \cdot (\mathbf{K} \nabla \mathbf{c}^{**}) & [0, \Delta t], \quad \mathbf{c}^{**}(\mathbf{x}, 0) = \mathbf{c}^*(\mathbf{x}, \Delta t/2) \\ \dfrac{\partial \mathbf{c}^{***}}{\partial t} = \mathbf{s}(\mathbf{c}^{***}) & [0, \Delta t/2], \quad \mathbf{c}^{***}(\mathbf{x}, 0) = \mathbf{c}^{**}(\mathbf{x}, \Delta t) \end{cases}$$

Rosembrock 2

$$\begin{cases} \mathbf{c}_{n+1} & = \mathbf{c}_n + \frac{3}{2}\tau k_1 + \frac{1}{2}\tau k_2 \\ ((\mathbf{I}) - \gamma \tau \mathbf{J}) k_1 & = \mathbf{s}(\mathbf{c}_n) \\ ((\mathbf{I}) - \gamma \tau \mathbf{J}) k_2 & = \mathbf{s}(\mathbf{c}_n + \tau k_1) - 2k_1 \end{cases}$$

$$\gamma = 1 \pm 1/\sqrt{2}$$

$$\tau = dt$$

J = Jacobian **s**(c)

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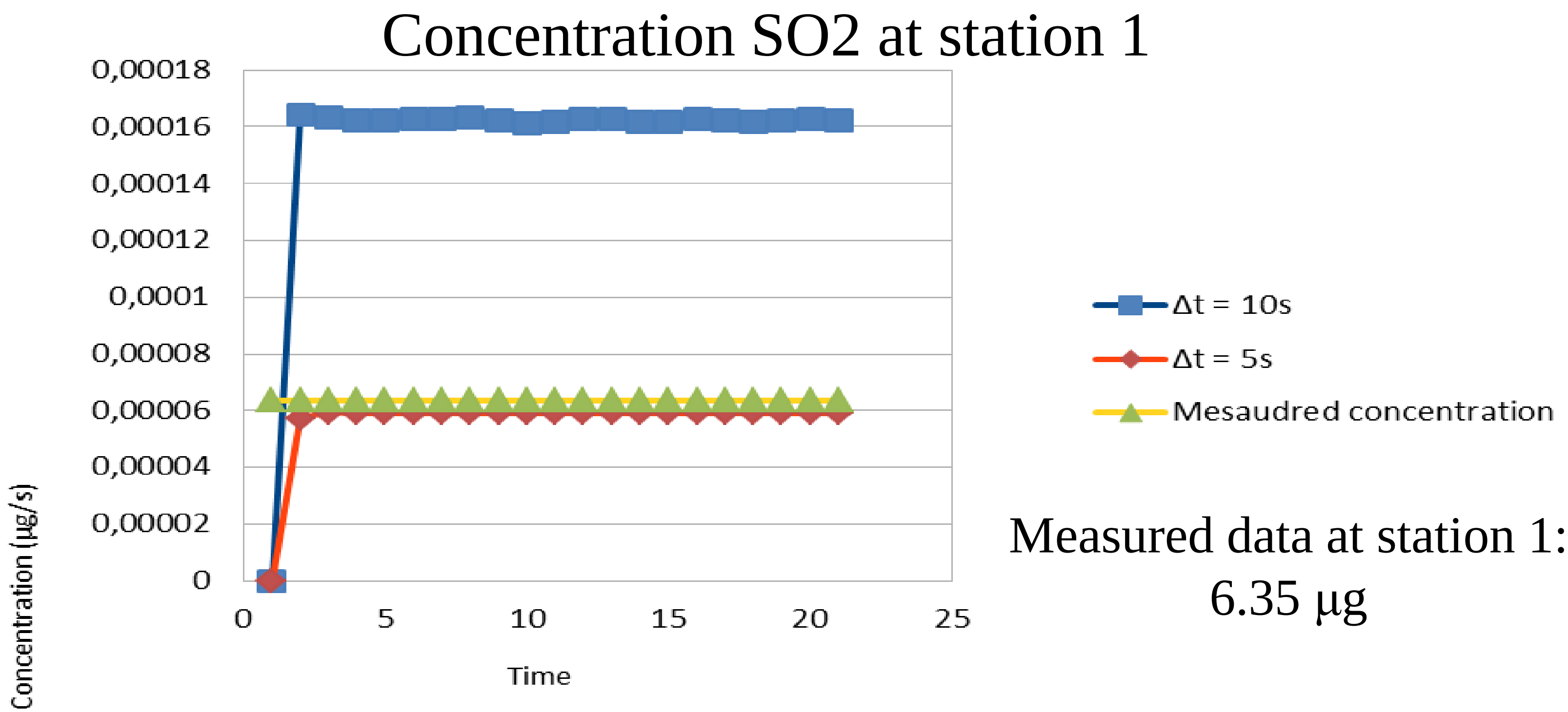
Air quality modeling

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

Air quality Calibration

- Calibration
  - Diffusion (K)
- Choose time step regarding numerical conditions (artificial diffusion)



Measured data at station 1: 6.35 µg

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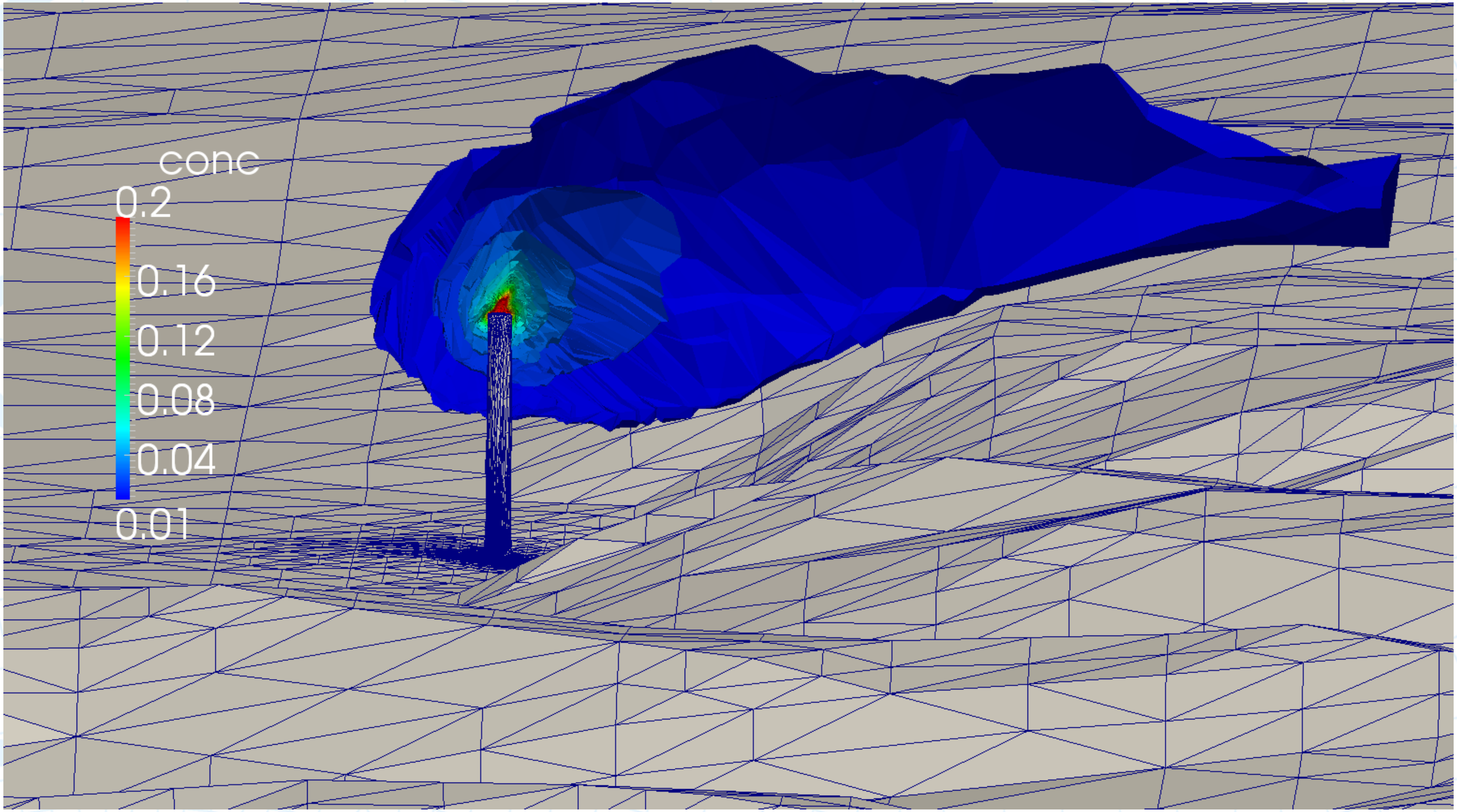
Air quality results

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



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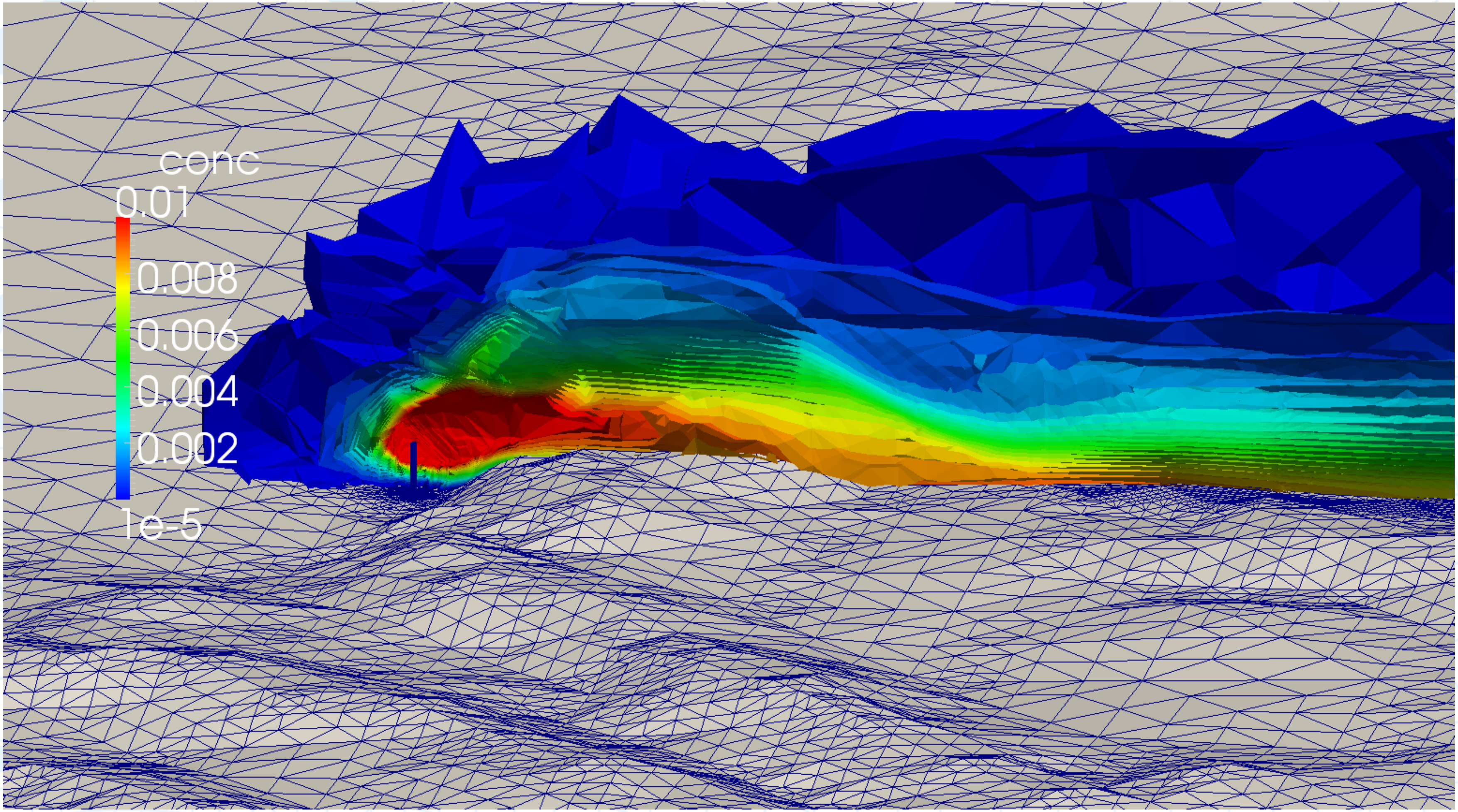
Air quality results

Concentration $S0_2$ (g/m^3) after 1000 seconds



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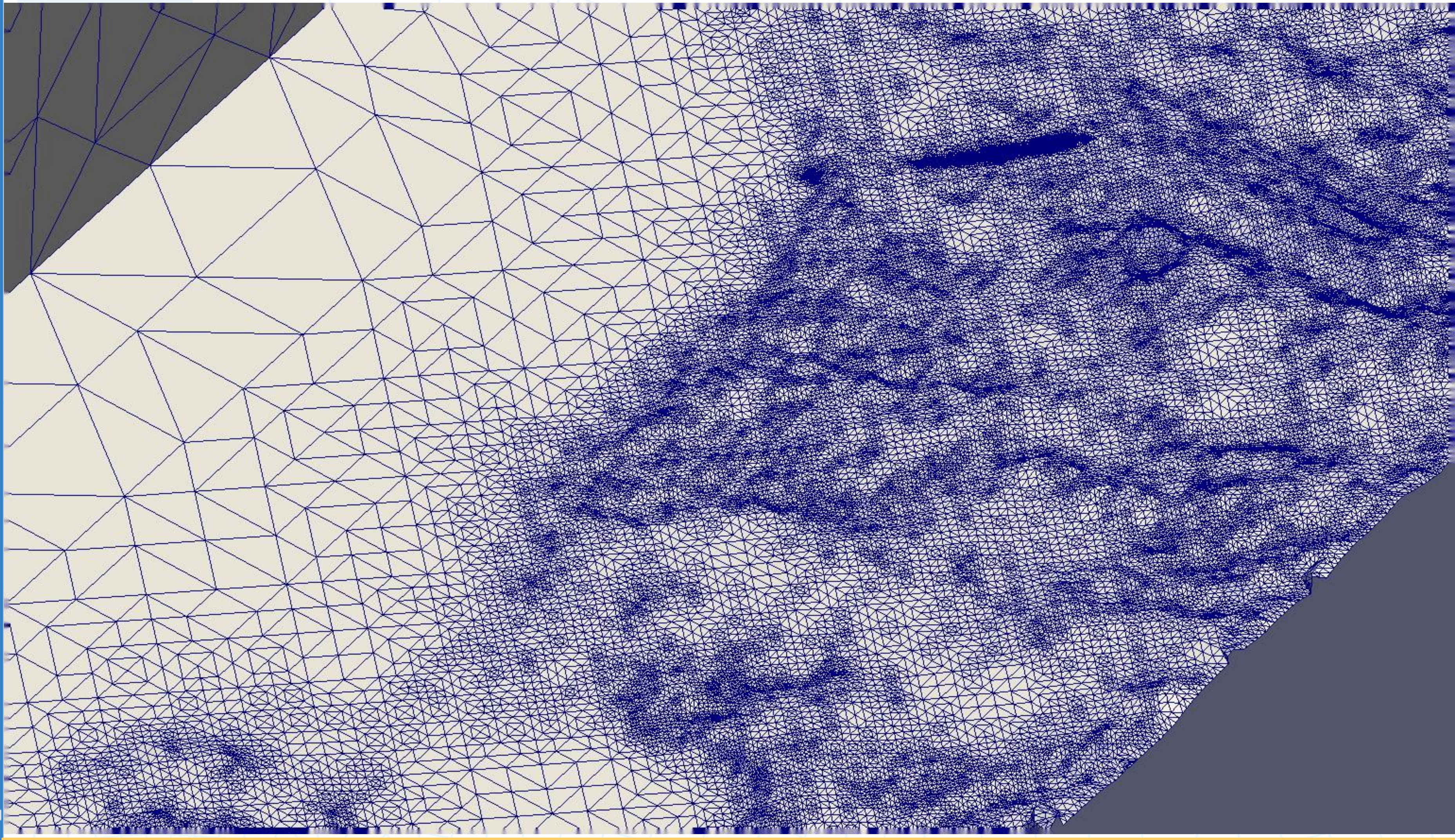
Air quality results

Isosurface evolution 1 μg/m^3



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Conclusions

- 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