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LABORATORI DE CÀLCUL NUMÈRIC

MODELOS NUMÉRICOS PREDICTORES PARA GESTIÓN MEDIOAMBIENTAL
Referencia: CGL2008-06003-C03 (2009-2011)

www-lacan.upc.edu

Workshop en la Agencia Estatal de Meteorología

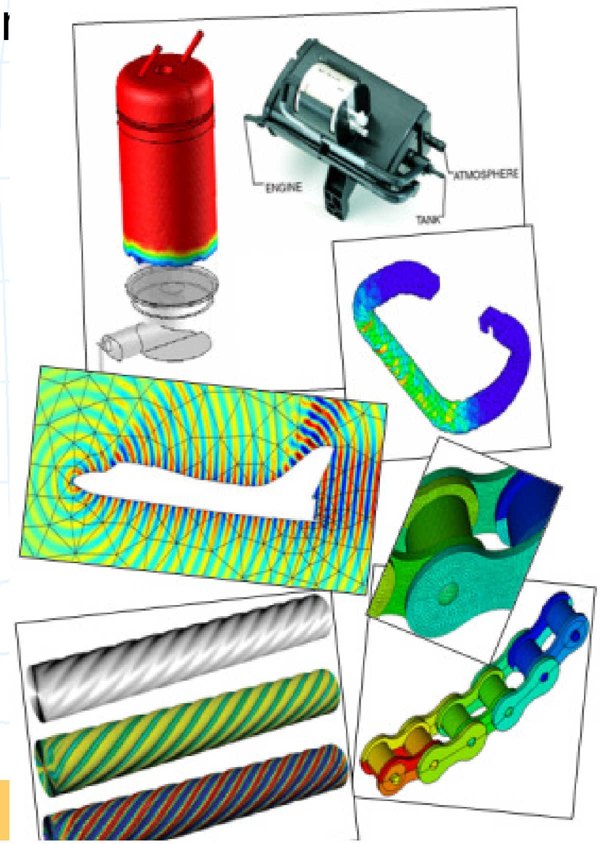
Jueves 16 de Abril de 2009

Índice

- Breve presentación grupo LaCàN (UPC)
- Temas planteados:
  - *Dispersión de contaminantes de grandes emisores puntuales*
  - *Acoplamiento de modelos de calidad del aire regionales con la dispersión a escala local*

LaCàN (UPC)

- Faculty: 13 people
- Research lines in computational methods and numerical analysis
  - Adaptivity and error estimation,
  - Mesh generation,
  - Advanced discretization methods,
  - Iterative methods for linear and non-linear probler
  - High-order time integrators,...



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LaCàN (UPC)

- ULPGC-USAL-UPC coordinated research projects (Spanish government):
  - Modelización numérica de problemas medioambientales de convección-difusión-reacción, (2001-2004)
  - Modelización numérica en tiempo real de la contaminación atmosférica por emisiones puntuales (Tit. UPC), (2004-2007)
  - Modelos numéricos para la diagnosis y predicción de la contaminación atmosférica (Tit. UPC), (2007-2008)
  - Modelos numéricos predictores para gestión medioambiental, (2009-2011)

- Technology transfer (EPO)
  - Modelización y simulación de la dispersión de contaminantes de La Oroya en el período 2007-2008, y alternativas de actuación para 2009-2010, (2008)

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Finite element local air quality modeling of punctual emissions

Laboratori de Càlcul Numèric (LaCàN), Dept. de Matemàtica Aplicada III,
Universitat Politècnica de Catalunya (Spain)

University Institute for Inteligent Systems and Numerical Applications in Engineering, University of Las Palmas de Gran Canaria

Outline

- Motivation and proposed approach
- Test case: 2 stacks plumes coupling
- Application to a complex topography: La Palma island
- Approach and results with non-linear chemistry
- Conclusions

Motivation

- Goal: Compute plumes of major punctual emissaries (stacks, chimneys, …) when:
  - Topography is complex
  - Wind data at some locations is available
  - Nonlinear reaction coupling between different plumes is relevant

- Plume models (stationary) or puff models (lagrangian) cannot manage properly these problems

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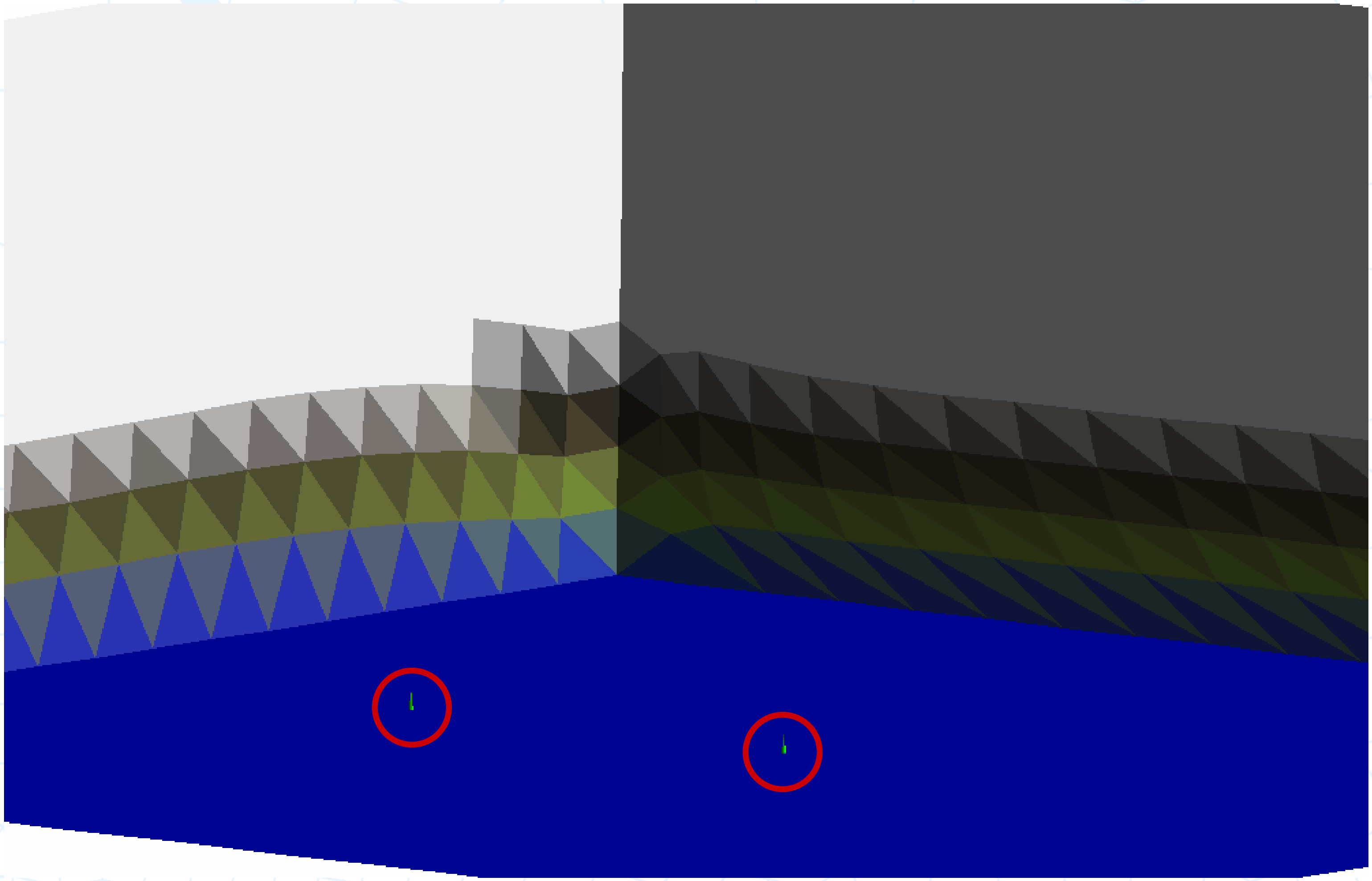
Proposed approach

- Approach:
  1. 3D Finite Element mesh adapted to topography, including punctual emissaries
  2. Approximation of overall wind field from punctual data using a mass consistent model
  3. Approximation of plume rise and meanline trajectory
  4. Refinement of FE mesh to capture approximated plume geometry and wind field
  5. Computation of transport and reaction of pollutants

- Specific goals of this presentation:
  - To show main steps of the overall approach
  - To solve transport-reaction problem with complex topographies
  - To test appropriate numerical linear and nonlinear solvers

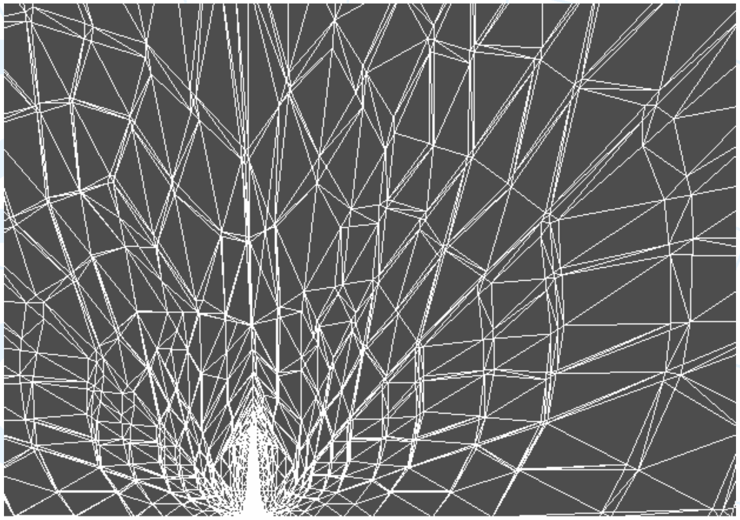
Example: Flat domain

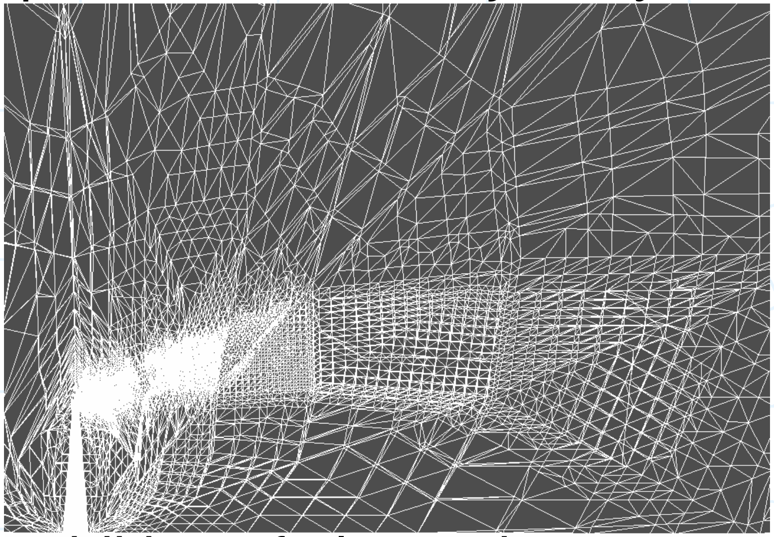
- Domain size: 20kmx20kmx7km
- Inclusion of two real-size stacks (200m height x 5m diameter)
- Mass consistent model is used to compute wind field from available punctual data



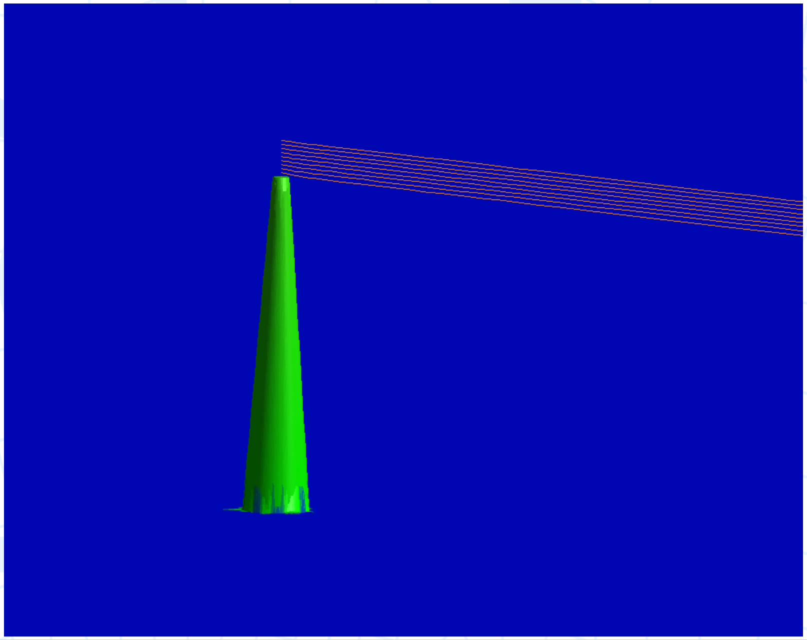
Example: Refinement & Plume rise

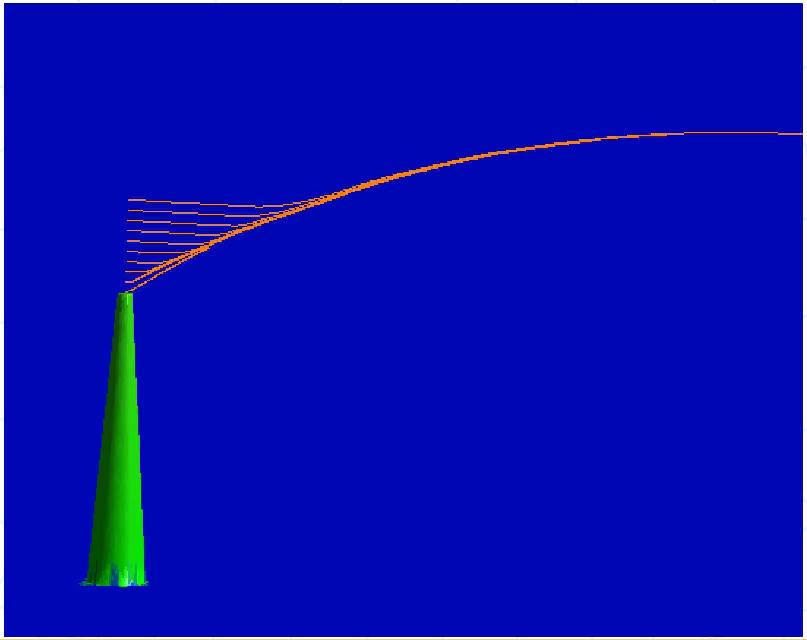
- Initial mesh and refined one to capture plume rise and trajectory





- Initial wind field and wind field with the addition of plume rise





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Transport – reaction model

Convection – diffusion – reaction equation:

$$\frac{\partial \mathbf{c}}{\partial t} + \overbrace{\mathbf{u} \cdot \nabla \mathbf{c}}^{\text{Convection term}} = \overbrace{\nabla \cdot (\mathbf{K} \nabla \mathbf{c})}^{\text{Diffusion term}} + \underbrace{\mathbf{e}}_{\text{Emissions within domain}} + \overbrace{\mathbf{s}(\mathbf{c})}^{\text{Reaction term}}$$

$$\begin{cases} \mathbf{n} \cdot \mathbf{K} \nabla u = \Phi & \text{in } \Gamma_N\text{: Stack source point} \\ \mathbf{n} \cdot \mathbf{K} \nabla \mathbf{c} = -\mathbf{V}^d \mathbf{c} & \text{in } \Gamma_R\text{: Terrain} \\ \mathbf{n} \cdot \nabla \mathbf{c} = 0 & \text{in } \Gamma_N = \partial\Omega \backslash (\Gamma_D \cup \Gamma_R) \end{cases}$$

$$\mathbf{c}(\mathbf{x}, 0) = \mathbf{c}^{ini}(\mathbf{x})$$

c = concentration (unknowns)
Φ = stack pollutant flow
$\mathbf{c}^{ini}$ = initial concentrations (null)
u = wind velocity

K = diffusion matrix (constant)
e = emission inside domain (null)
s(c) = reaction term (linear or nonlinear)
$\mathbf{V}^d$ = deposition velocity (constant)

Numerical solver linear model

- Temporal discretization: Cranck-Nicolson
- Spatial discretization: Least Squares

see Huerta & Donea, 2002

- Linear system solver:
  - Conjugate gradient preconditioned with an Incomplete Cholesky Factorisation

see Rodríguez-Ferran & Sandoval, 2006

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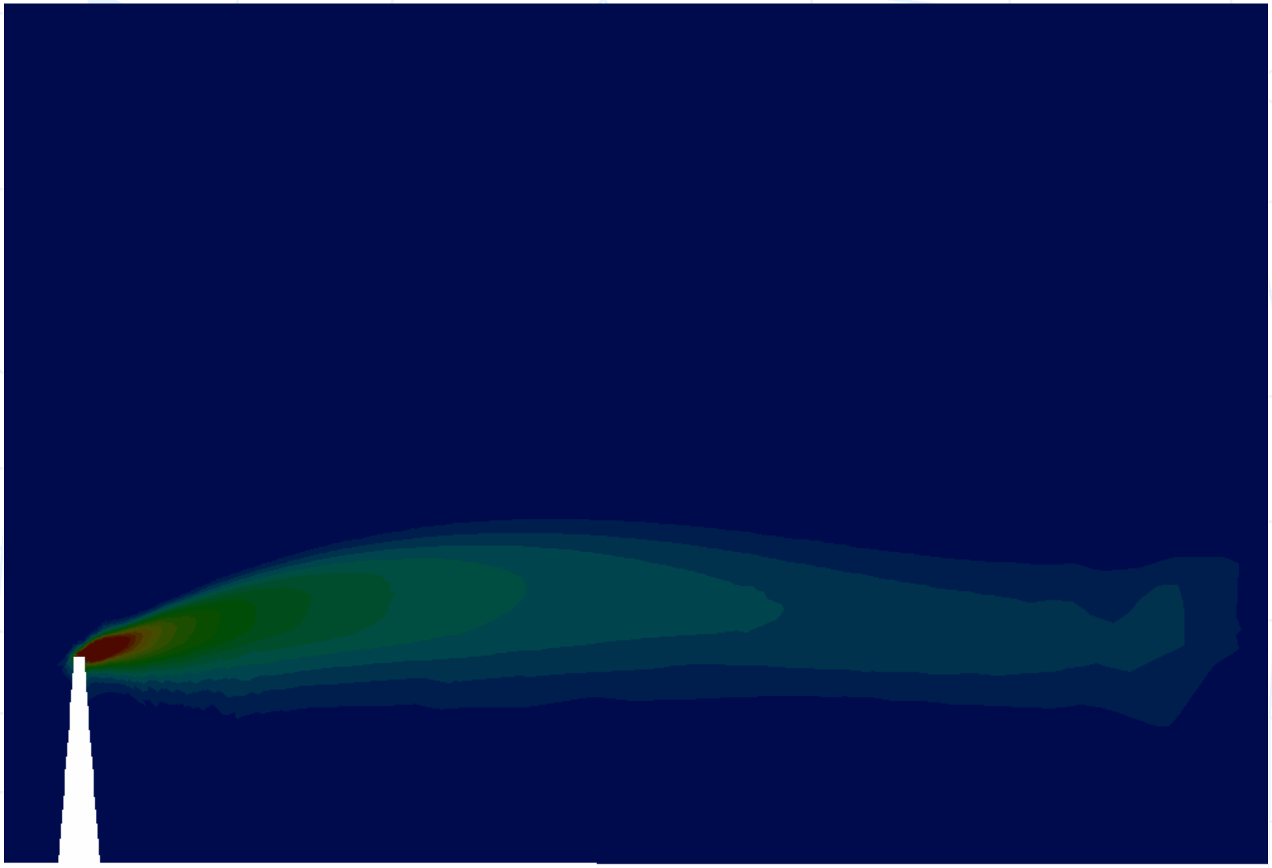
Example: Results

- Firsts time steps



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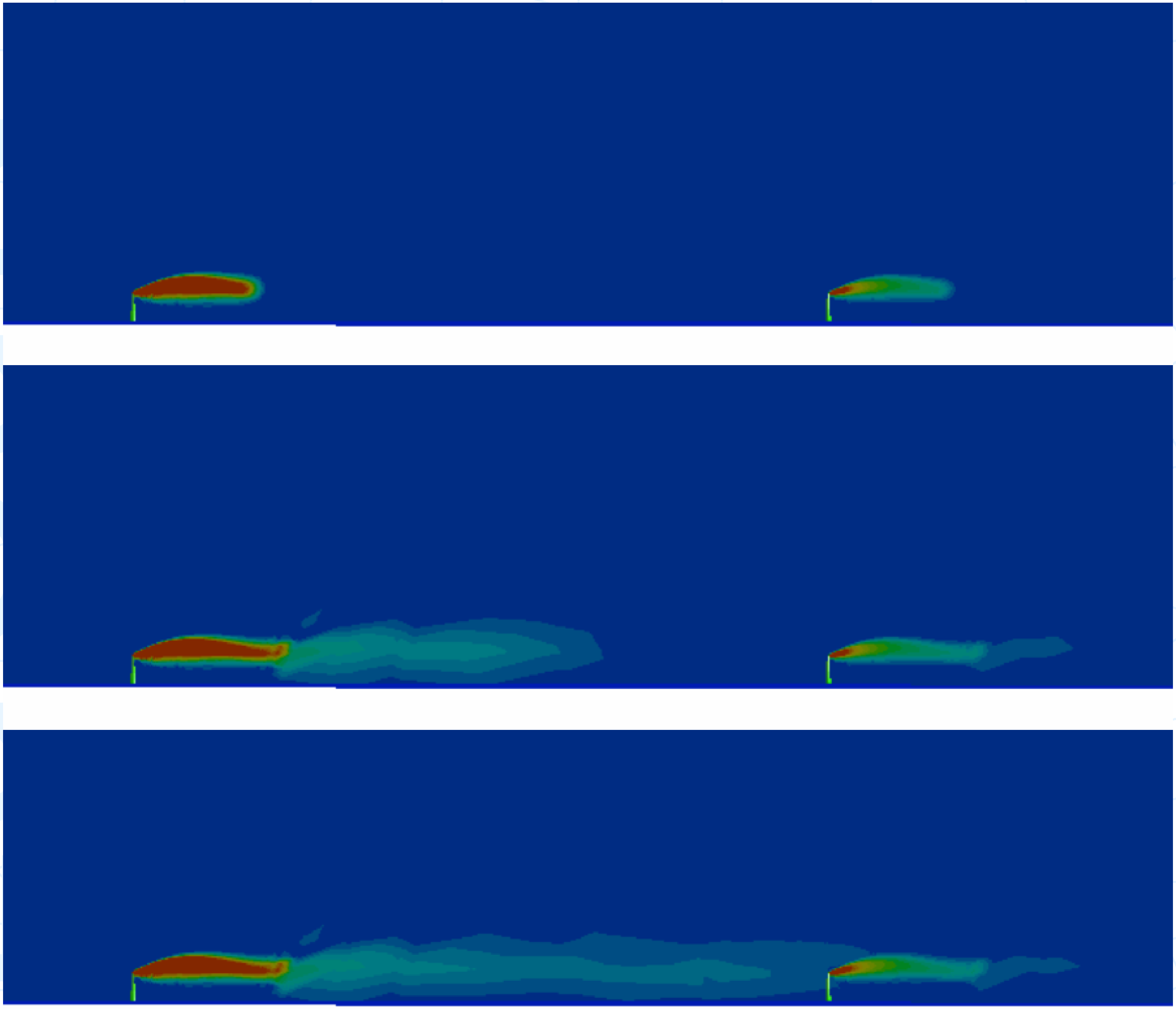
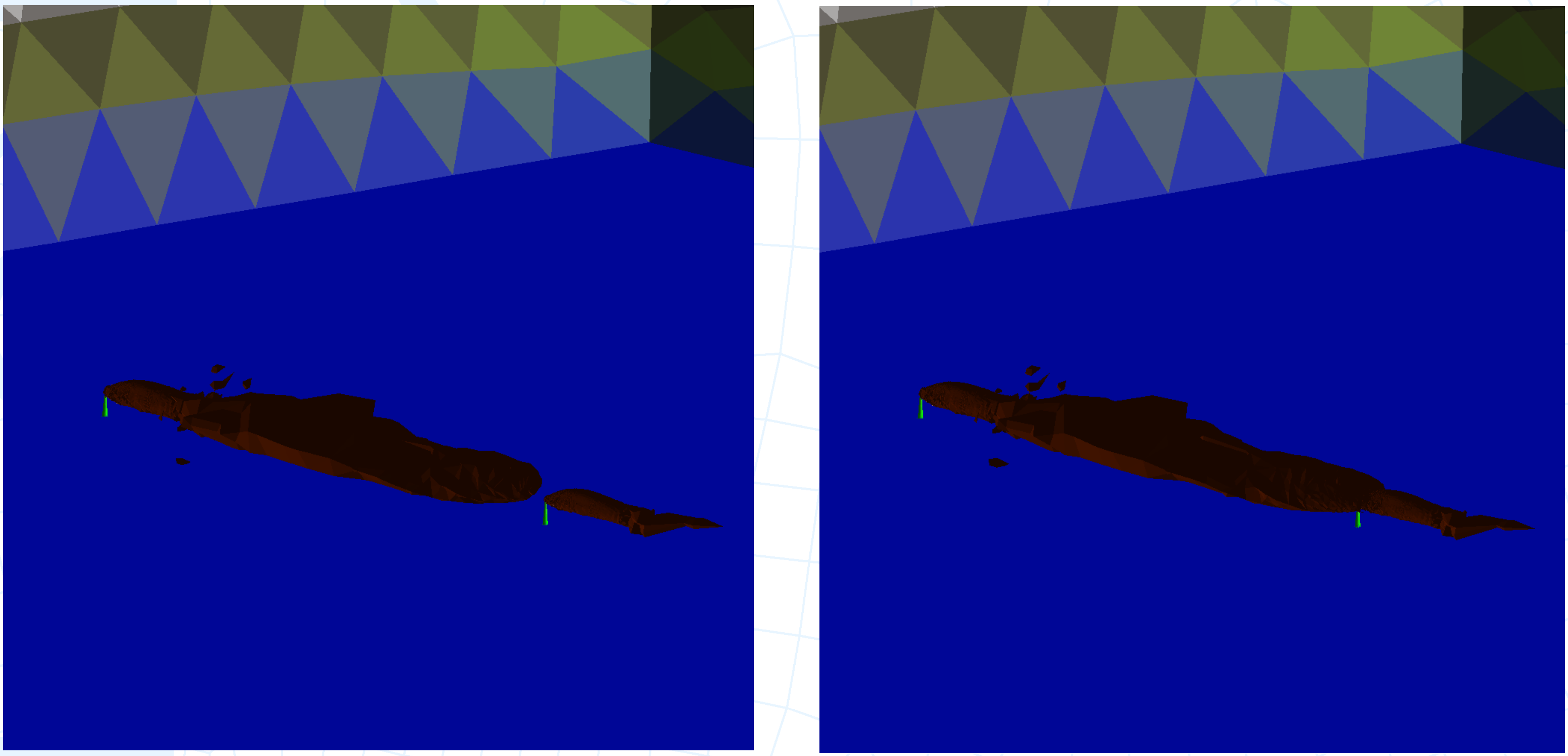
Example: Results



Coupling between plumes

Example: Results

- 3D view of coupling of plumes



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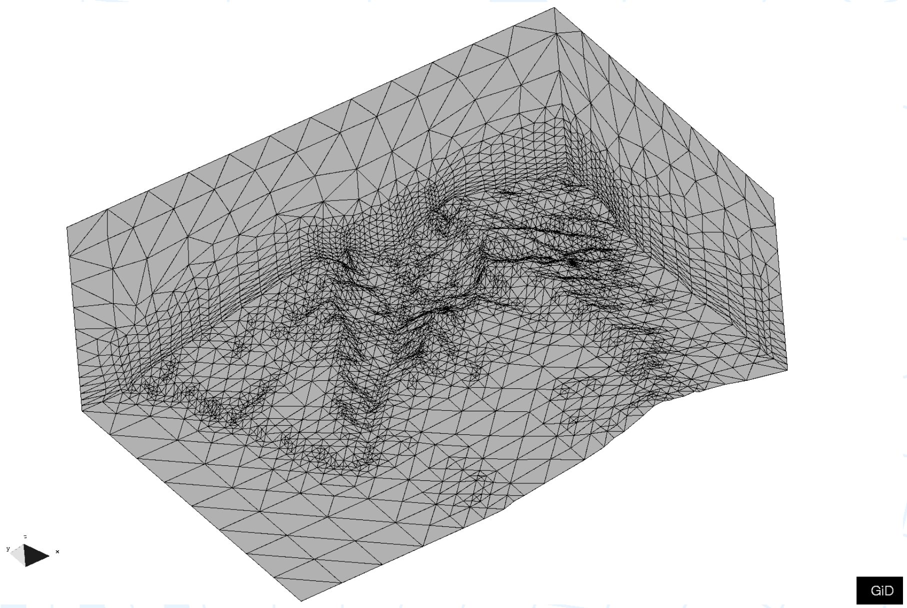
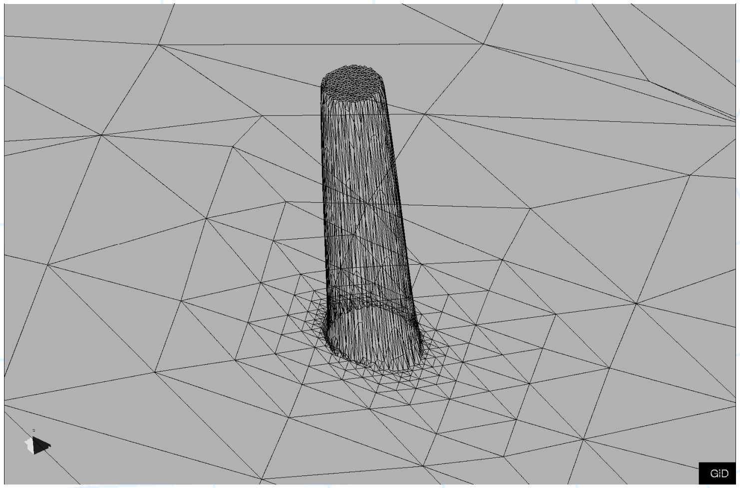
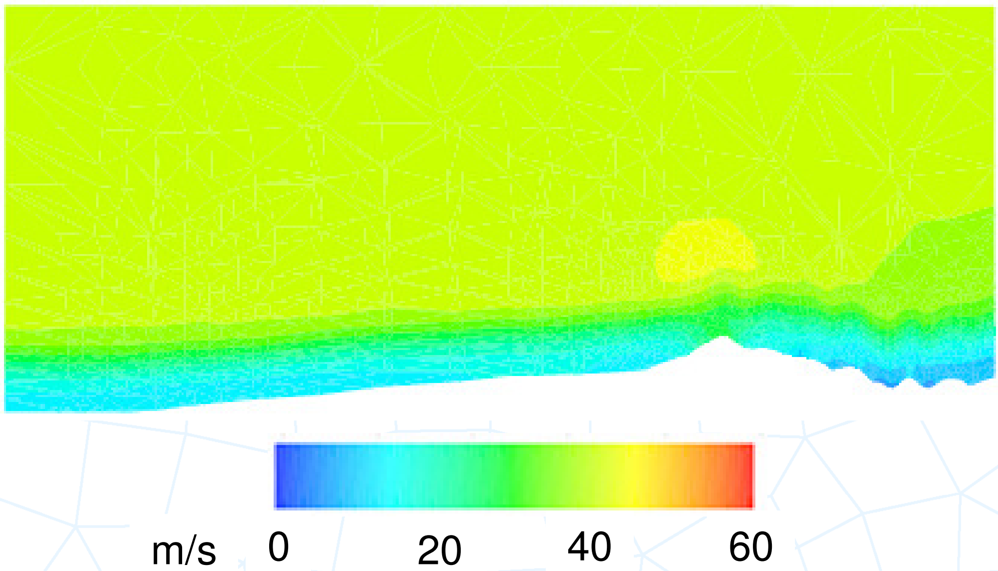
Test in a complex topography domain

- Part of La Palma island (15x18x9 km³)
- Inclusion of major emissary
- Strong wind field







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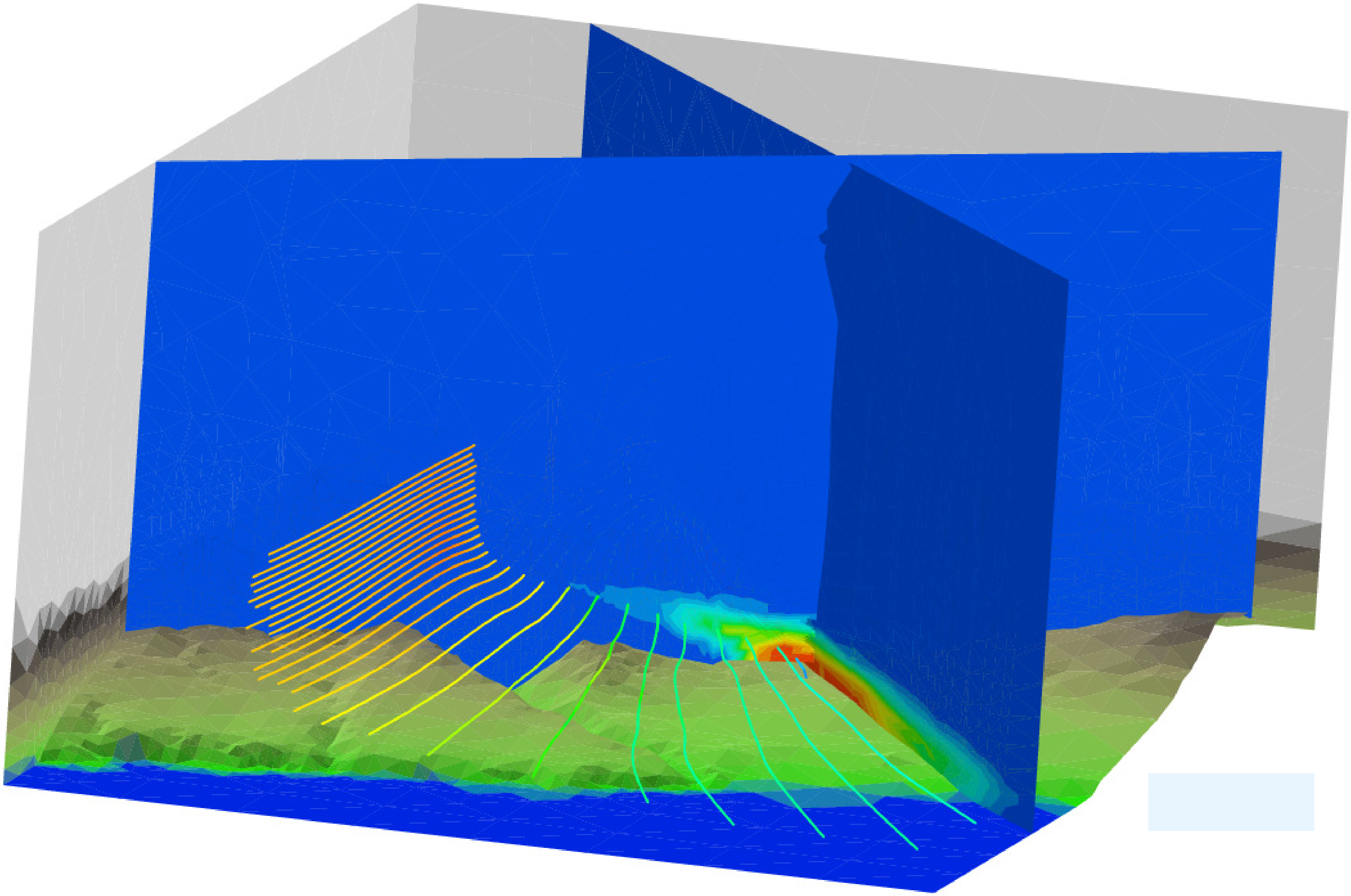
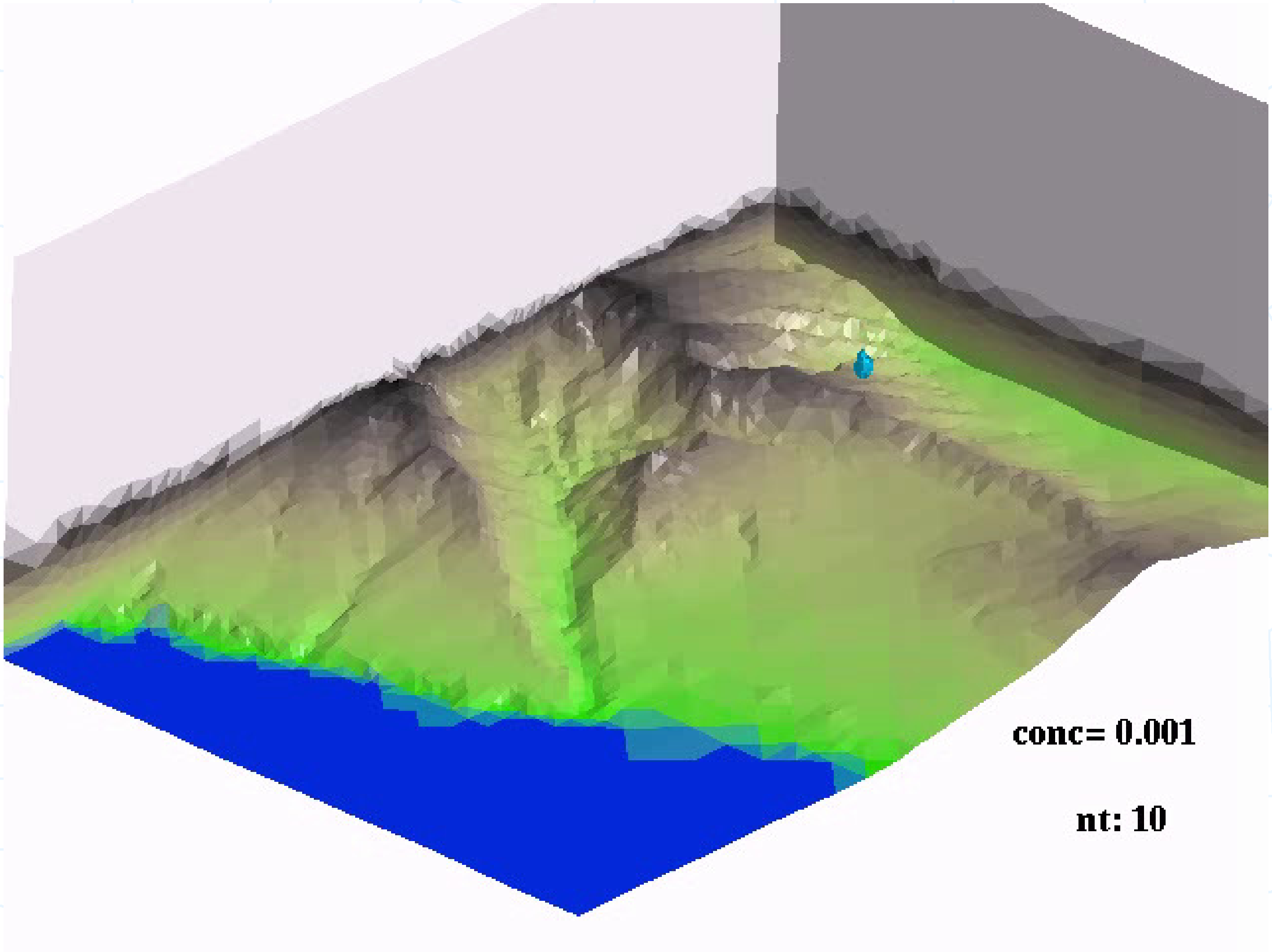
Complex topography results

- Pollutant cross sections and wind field streamlines



Complex topography results

Evolution of primary pollutant



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Test: Influence of Δt

- Maximum Courant Number >> 1 ?

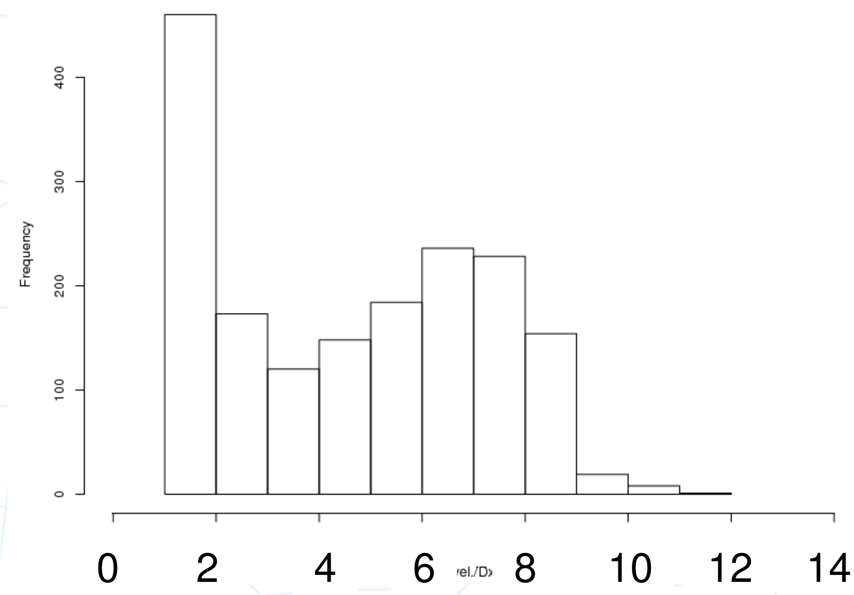
$$C = \frac{||\mathbf{u}||}{\Delta x} \Delta t$$

$\Delta t^{I}_{ref,1,2,3}$(s)	% elements with C< 1	Maximum C
0.09	100%	1
0.9	99%	10
9	76%	100

||u||/Δx histogram

Most part of domain < 1

Tail due to stack discretization



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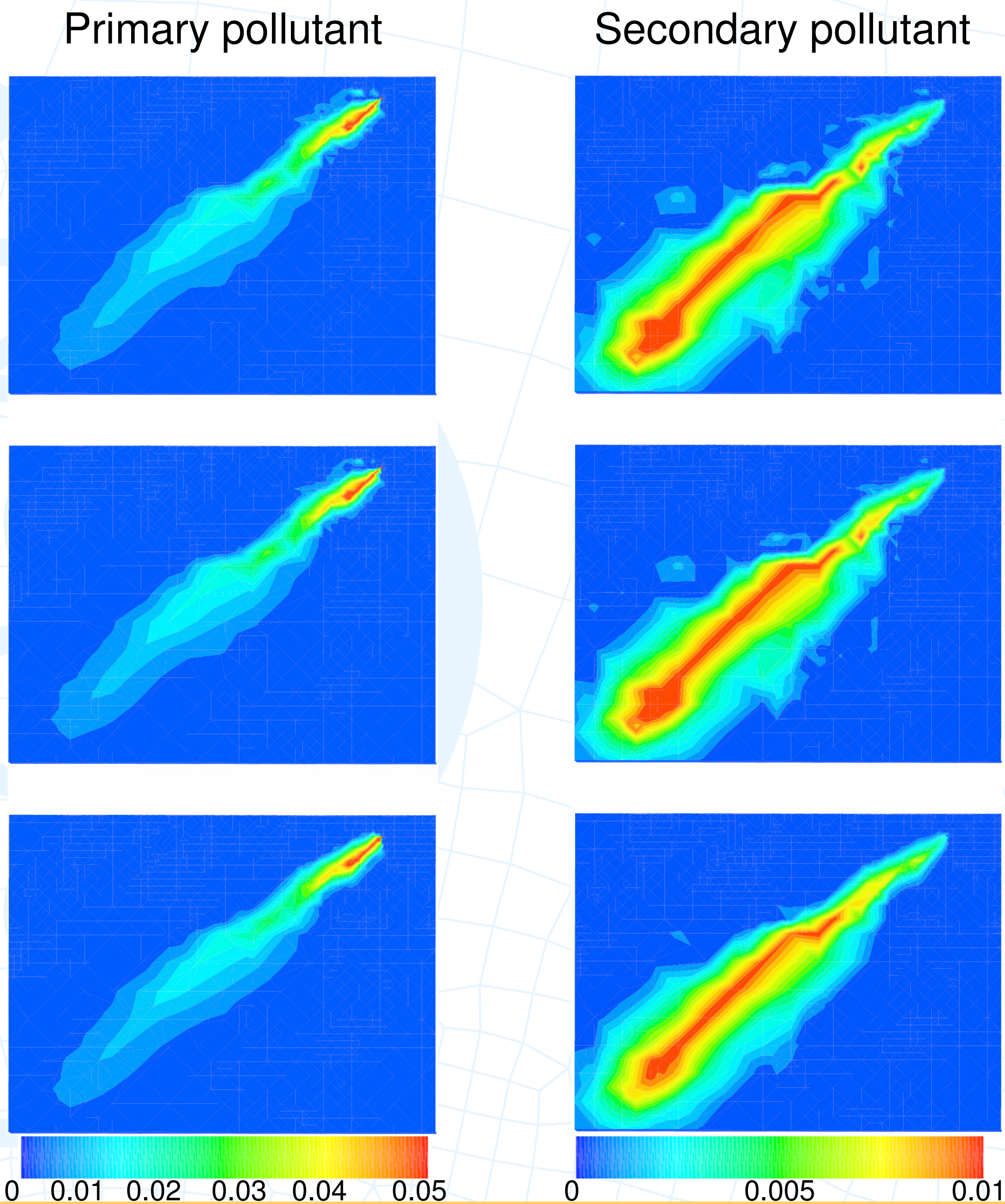
Influence of Δt



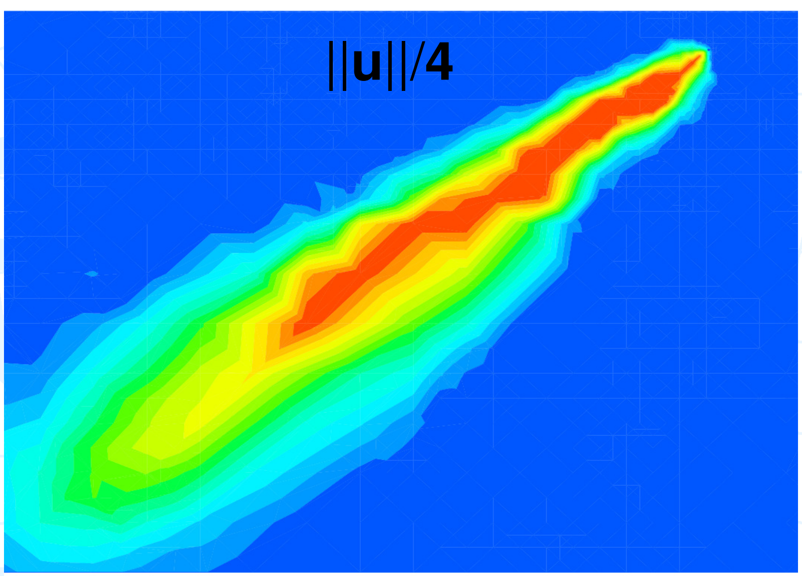
$\Delta t^{I}_{ref,1}$

$\Delta t^{I}_{ref,2}$

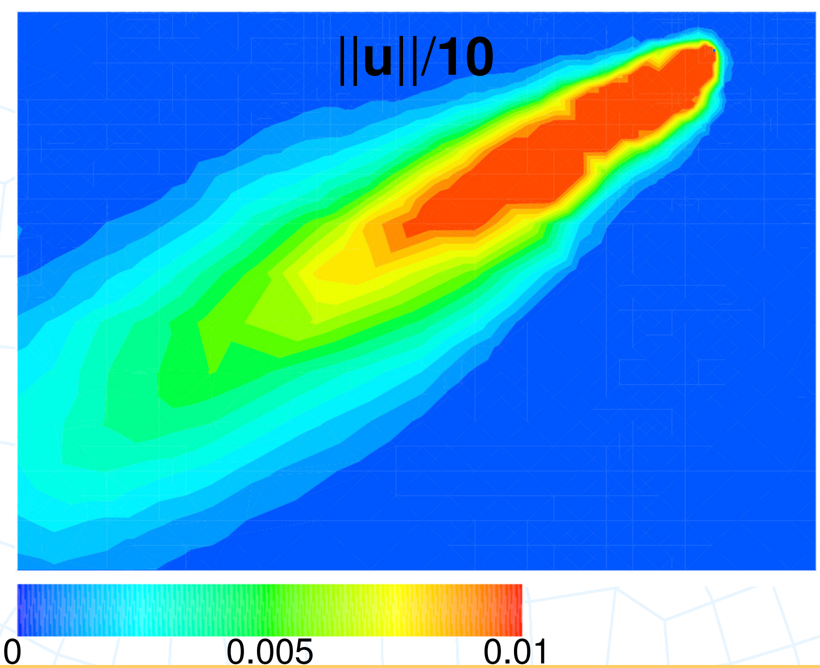
$\Delta t^{I}_{ref,3}$

Influence of velocity: Results

- Good results with winds up to 100 km/h
- Results with weaker wind fields:



Secondary pollutant



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Numerical solver nonlinear model

- Transport – Reaction splitting:
  - First order direct splitting (2 steps)

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

  - Second order strang splitting (3 steps)

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

- Rosembrock-2 solver for reaction step:

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

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

$\tau = dt$

J = Jacobian of **s**(c)

  - Uncoupled node by node

Nonlineal chemistry

- Simple nonlinear chemistry models

Simplified photochemical scheme (10 species)

Quadratic source terms

$$\mathbf{s}_k(\mathbf{c}) = \sum_{i=1}^{n_c} \left(\sum_{j=1}^{n_c} \alpha_{ij}^k \mathbf{c}_j + \beta_i^k \right) \mathbf{c}_i$$

Linear Jacobian

$$\frac{\partial \mathbf{s}_k}{\partial \mathbf{c}_l} = \sum_{i=1}^{n_c} \left(\alpha_{il}^k + \alpha_{li}^k \right) \mathbf{c}_i + \beta_l^k$$

RIVAD model (4 species)

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

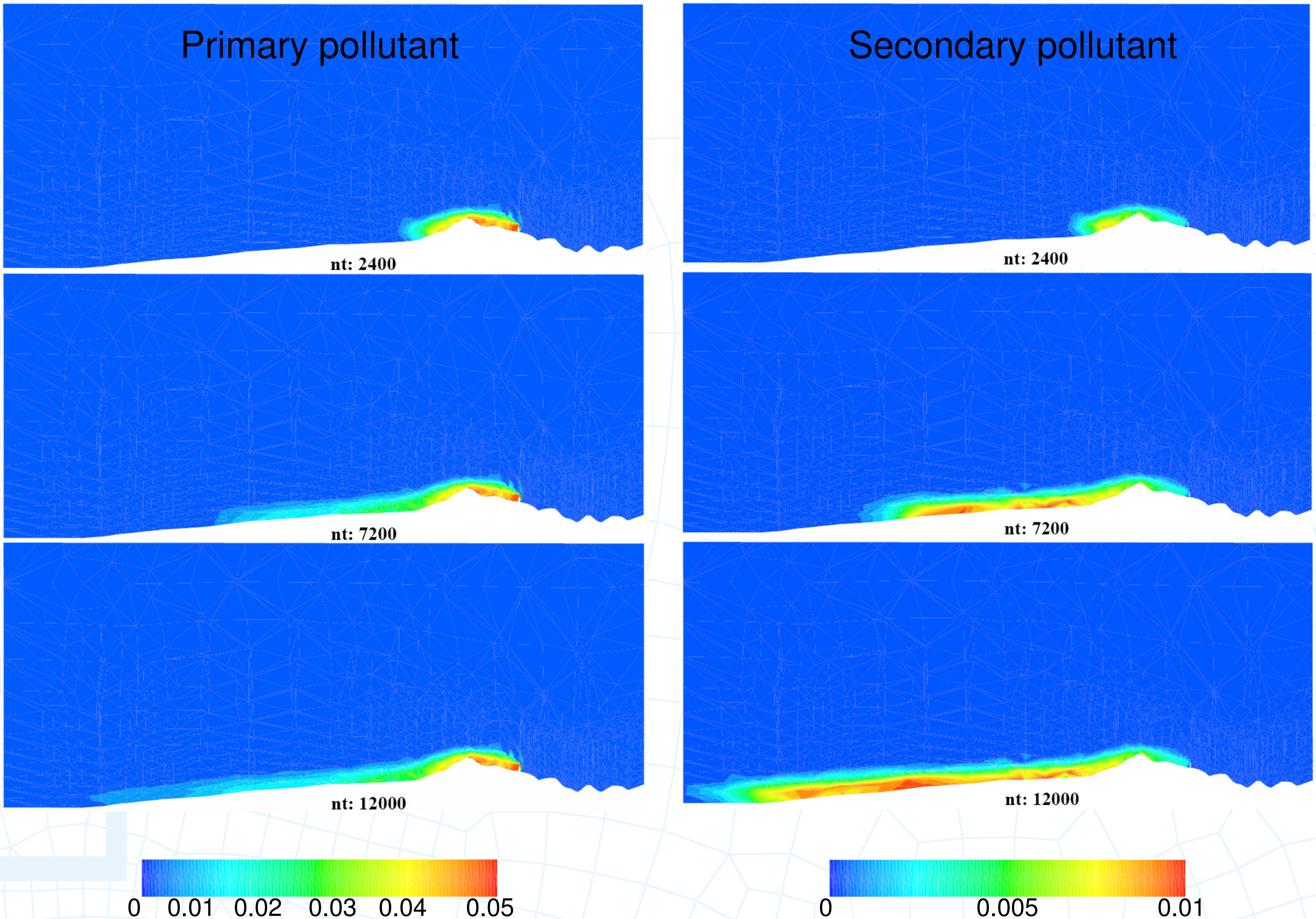
$$\mathbf{s}_3(\mathbf{c}) = -\alpha_3(\mathbf{c})\mathbf{c}_3 = -\mathbf{s}_4(\mathbf{c})$$

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

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

Nonlinear Jacobian

Nonlineal chemistry results



Conclusions

- FE computation of plumes of major punctual emissaries can deal with:
  - Complex topographies
  - Nonlinear reaction coupling between different plumes
- Proposed approach useful to solve transport – reaction of punctual emissions
  - FE mesh & Mass consistent wind model with effect of plume rise
  - CN + Least Squares for linear chemistry
  - Strang splitting + Ros2 + CN for nonlinear chemistry
- Time-step of the convection-reaction problem is not affected by the small elements from stack discretization (Courant numbers greater than one in small part of the domain can be allowed).

Simulación de la dispersión de contaminantes atmosféricos en la Zona Andina

LaCàN, UPC

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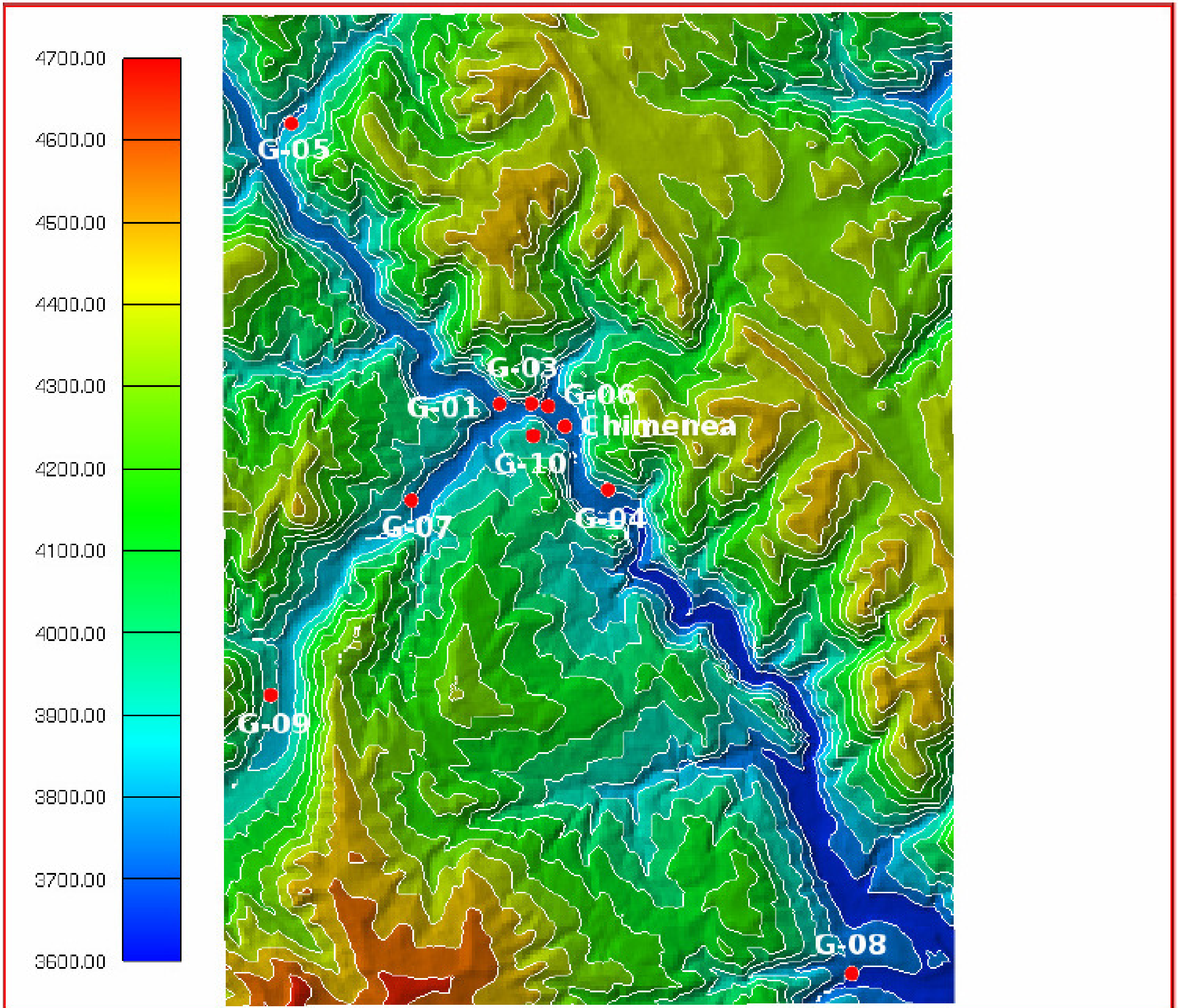
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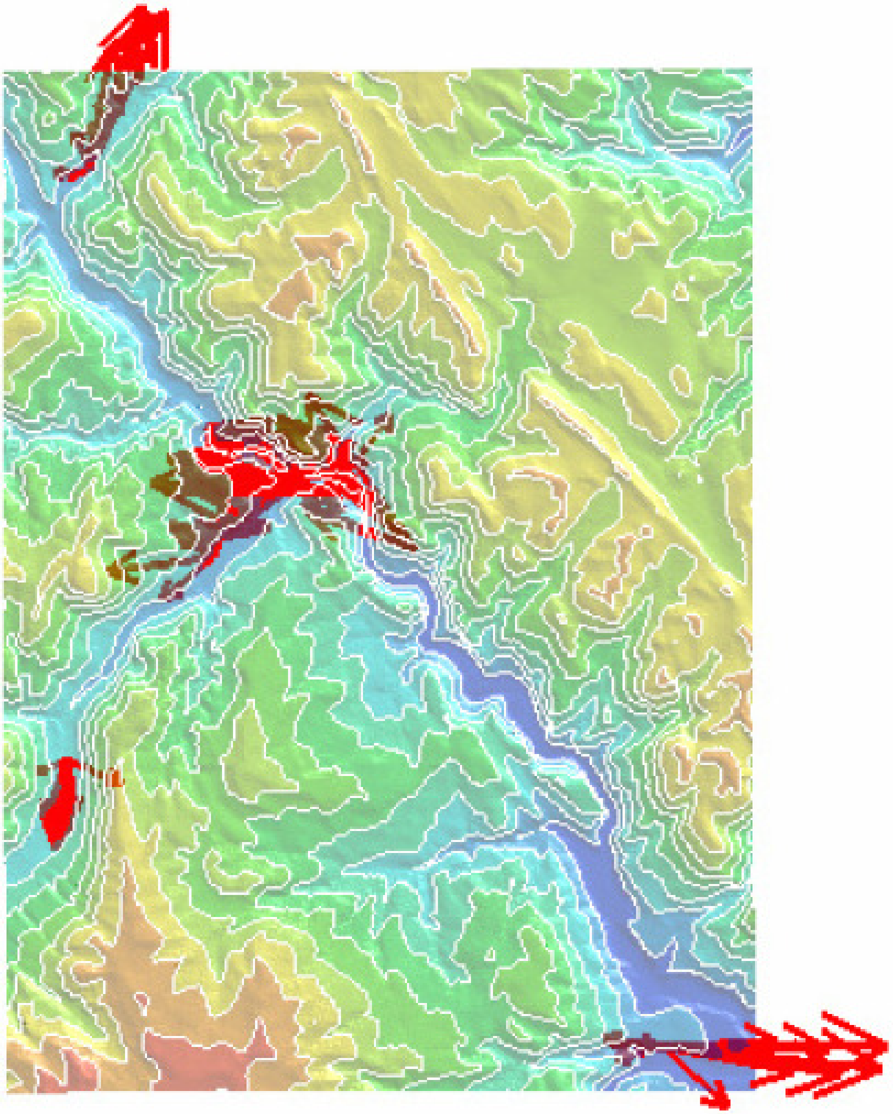
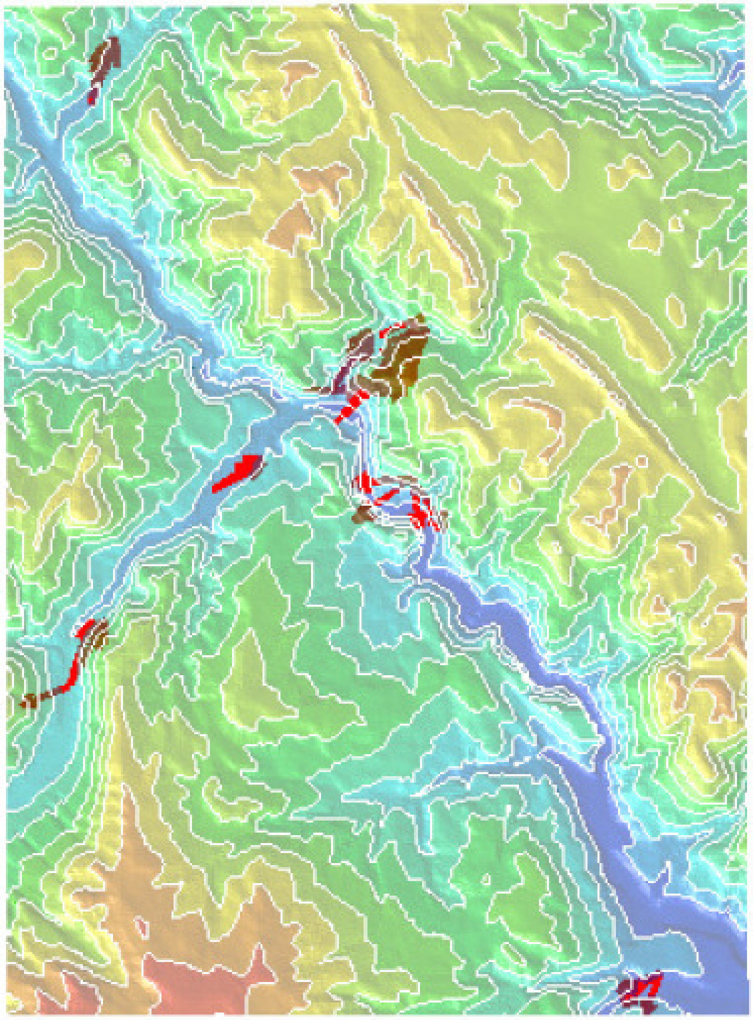
Noche



Dia (x4)



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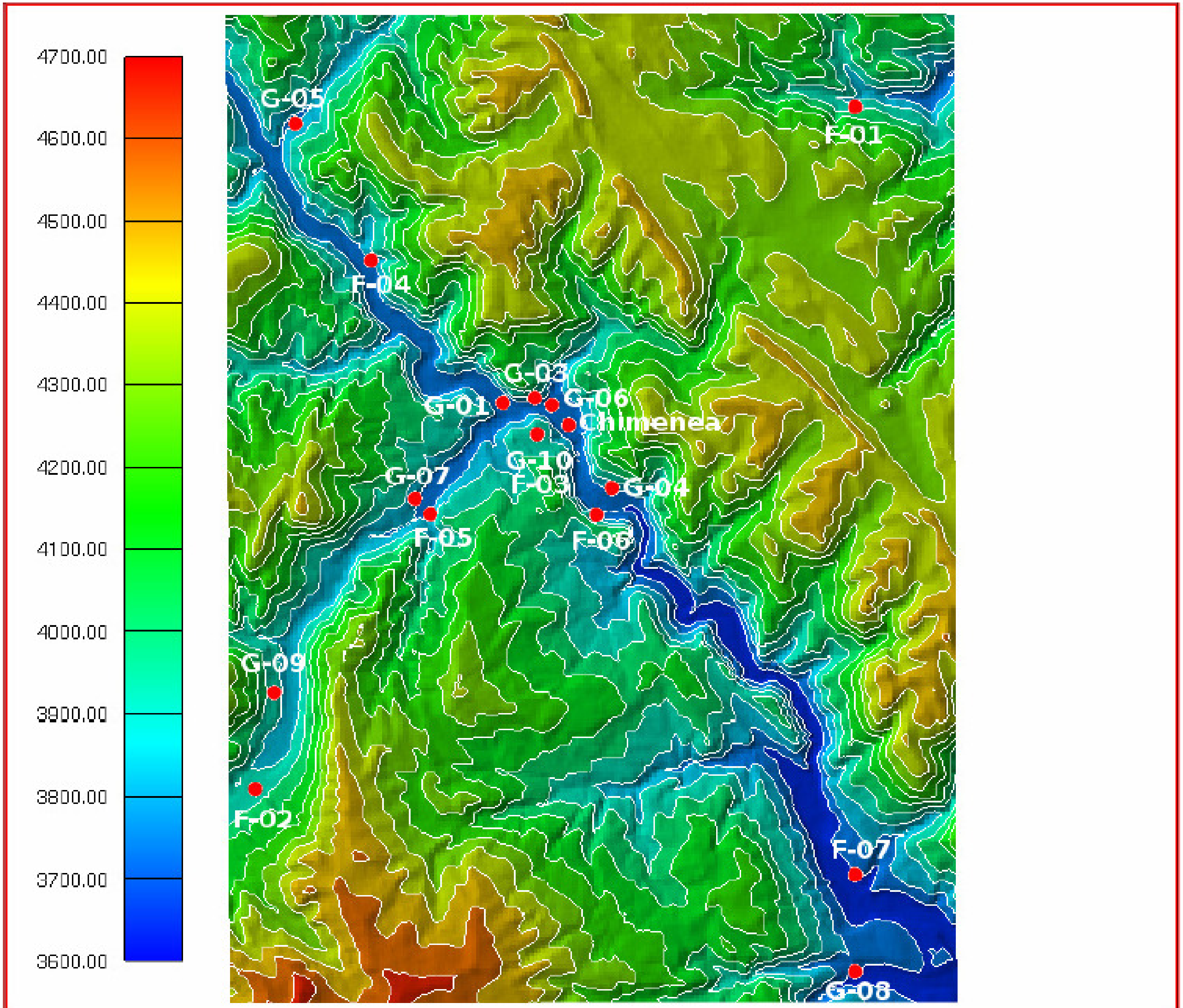

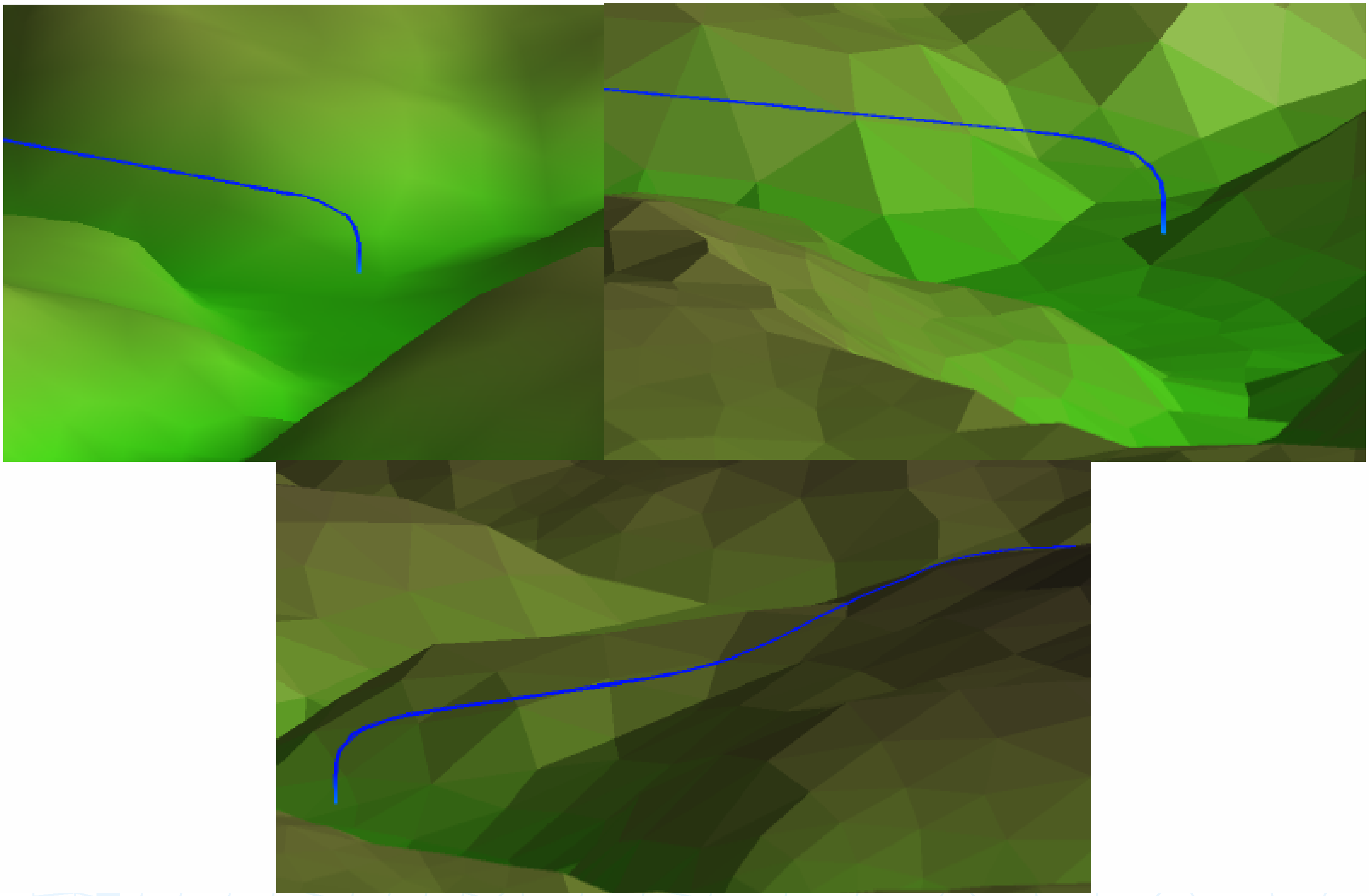

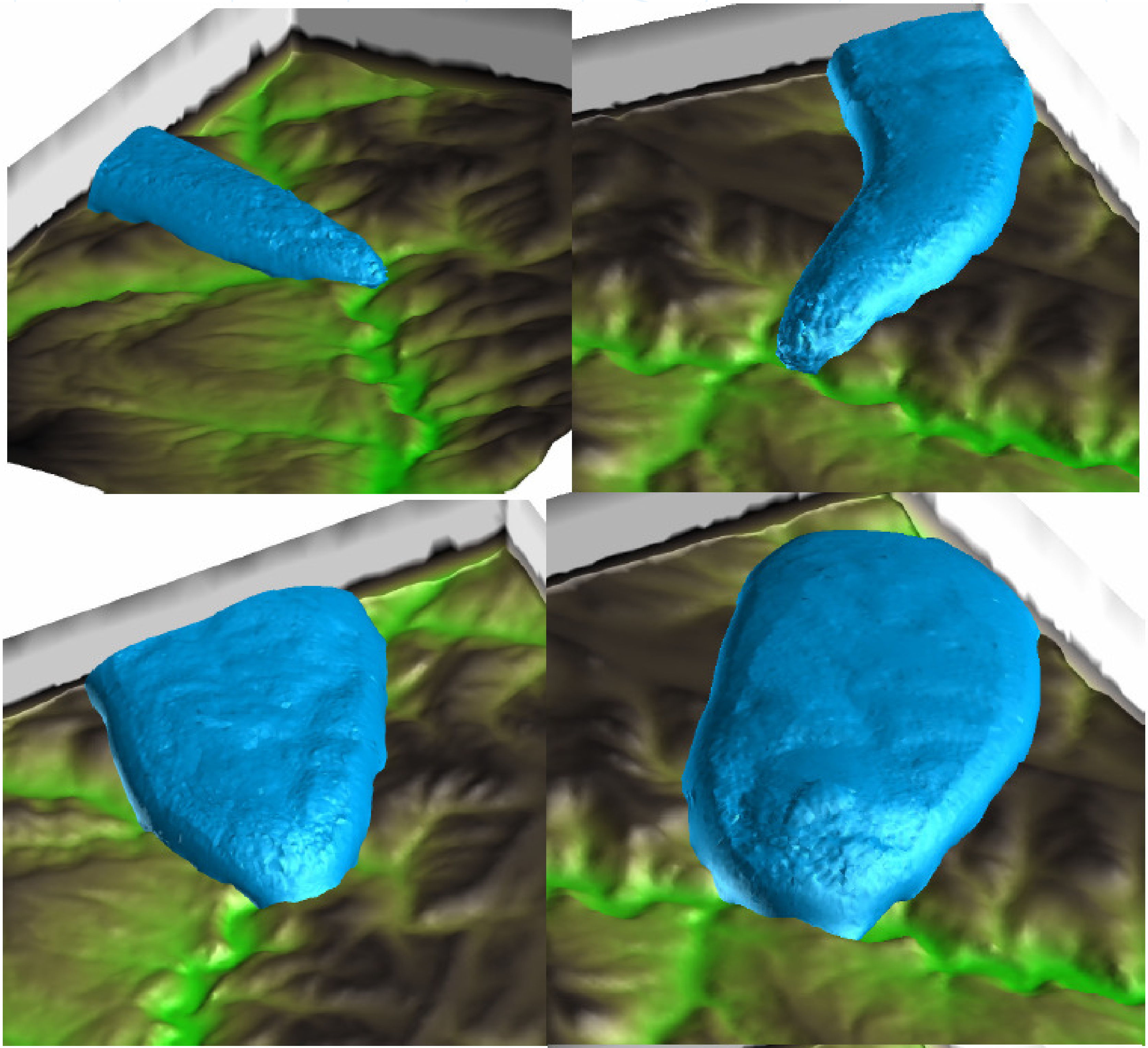

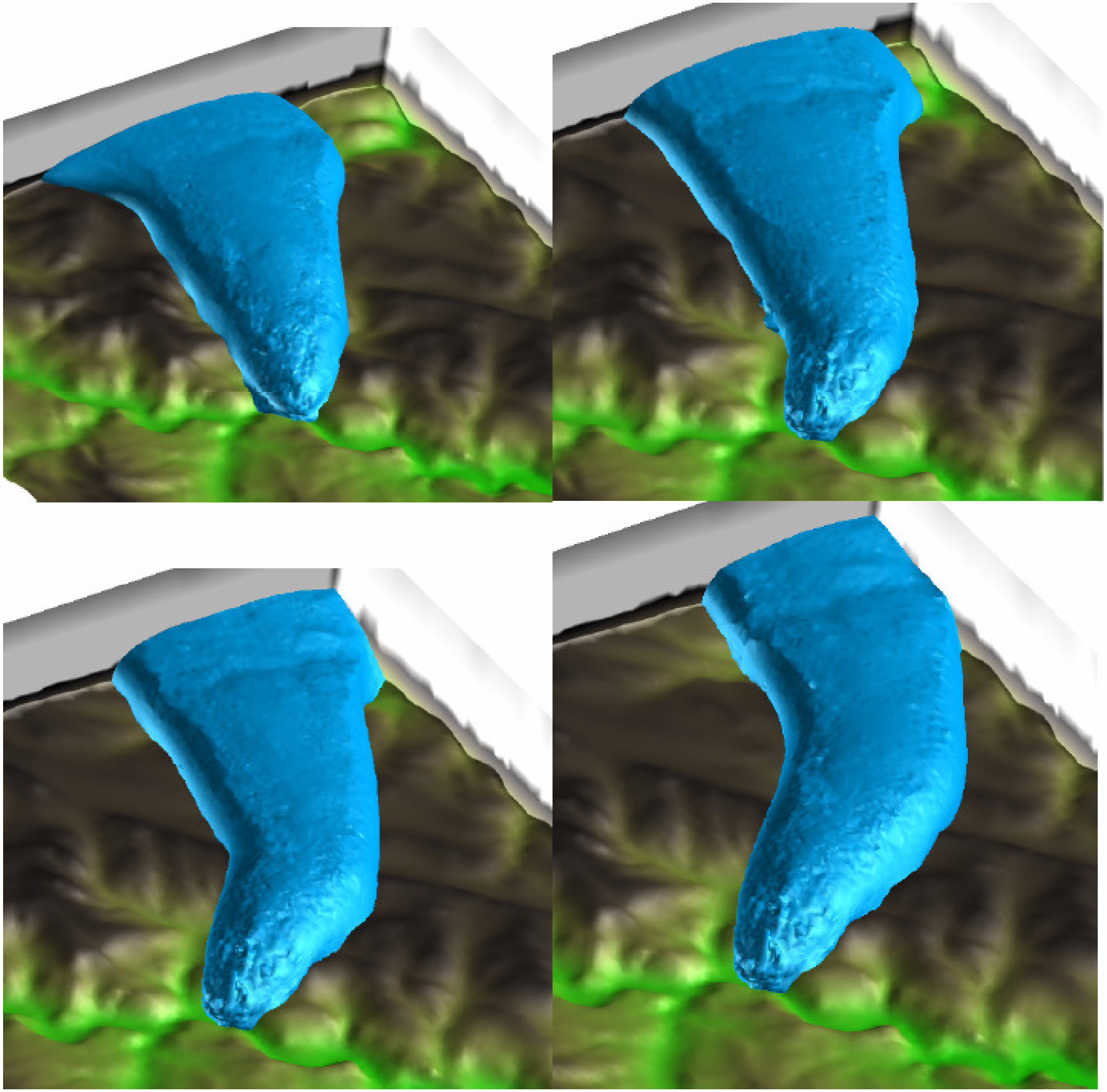

Figura A2.5. Resultados de la simulación del transporte para las 13:00 (sup. izq.), 13:20 (sup. der.), 13:40 (inf. izq.) y 14:00 (inf. der.) del 17/7/2008 (escenario de emisión 2008, parámetros D1). Isosuperficies de valores relativos de concentración igual a 1 10^-3.

- Dificultades detectadas:
  - Modelización de los efectos locales en el campo de viento (corrientes térmicas en los valles):
    - Es necesario calibrar la interpolación del campo de viento en los valles a lo largo del ciclo diario
  - Información sobre los vientos "en altura" (no sólo en superficie):
    - Es necesario acoplar las simulaciones de transporte con modelos meteorológicos que proporcionen información del viento dominante a escala regional (para este caso, según el SENAMHI de Perú, existen predicciones elaboradas cada 6 h, a 72 h vista, en intervalos de 6 h, en grids de 32x32 km2, modelo ETA, http://etamodel.cptec.inpe.br/).
  - Modelización del transporte en la zona con estratificación (bajo la capa de inversión térmica)
    - La calibración de la difusión vertical ofrece valores mucho más bajos que las difusiones horizontales.
    - Es necesario desarrollar esquemas numéricos específicos para las situaciones muy anisotrópicas

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Coupling regional and local air quality models for short-time prediction around punctual pollutant sources using finite elements

LaCàN, UPC

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Outline

- Introduction
- Proposed approach
- Regional AQM and their treatment of major punctual emissaries
- Coupling regional AQM and local Finite Elements AQM
  - Specific FE meshing strategy
  - Specific interpolation scheme
- Conclusions

Introduction

- Goal: To simulate air quality around punctual emissaries using short-time meteorological predictions, linking regional AQM with local Finite Elements AQM.

- Regional AQM uses information from Meteorological models (predictive behaviour)
  - Hourly prediction (typically 24 hours): Wind velocity, concentrations, solar radiation,…
  - BUT: Low spatial resolution (several km) and severe restrictions to accurate modeling of punctual emissaries

- Local FE AQM: transport – reaction of pollutants from punctual emissaries with resolutions of few hm (or less), and including complex topography and interaction of plumes

Introduction

- Regional AQM are not enough:
  - They can include the effect of major punctual emissaries
    - Specific models embedded within coarse grids (32x32 km2)
    - BUT: Conceived for chemical influence at regional scale not for accurate description at local scale
  - Alternatively, precision can be increased using nested grids:
    - Uniform 4x4 km2 nested grids has been reported
    - BUT: Major punctual emissaries cannot be included
- One-way link (from regional to local level):
  - Approach for short-time prediction at local level
- Two-way link (feddback from local to regional level):
  - Useful to improve accuracy of embedded models in regional AQM

Proposed approach

- Use predicted data from regional AQM for the local FE AQM simulation:
  - Wind field, Initial conditions, Boundary conditions, Parameters

- Approach:
  1. 3D Finite Element mesh adapted to topography, including geometry of punctual emissaries, and adapted to layer-structure of regional AQM
  2. Interpolation of wind field, initial conditions and complementary data
  3. Approximation of plume rise and mean-line trajectory
  4. Refinement of FE mesh to capture approximated plume geometry and wind field
  5. Computation of transport and reaction of pollutants
  6. [Return of pollutant masses to regional AQM, within FE domain and throughout FE boundaries]

Proposed approach

- Specific goals of this presentation:

1. To summarize main computational features of a regional AQM and coupling with local FE AQM

1. To present 3D meshing procedure that captures layer-structure of AQM and includes geometry of punctual emissaries

1. To present interpolation approach for local FE AQM input data

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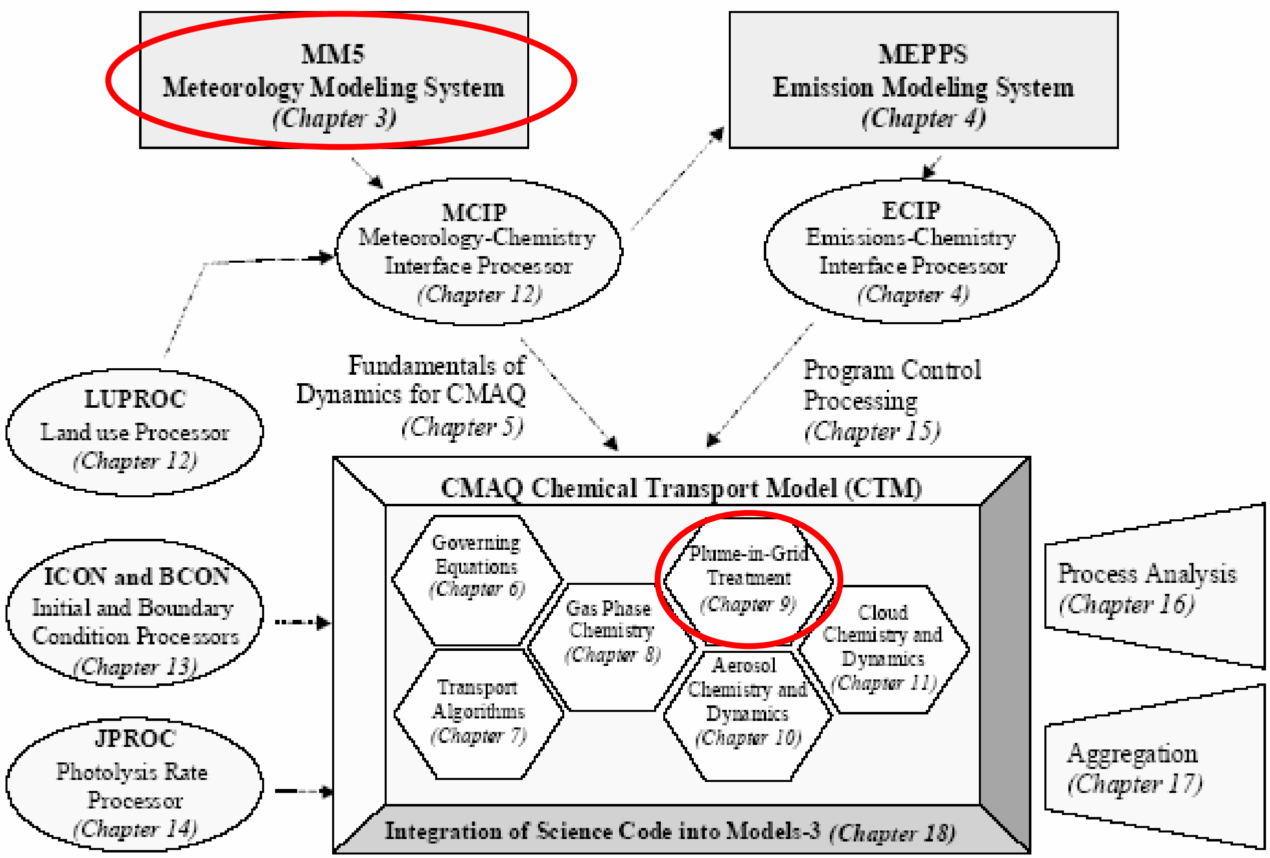
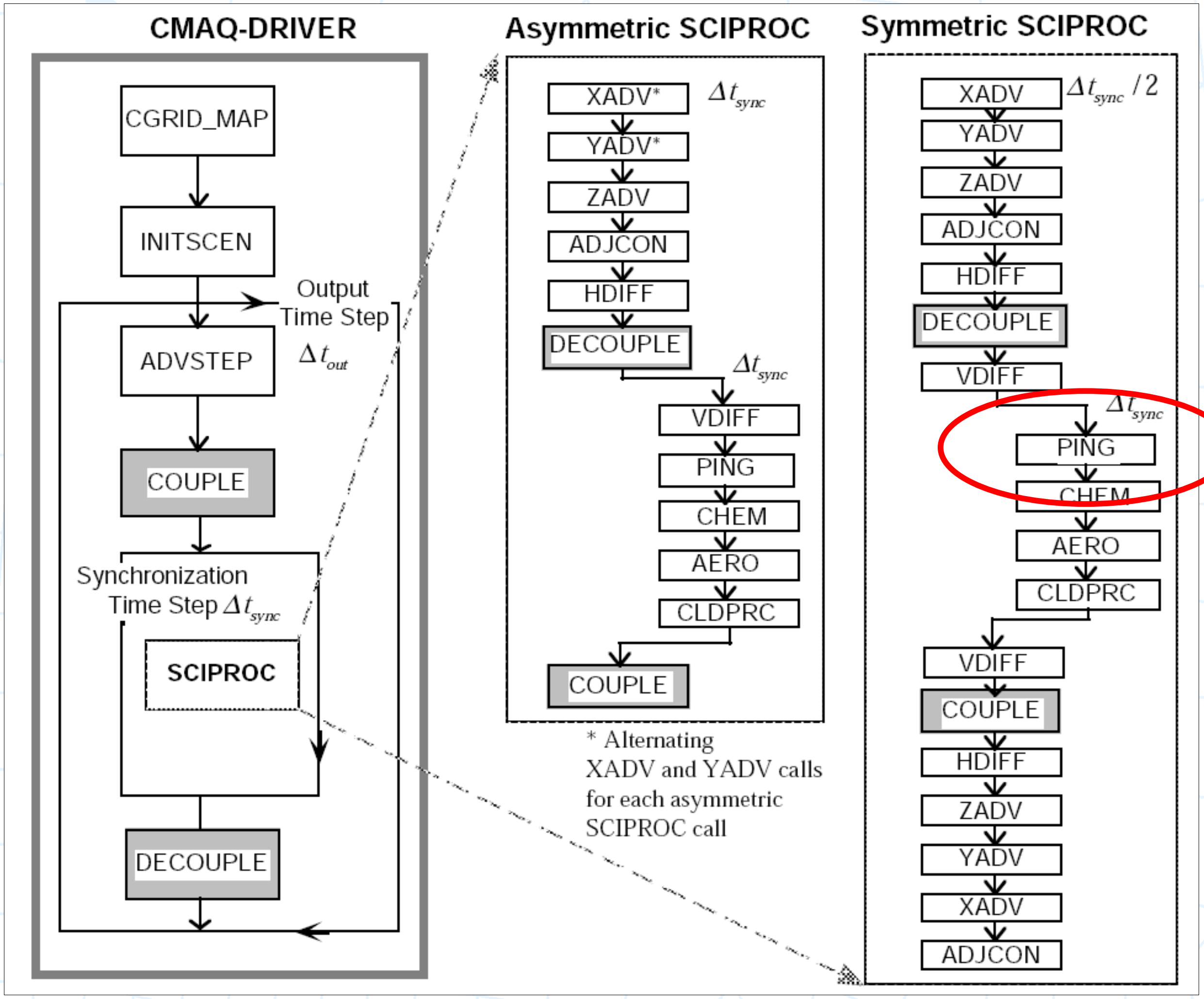
1. Regional AQM: CMAQ

- Key features of CMAQ:
  - Related with MM5 (meteorology model)
  - Finite Volume schemes
  - Complete non-lineal chemical reaction models (CB4, RADM2,…)
  - Plume-in-Grid treatment of major emissaries



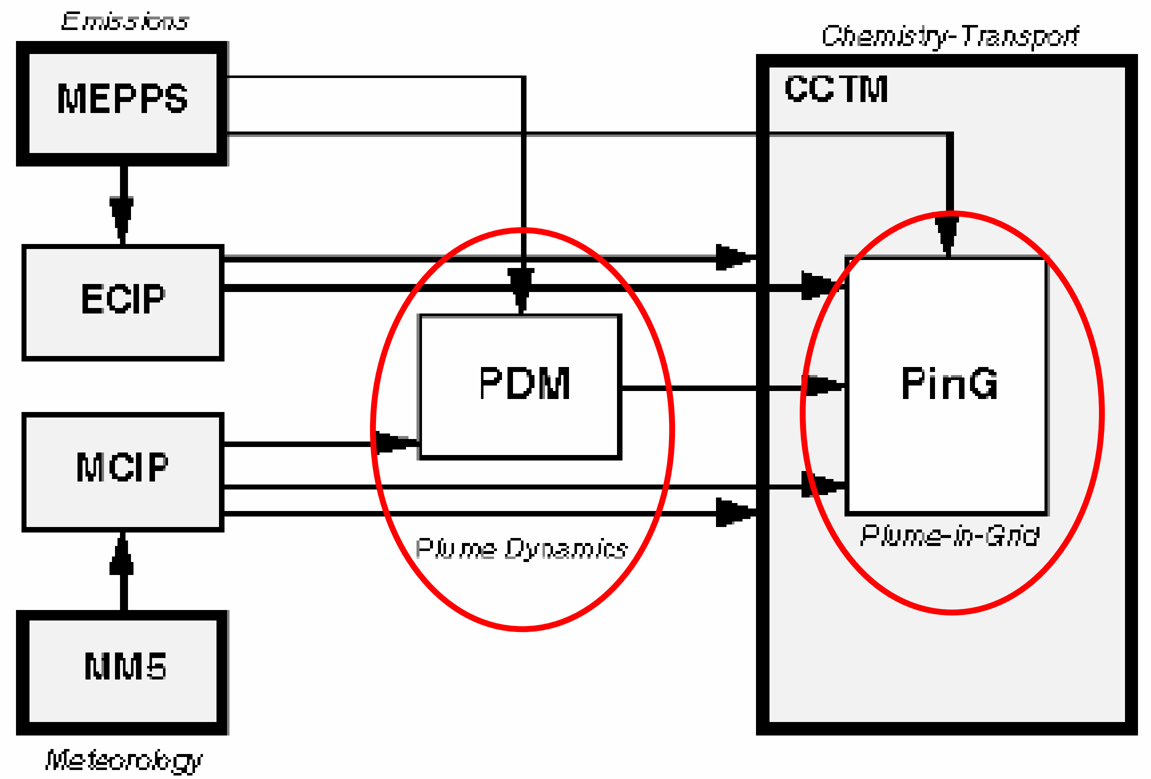
1. Regional AQM: CMAQ

- Chemical Transport Model algorithm: Splits all processes



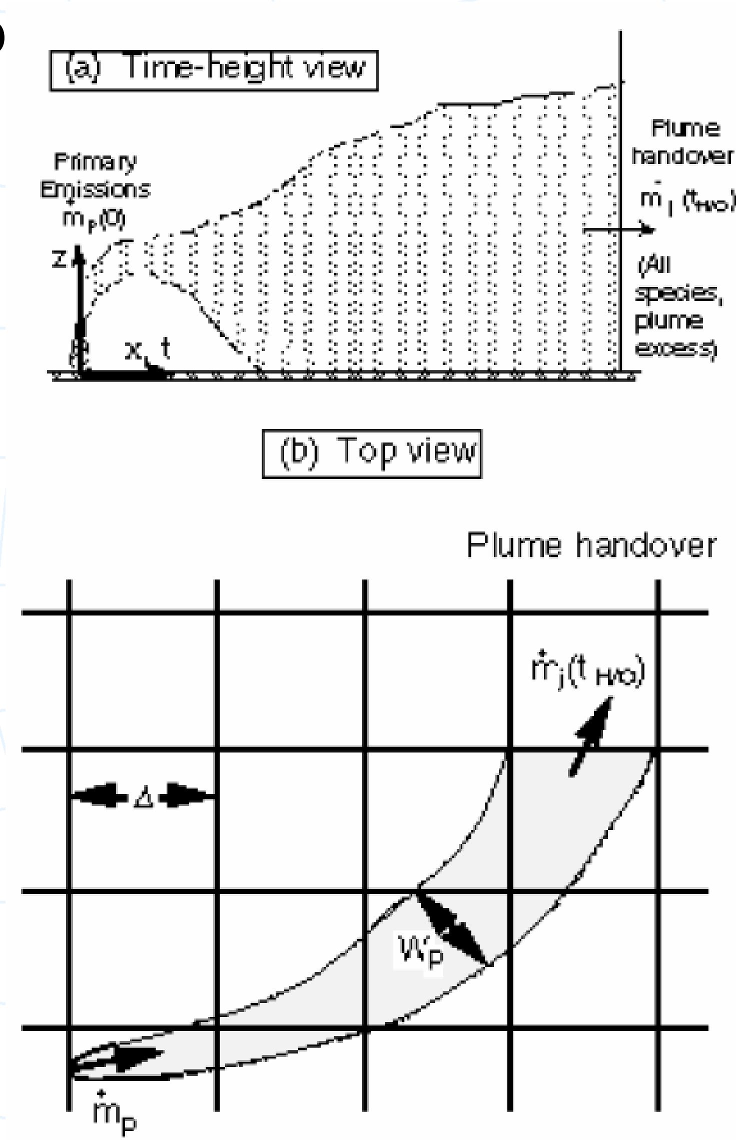
1. Regional AQM: Plume-in-Grid model

- PiG is used for solving chemical reaction within major point source pollutant plumes
- PiG needs a Plume Dynamics Model (PDM) as a preprocessor to know plume position and geometric characteristics



1. Regional AQM: Plume-in-Grid model

- PDM is a one-layer lagrangian method used to approximate (for each global time step):
  - Trajectory of plume (x-y plane)
  - Plume size: Plume rise and dispersion.
  - Plume end: Horizontal size same as CMAQ cell size



- PiG solves chemical reactions and update values at subgrid nodes defined by PDM.

- Mass from subgrid scale is added to CMAQ cells at plume handover:
  - Indicated by PDM
  - Chemical maturity of the plume
  - Coupling with other emissions
  - Excessive wind-shear, wet deposition,…

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1. Coupling CMAQ and local FE AQM

- Replace PDM preprocessor with
  - Local FE mesh adapted to geometry, and for each global time step:
    - Interpolation of wind data on local FE mesh
    - Approximation of plume rise and trajectory
    - Refine mesh to approximate plume and wind field
- Replace PiG module with:
  - Interpolation of initial and boundary conditions
  - Computation of transport – reaction of pollutants
  - [Return FE results to CMAQ]

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2. FE Mesh adapted to CMAQ layers

- Mesh requirements
  - Adapted to topography, including punctual emissaries
  - Adapted to CMAQ layers (10 to 15,…)
    - Reference heights (e.g.): 0, 30, 70, 150, 300, 700, 1500,…, 10000,…
    - Large punctual emissaries cross some bottom layers!

- Strategy (without punctual emissaries):
  - Define first layer (terrain) with a digital elevation model
  - Define following layers using CMAQ heights, but reducing curvature recursively, until the top one (plane)
  - Mesh each layer (2D) with element-size based on curvature
  - Mesh domain lateral boundaries connecting layers boundaries
  - Mesh the overall domain (3D) based on previous 2D meshes
    - Computed with a constrained Delaunay tetrahedralization

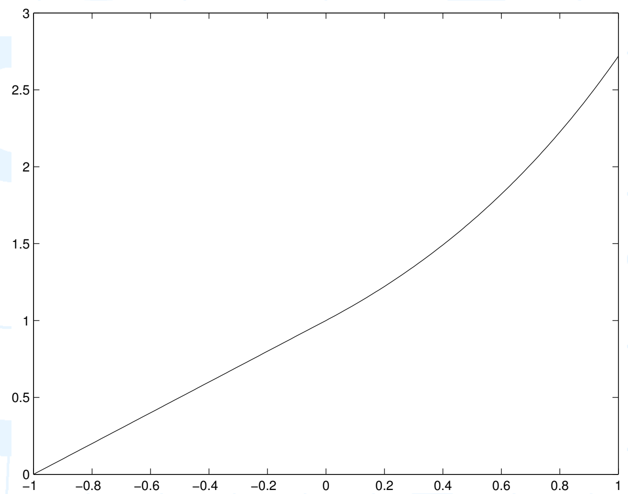
2. Test example

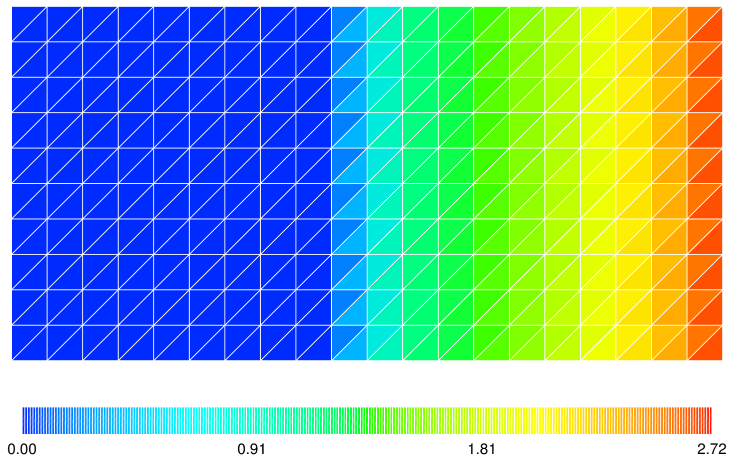
- Terrain example

$$f(x,y) = \begin{cases} x+1 & x<0 \\ e^x & x \geq 0 \end{cases}$$

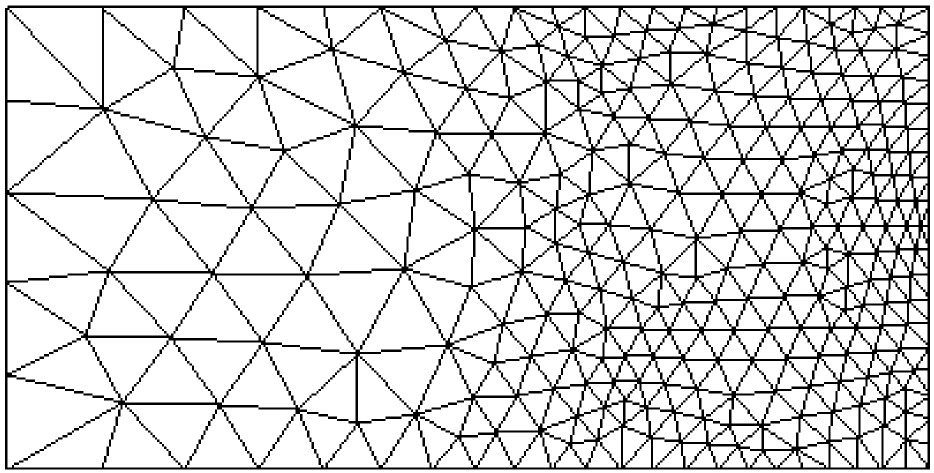
X=[-1,1]

Y=[-1,1]





Terrain curvature (x dir.)



Top view of terrain mesh

- Element size imposed with a background mesh

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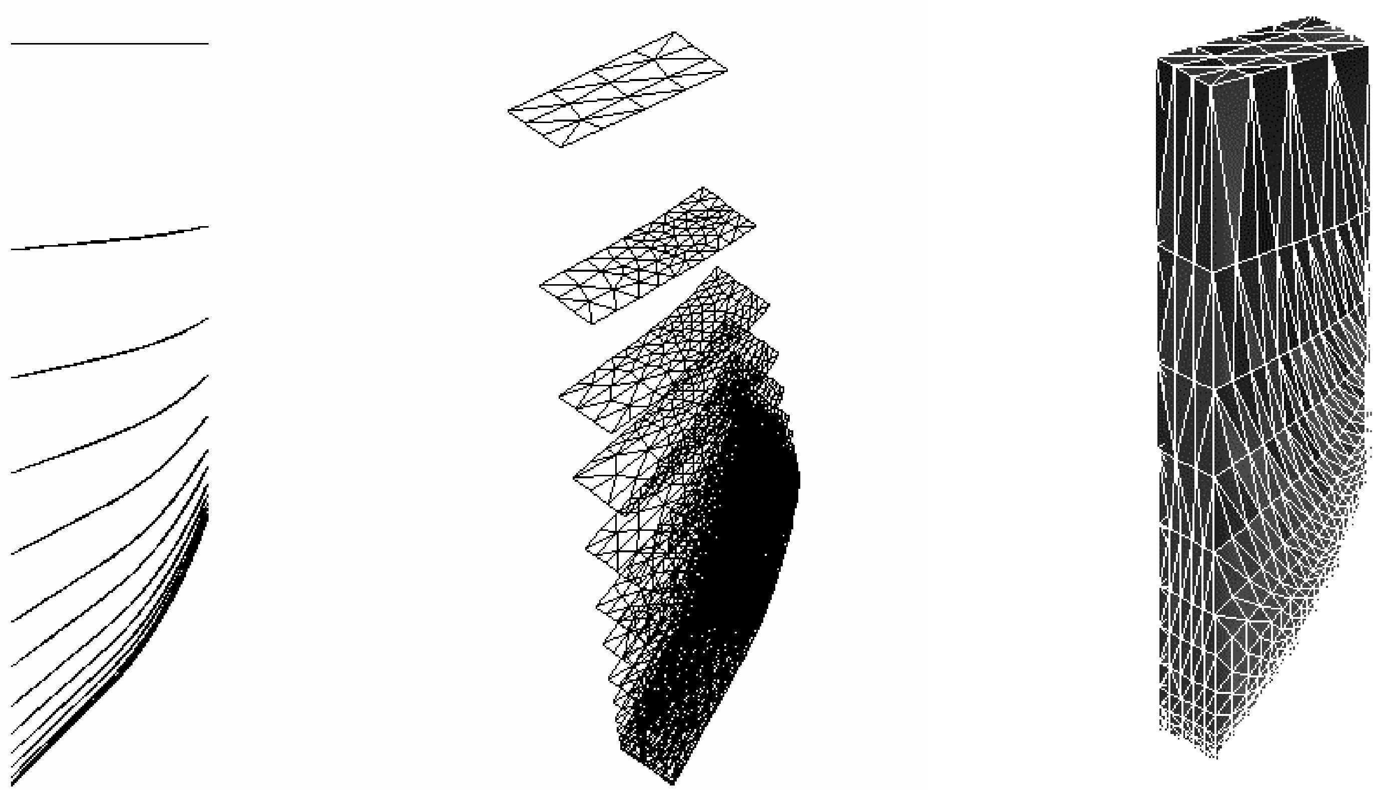
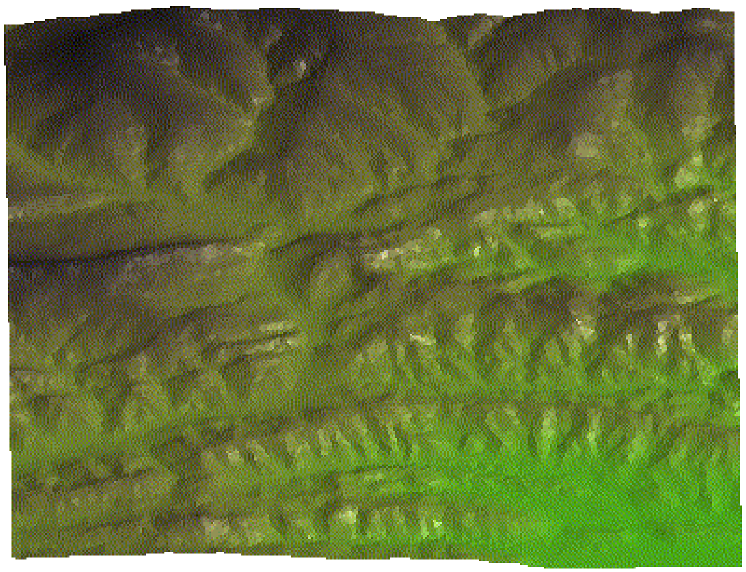
2. Test example

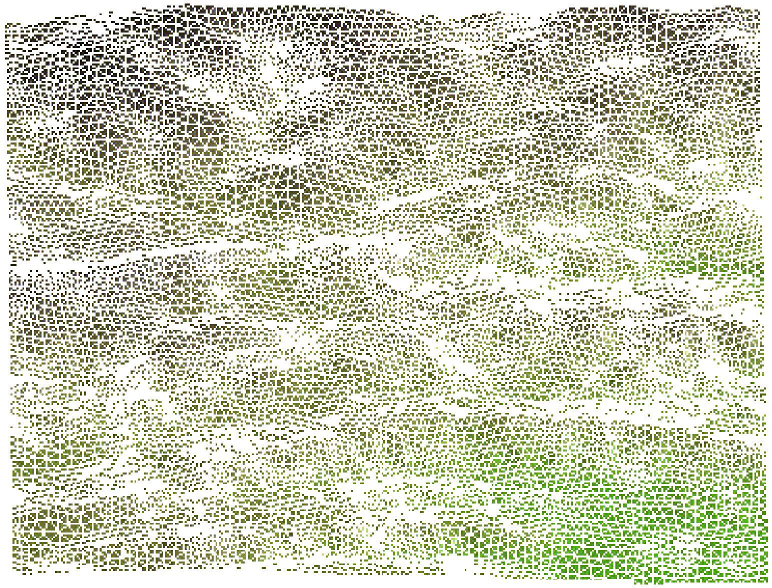
- Definition of following layers:
  - Mean distance between layers is imposed equal to distance between CMAQ layers
  - Within a layer: Vertical distance to mean height is smoothed w.r.t. that of previous layer. Nonlinear reduction:
    - Lower for bottom layers (to avoid layer crossing in complex topographies)
    - Higher for top layers (to reduce the number of elements)



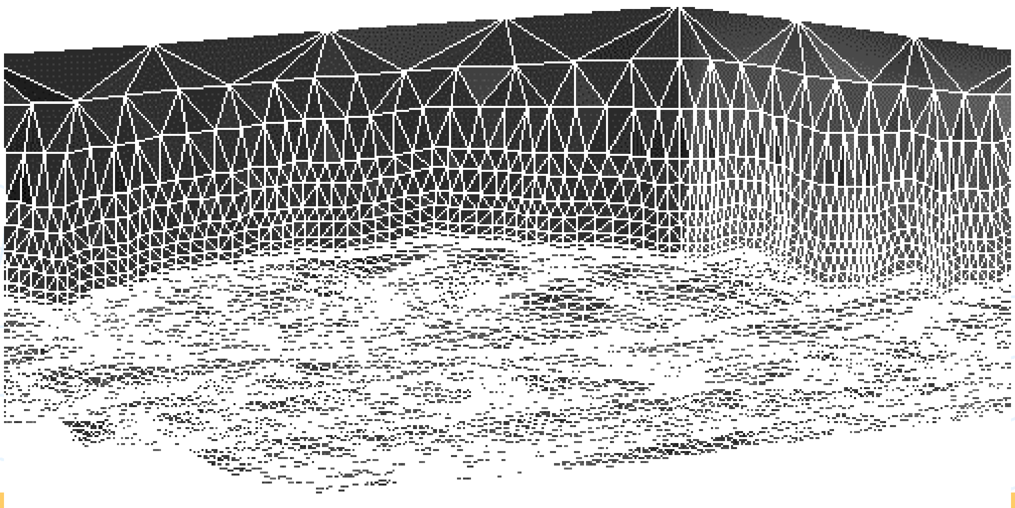
2. Example (Pyrenees)

- Domain size: 9x9 Km2
- DEM grid size: 90x90 m2



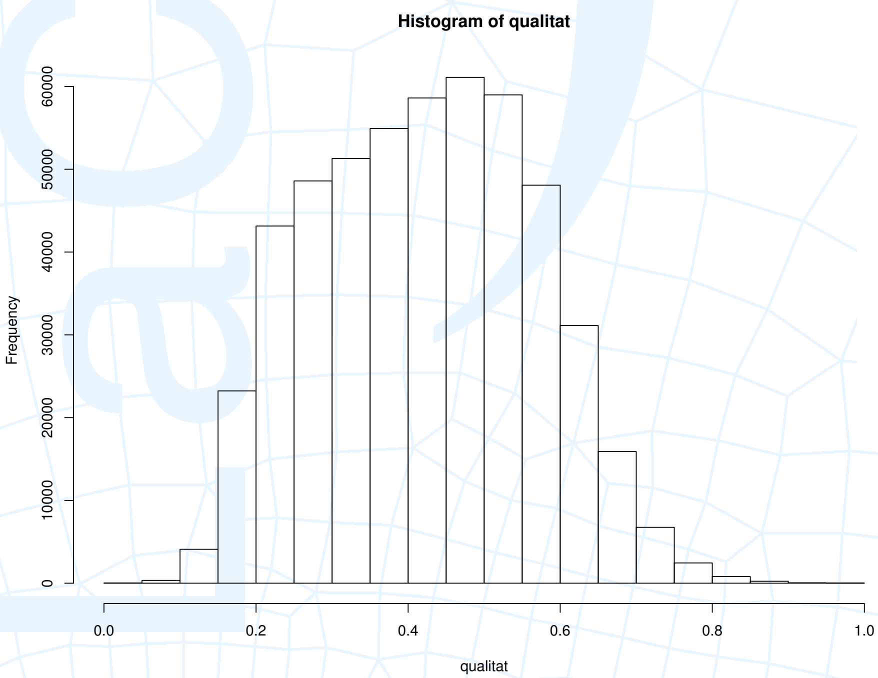


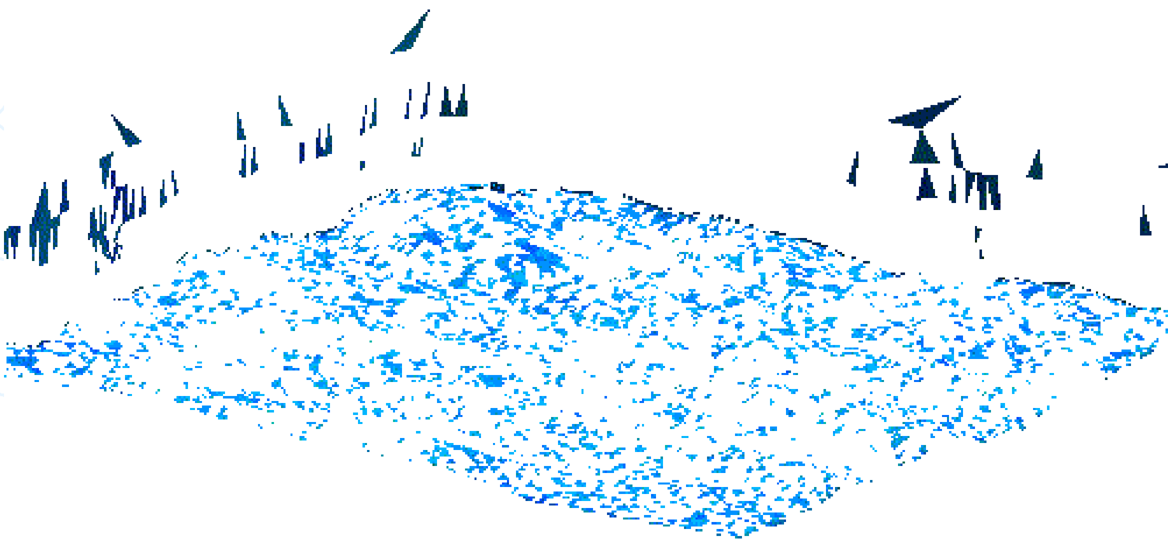
- 3D Mesh:



2. Example (Pyrenees): Mesh quality

- Shape quality measure (Q)
- Good results:
  - Min: 0.03
  - 1st quartile: 0.30
  - Mean value: 0.42
  - 3rd quartile: 0.53
  - Max: 0.99





Bad quality elements (Q < 0.2), concentrated in flat zones of terrain layer:

- Low height & large triangles

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2. FE Mesh including punctual emissaries

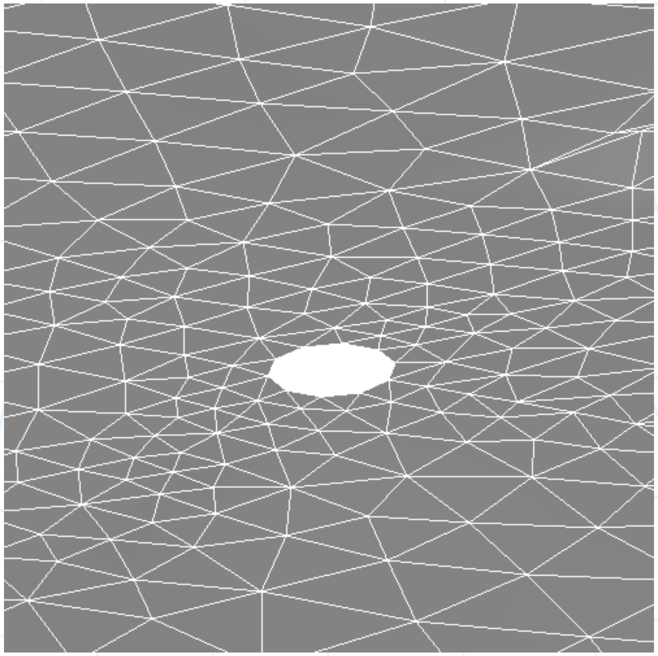
- Identify layers that intersects emissary and include a hole in their geometries (typical size: 5-10 meters diameter)

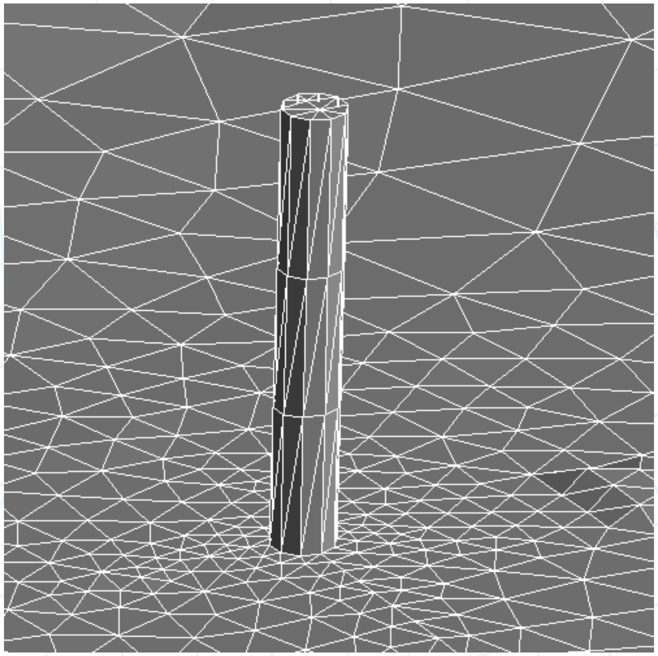
- Use background meshes with element size able to discretize holes
  - Lower than curvature-based value
  - Common to all intersected layers

- Mesh the hole (the circle) with the same background mesh (to have same nodes at the boundary)

- Connect nodes of layer holes between them and with the emissary top (the circle)

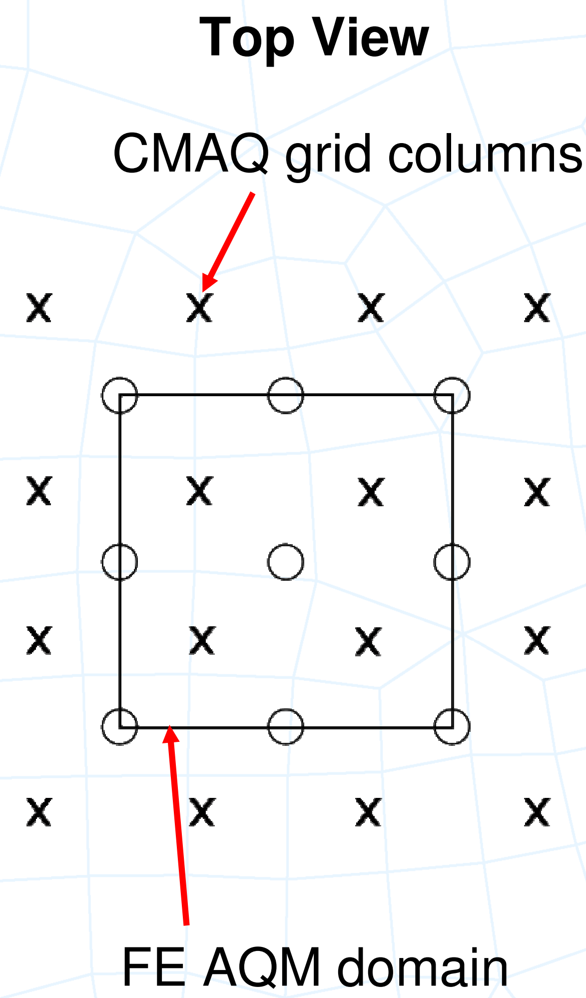
- Mesh 3D domain with a constrained Delaunay tetrahedralization





3. Interpolation of CMAQ data for FE AQM

- CMAQ data defined at CMAQ grid (cross points):
  - Layer vertical positions
  - Vertical velocities (Vz)
  - Concentrations of all species at all layers
- CMAQ data defined at CMAQ Gauss points, located in the middle of CMAQ grid (dot points):
  - Horizontal velocity (Vx-Vy) at all layers



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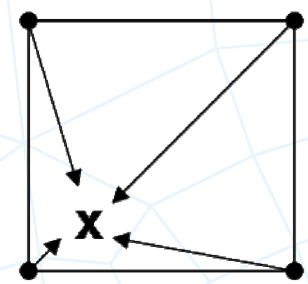
3. Interpolation of CMAQ data for FE AQM

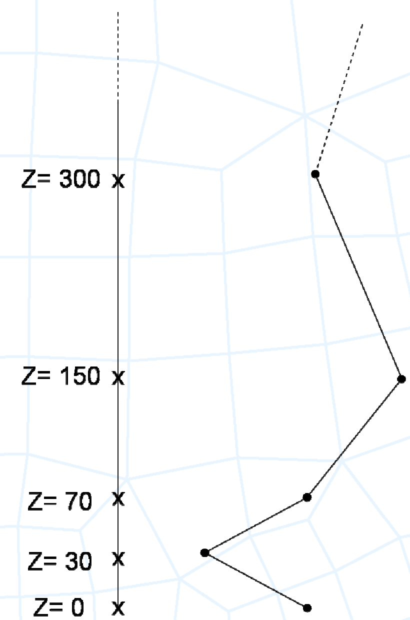
- Strategy to interpolate data:
  - For a given X-Y bilinear interpolation of data defined at CMAQ grid nodes (or at Gauss points):
    - Including layer heights!



  - Correction of interpolated layer vertical positions to match terrain

$$z^{corr} = z^{CMAQ} - \left(\frac{z^{max} - z^{CMAQ}}{z^{max} - z^{min}} \right) \left(z^{min} - z^{terr} \right)$$

  - For a given Z, linear interpolation of interest data



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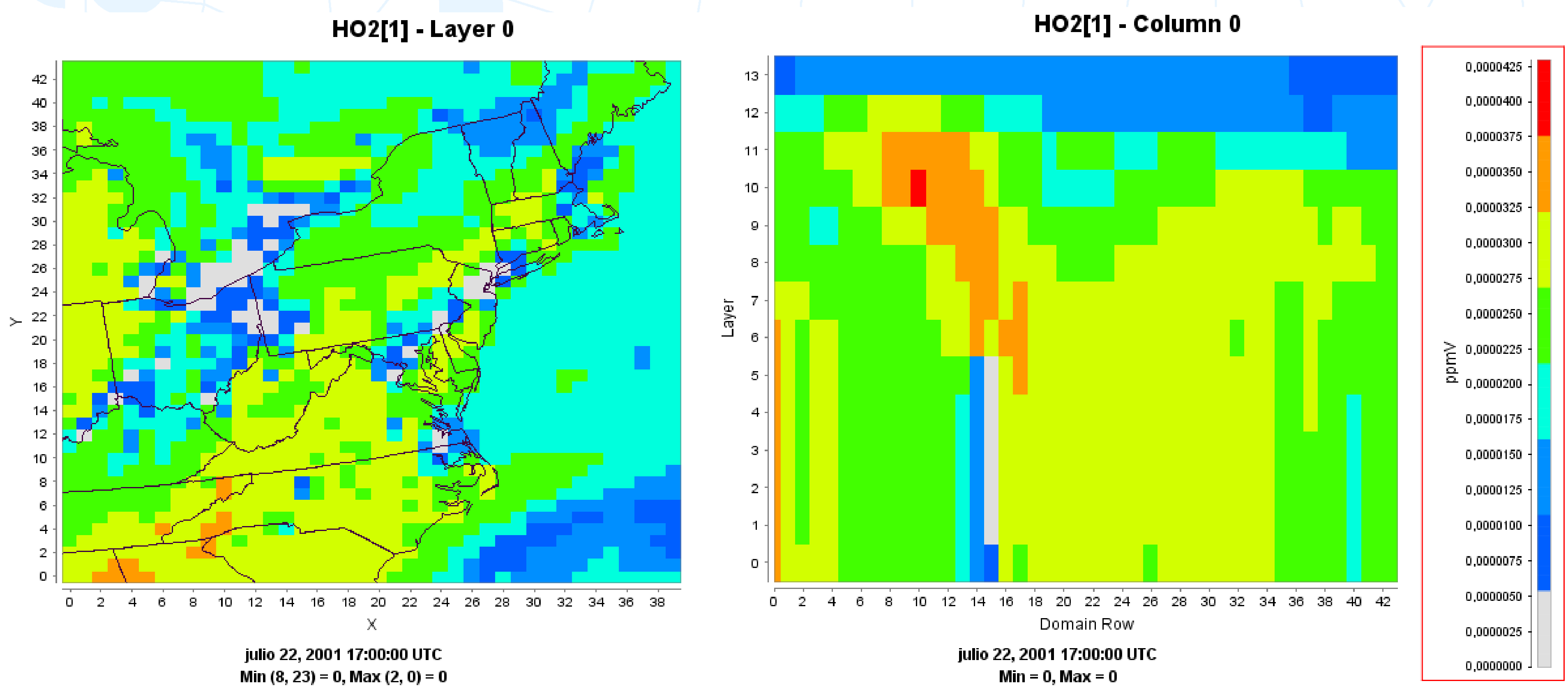
3. Example: CMAQ data

- CMAQ tutorial example:
  - Grid of 40x44 cells. Cells size 32x32 km2.
  - 14 layers, top height 15000 m
  - Nested grid of 8x8 km2 cells in a part of the domain

- Standard CMAQ visualization tool:



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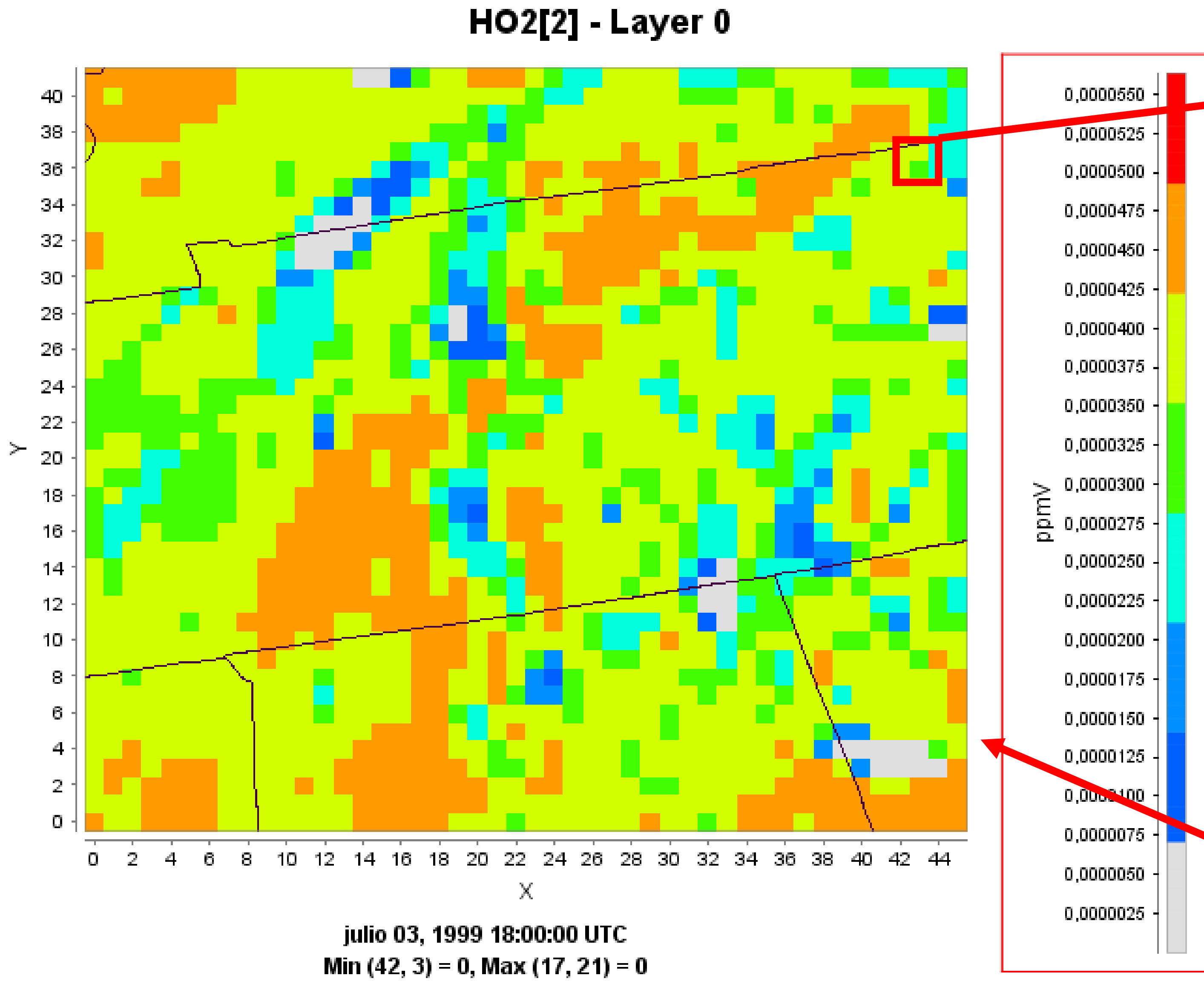
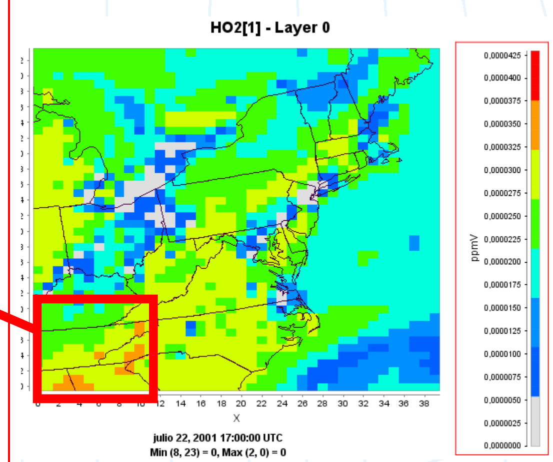
3. Example: CMAQ data

- Nested grid of 45x41 cells. Cells size 8x8 km2

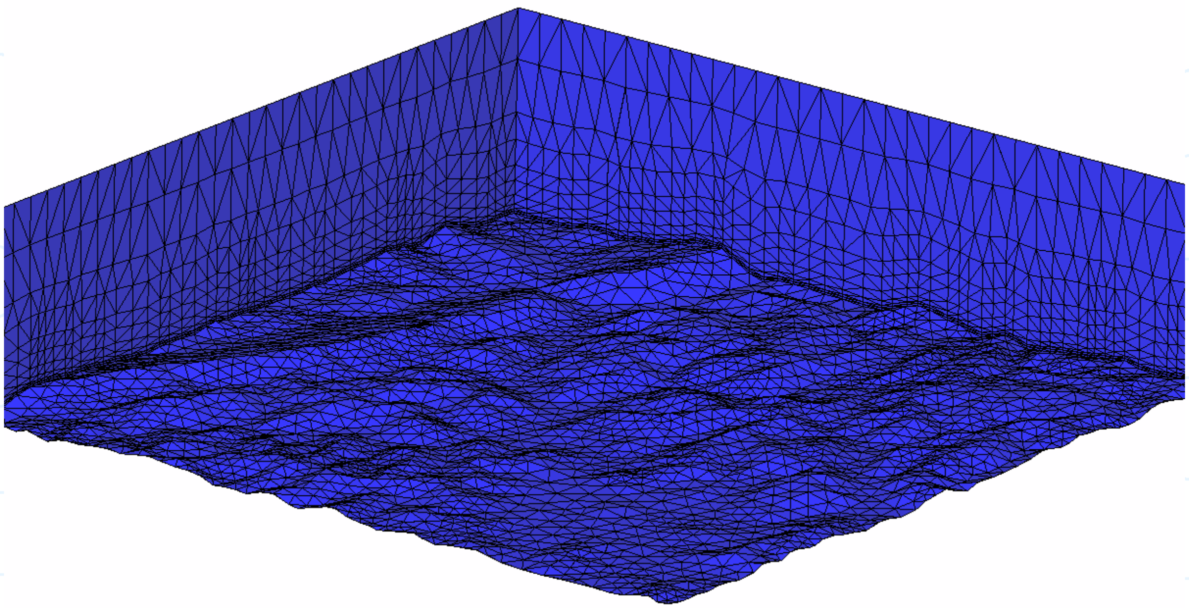


Local FE AQM domain: 16x16 km2



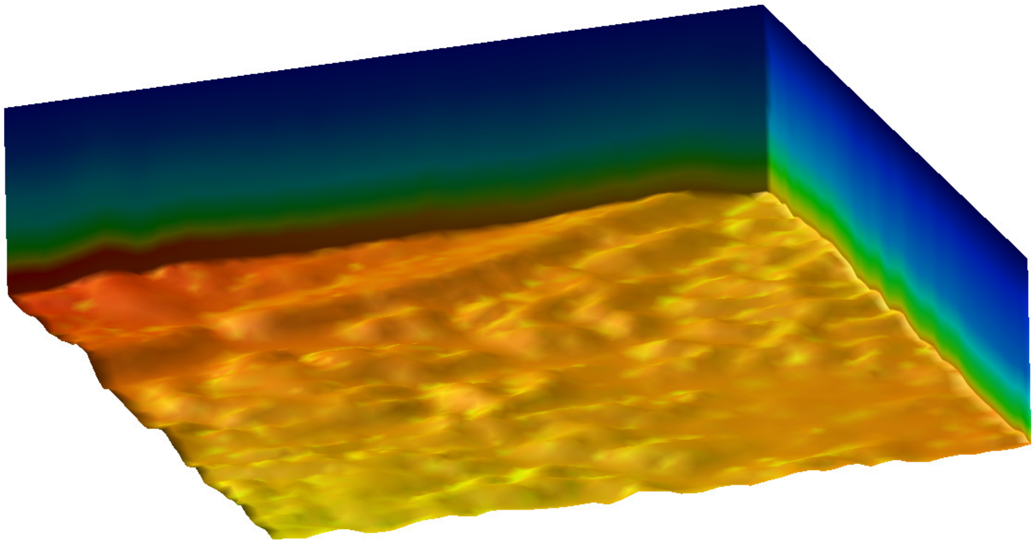
3. Example: FE Mesh

- 16x16 km2 x 4000 m

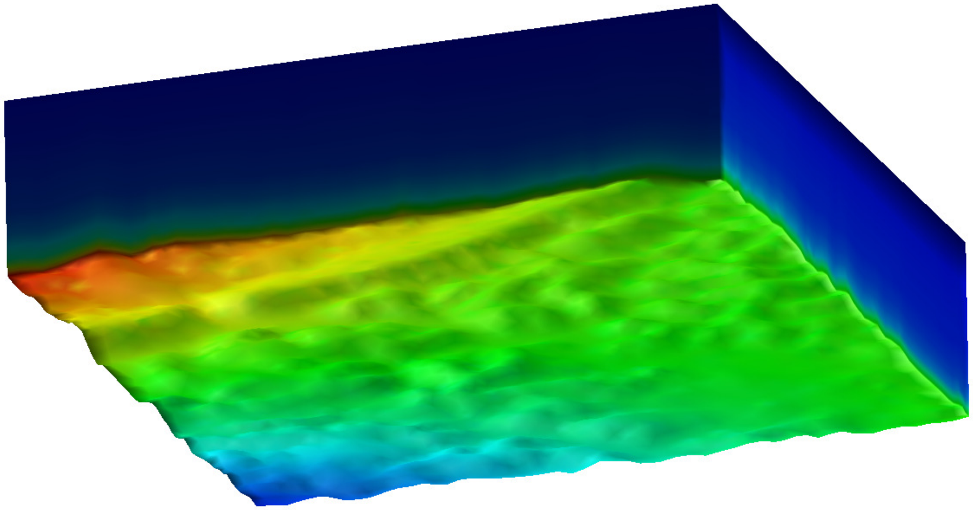


3. Example: Initial conditions for FE AQM

- Interpolated data from 4x4 columns of CMAQ nested grid data (covering 32x32 km2):
  - FE domain centered in CMAQ one (with 2x2 columns of cells in it)



NO3; most variation in height



NO2; most variation at bottom layers

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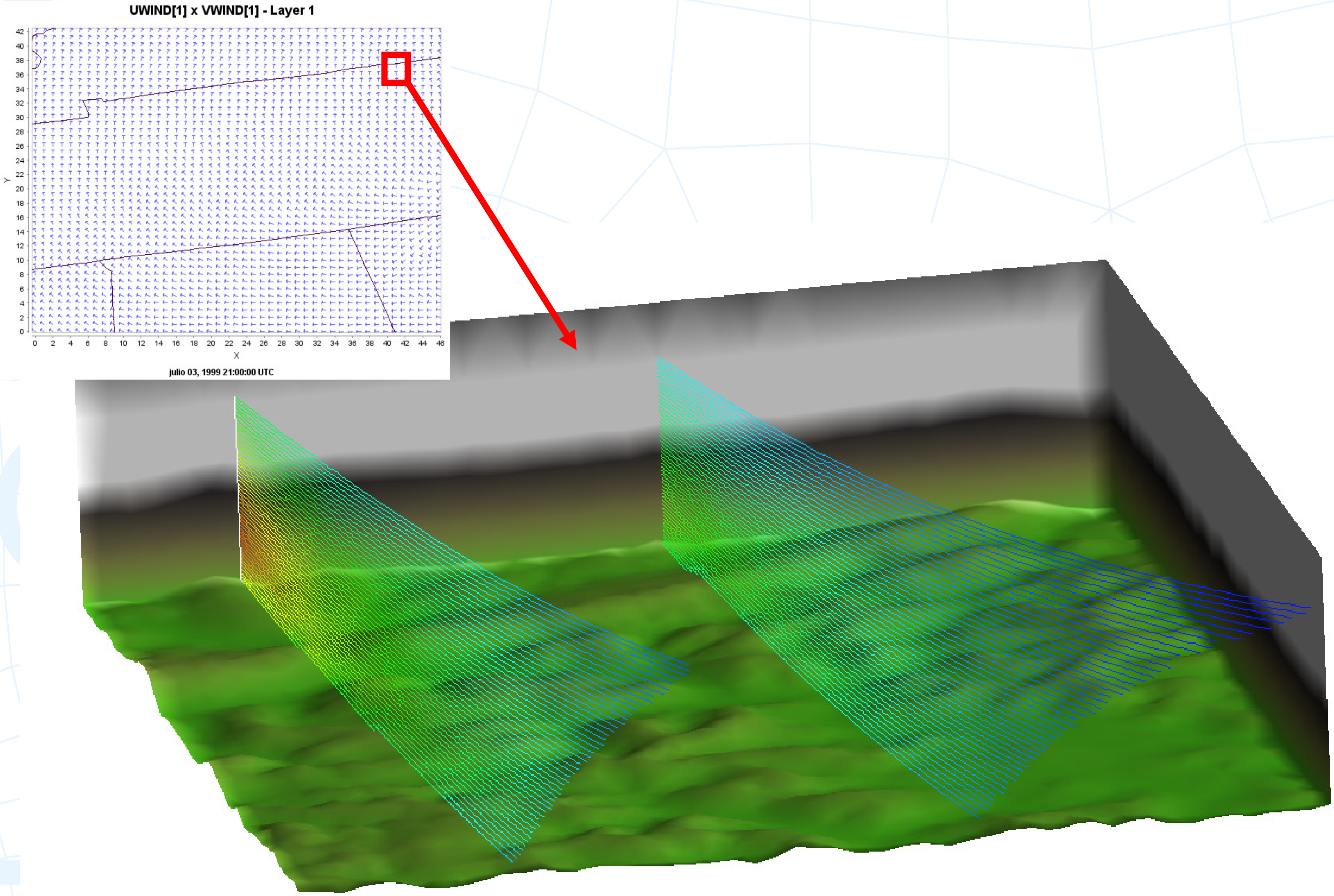
3. Example: Interpolated wind field



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Conclusions

- Short-time prediction of air quality at local level can be obtained coupling local FE AQM with regional AQM
  - Regional AQM gives the predictive character thanks to link with meteorological models
  - Regional AQM alone are not suited for accurate description of major emissaries at local scale
- One-way / two-way links between scales have been defined without modifying structure of regional AQM algorithm
- 3D meshes including geometry of punctual emissaries and respecting layer-structure of regional AQM have been defined
- Specific interpolation schemes adapted to fine description of topography have been defined

Next steps...

- Tesis doctoral “en marcha”
- Casos de estudio “realistas”:
  - Zona Andina ?
  - España ?

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