Inspira Crea Transforma

Model Based Predictive Control for Air Quality in Colombia

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The Netherlands

Sensitivity and uncertainty sources in numerical modeling to forecast atmospheric systems: High-resolution WRF model simulations in urban valleys applied to air quality issues.
Part I

Research Grants – EAFIT 2018

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Outline

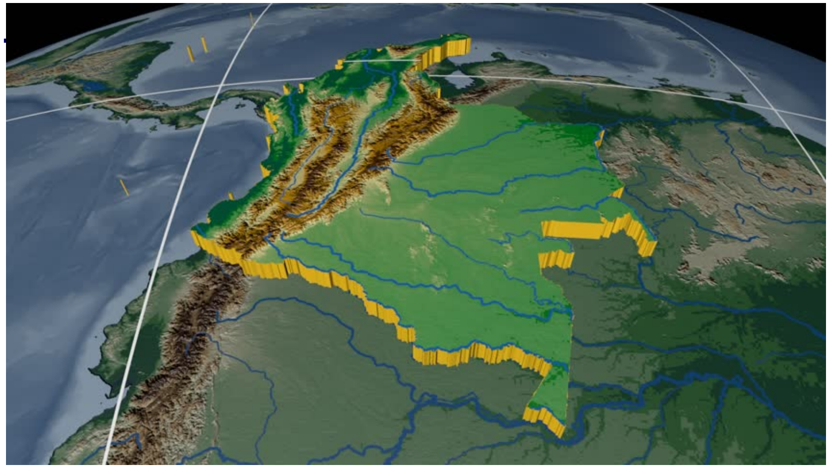
Introduction

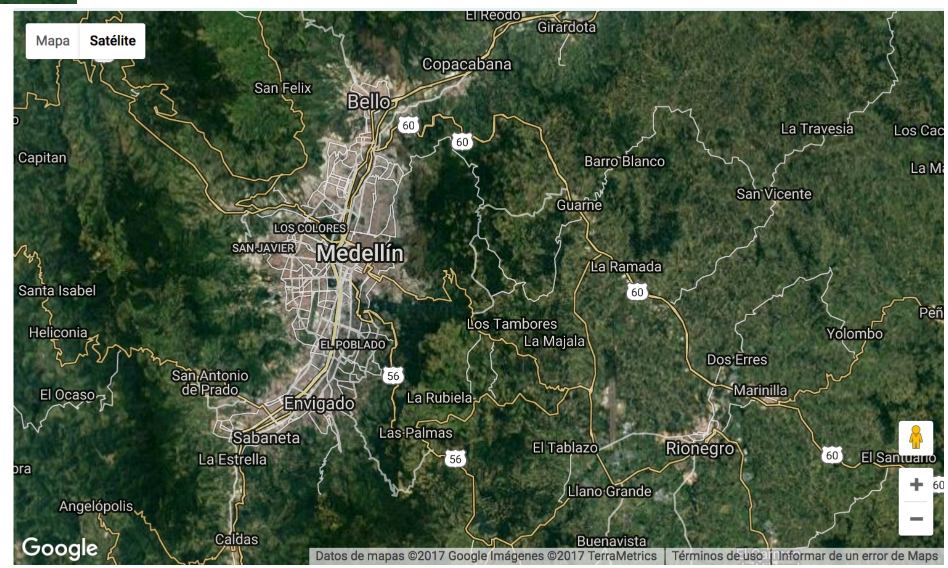
- Model Based Predictive Control Scheme
- Modeling
- Instrumentation and Sensing
- Controller design

Challenges

Proposal

Introduction



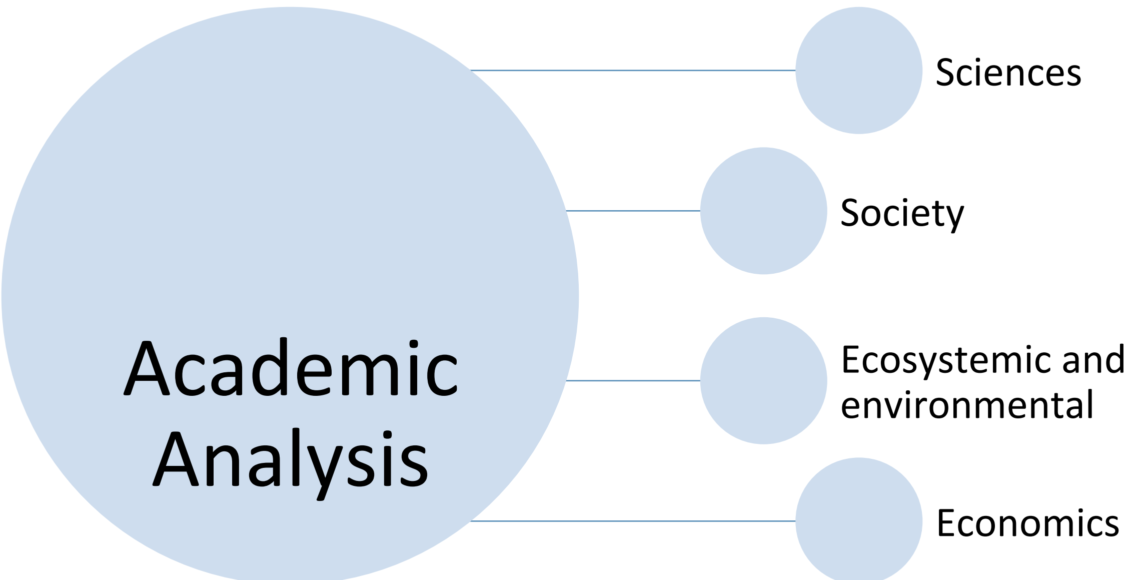


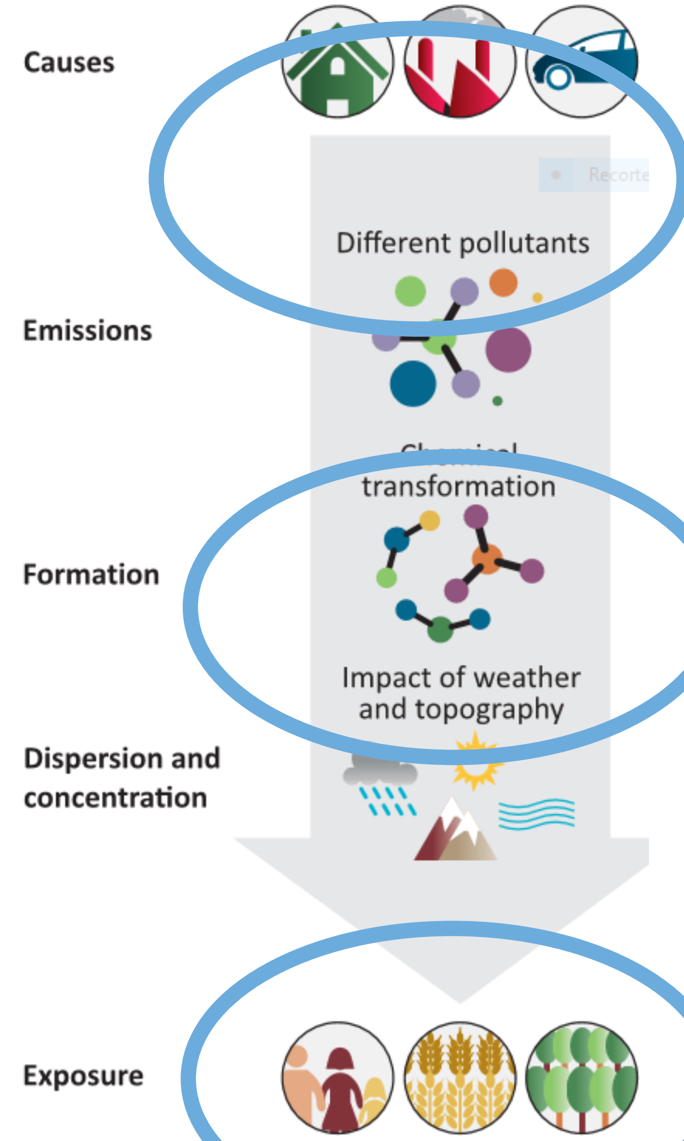
Environmental Emergency (a.k.a. Contingency) Medellin, Mar-Apr 2016

Environmental Emergency (a.k.a. Contingency) Medellin - Mar 18-Apr 19, 2016

PM2.5 > 125 μg/m3
(WHO guidelines max. 25 μg/m3)
Days without car & motorcycles
Restricted truck (volquetas) movement
Cease of outdoor activities
Regional rush hour traffic restrictions (pico y placa)
Free Metro

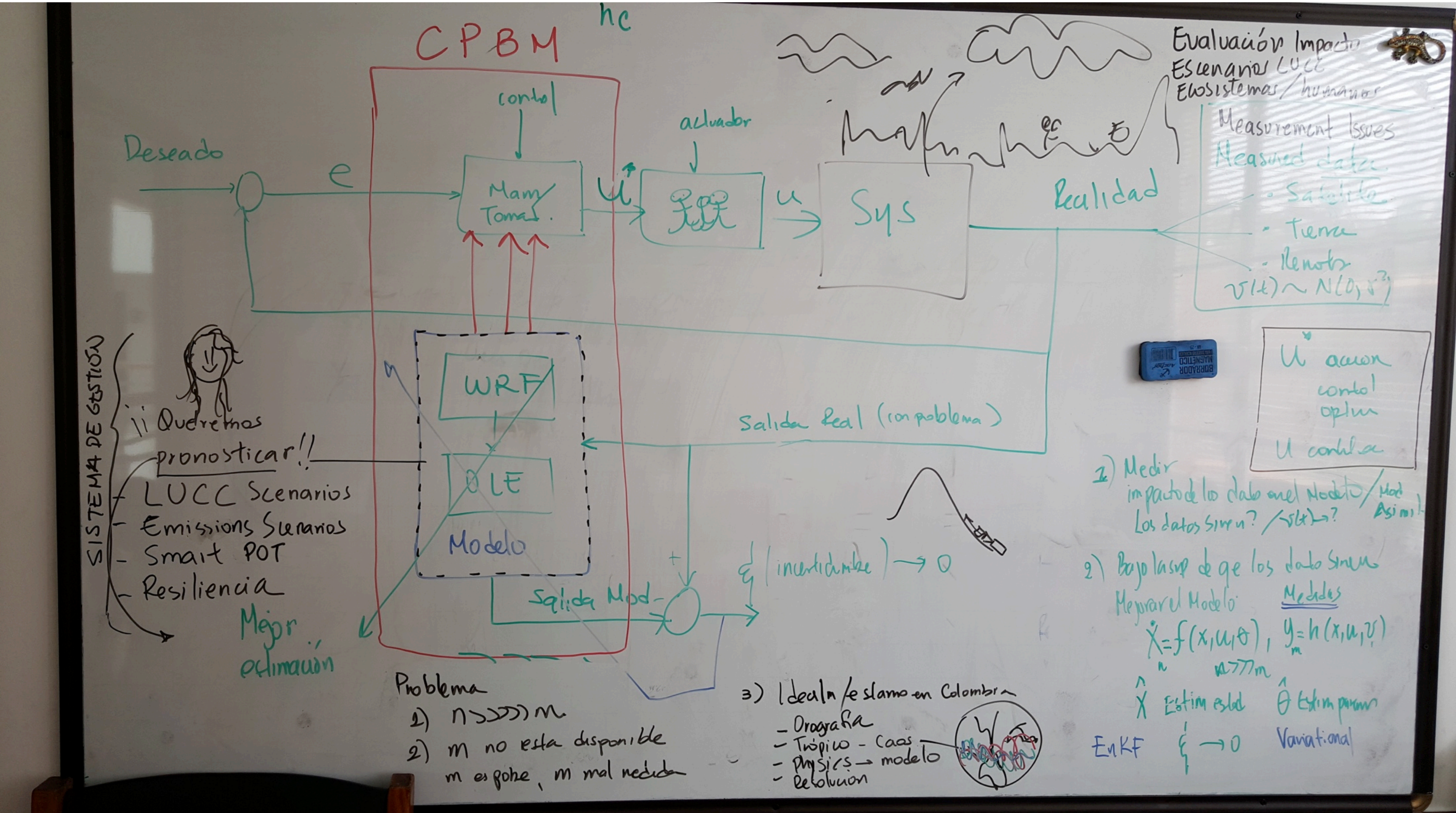
2017 – 2018? – 2019??????



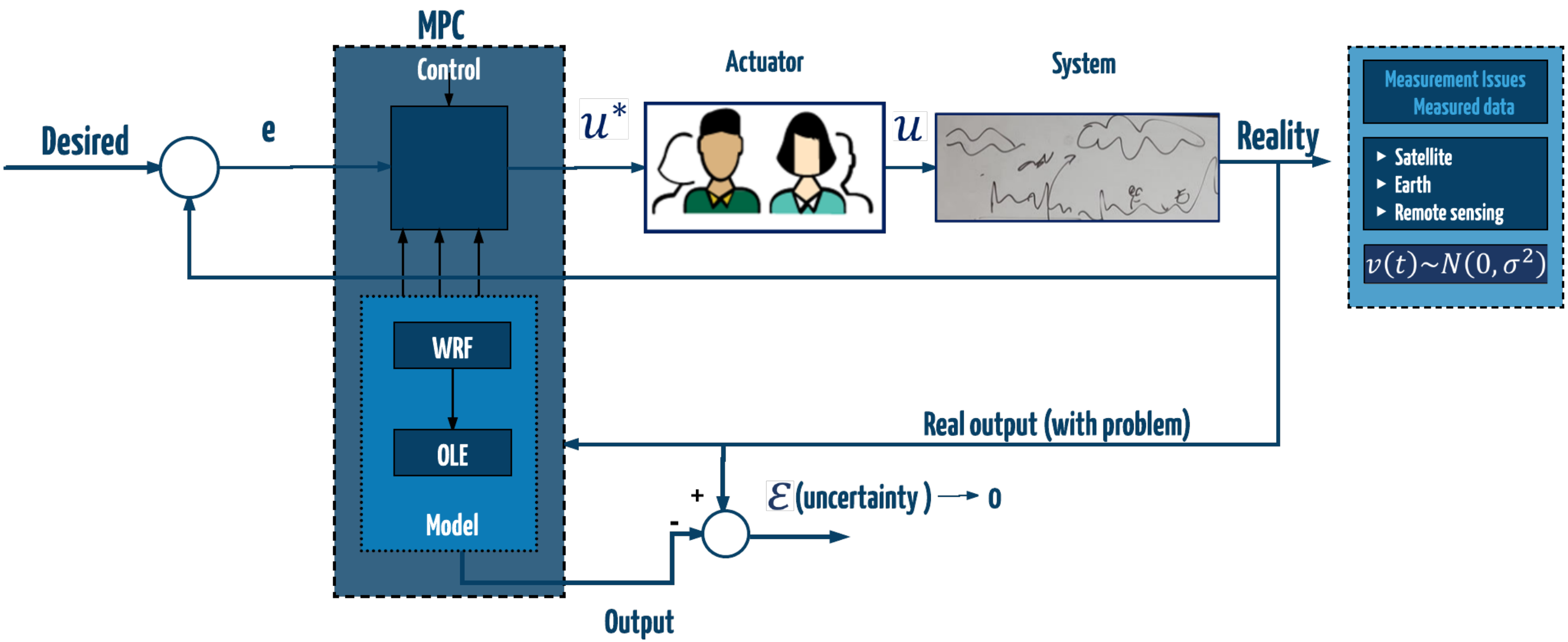


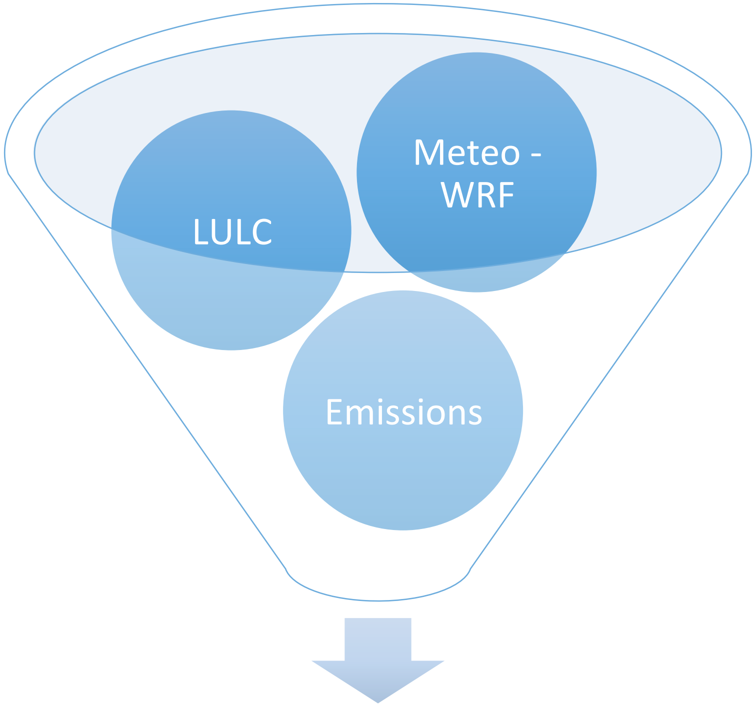
Source: IEA adapted from (EEA, 2016).

Model Based Predictive Control Scheme

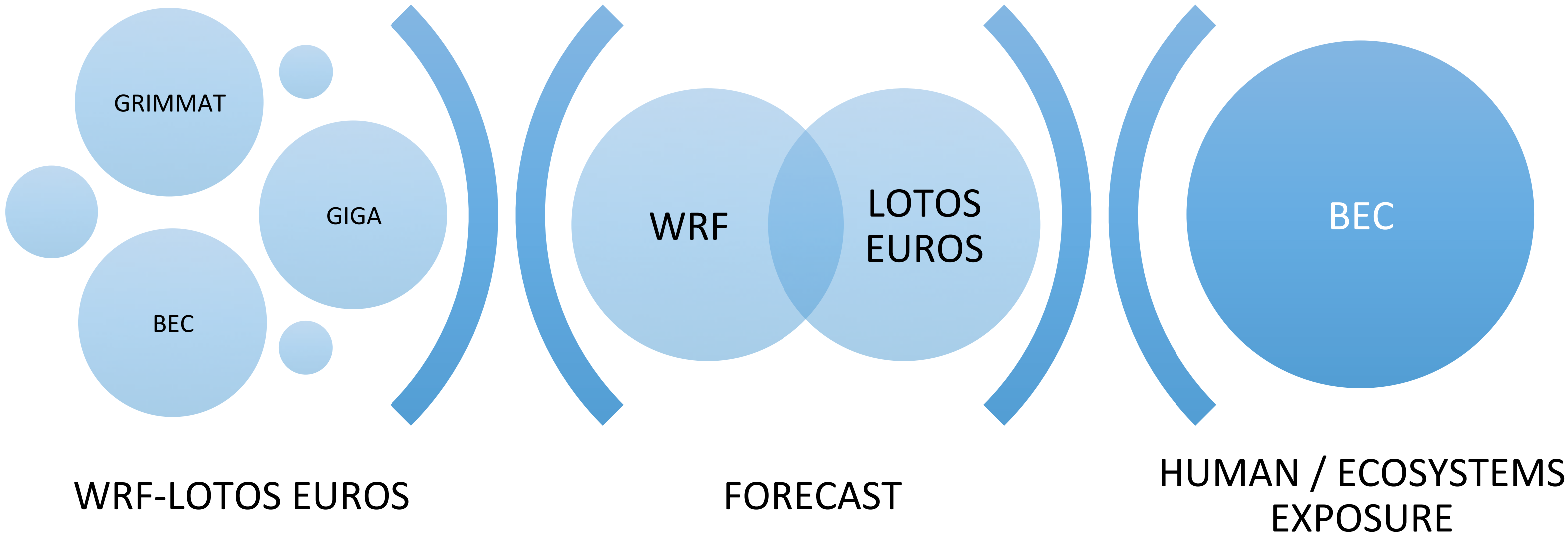


Model Based Predictive Control Scheme

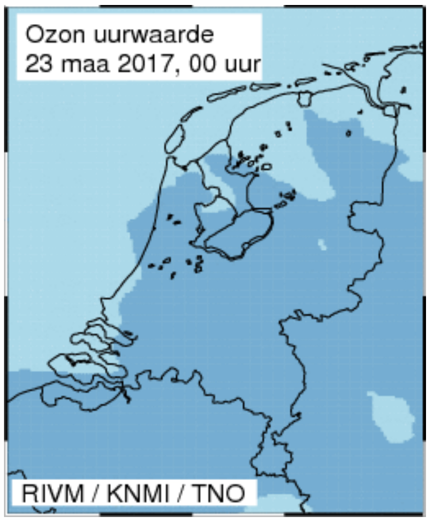




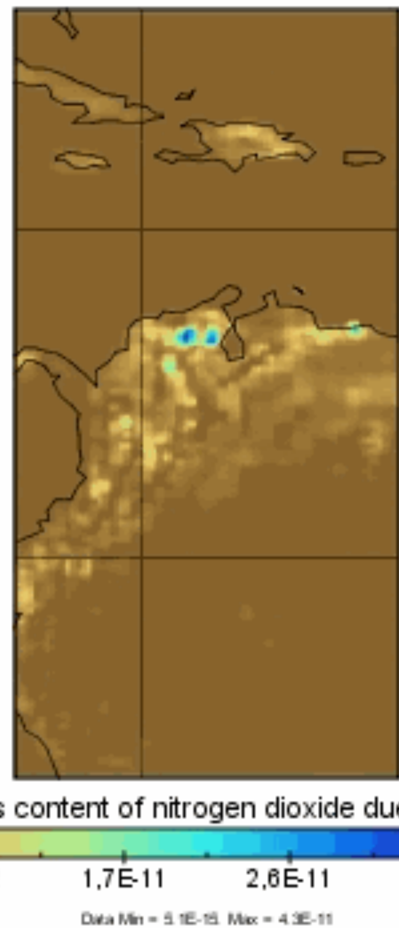
LOTOS EUROS


GRIMMAT
GIGA
BEC
WRF
LOTOS EUROS
BEC
WRF-LOTOS EUROS
FORECAST
HUMAN / ECOSYSTEMS EXPOSURE

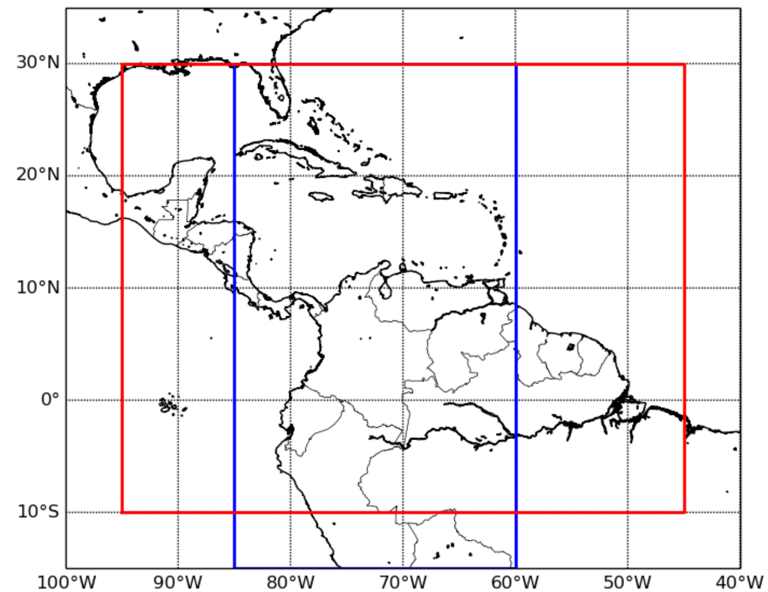
Modeling



Ozon uurwaarde
23 maa 2017, 00 uur
RIVM / KNMI / TNO



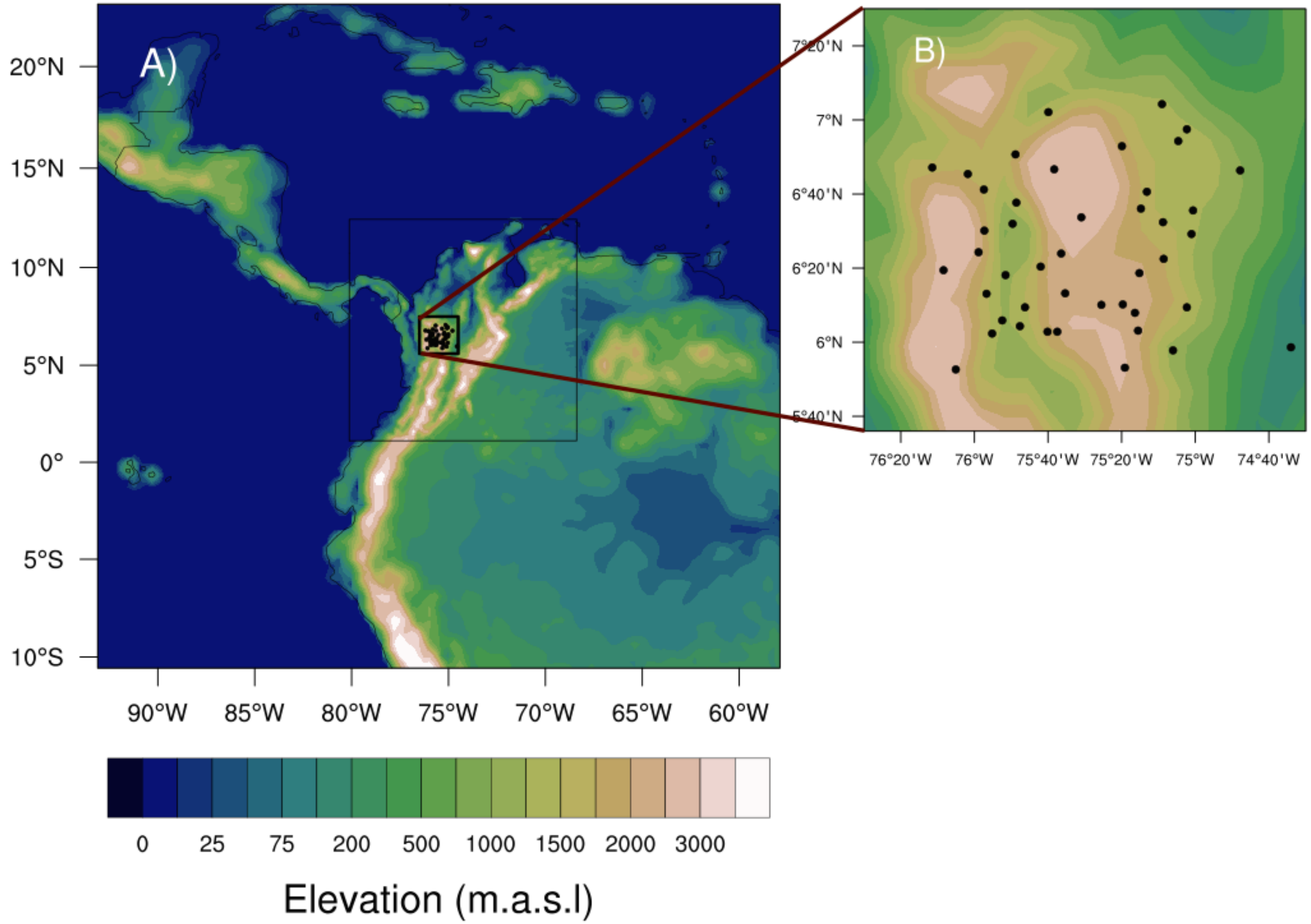
tendency of atmosphere mass content of nitrogen dioxide due to dry deposition
Time: 2016-03-24 01:00:00
tendency of atmosphere mass content of nitrogen dioxide due to dry deposition (kg m-2 s-1)
5,1E-15
8,6E-12
1,7E-11
2,6E-11
3,4E-11
4,3E-11
Data Min = 5.1E-15, Max = 4.3E-11



30°N
20°N
10°N
0°
10°S
100°W
90°W
80°W
70°W
60°W
50°W
40°W

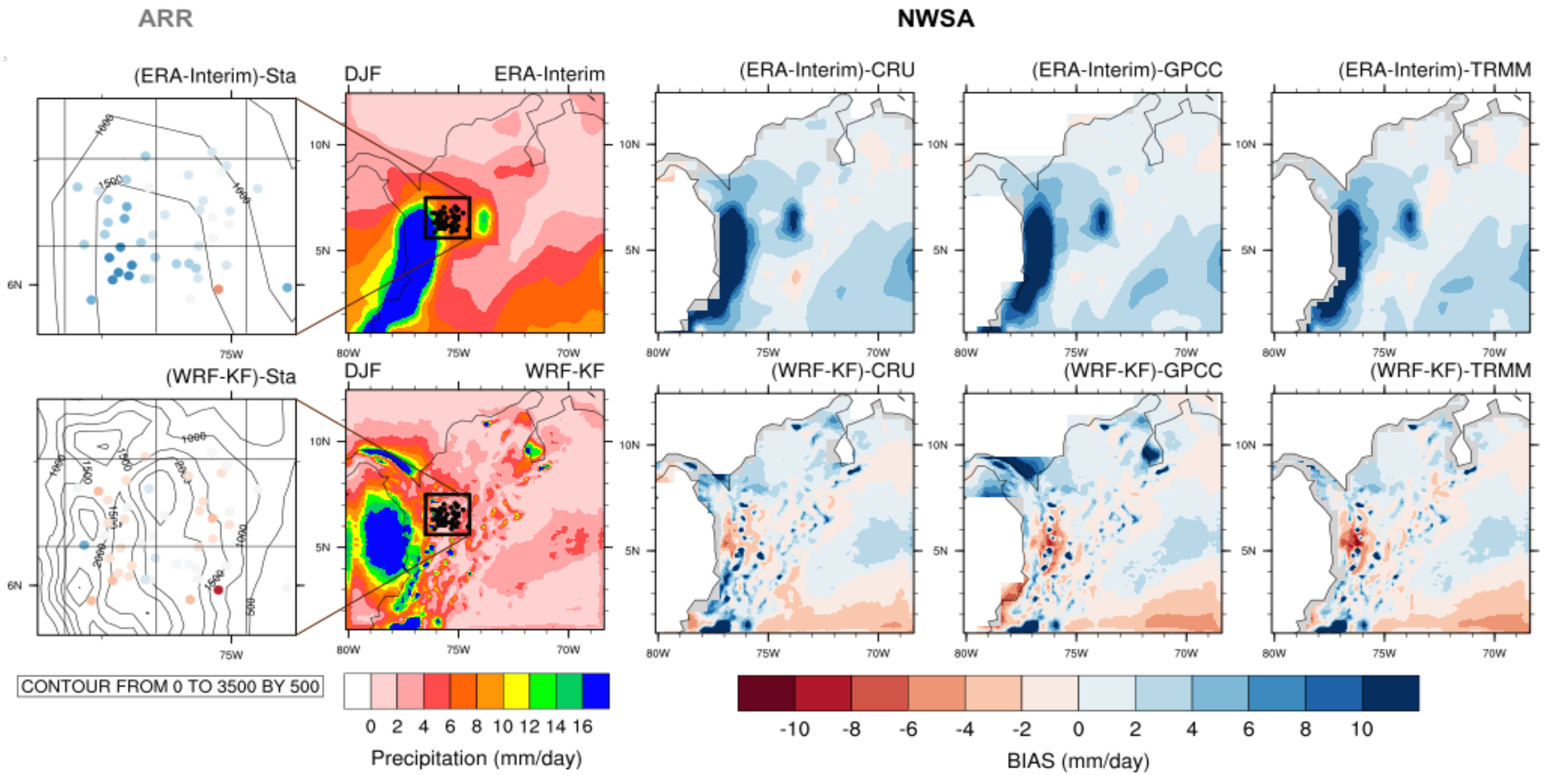
Modeling

Meteorological Modeling



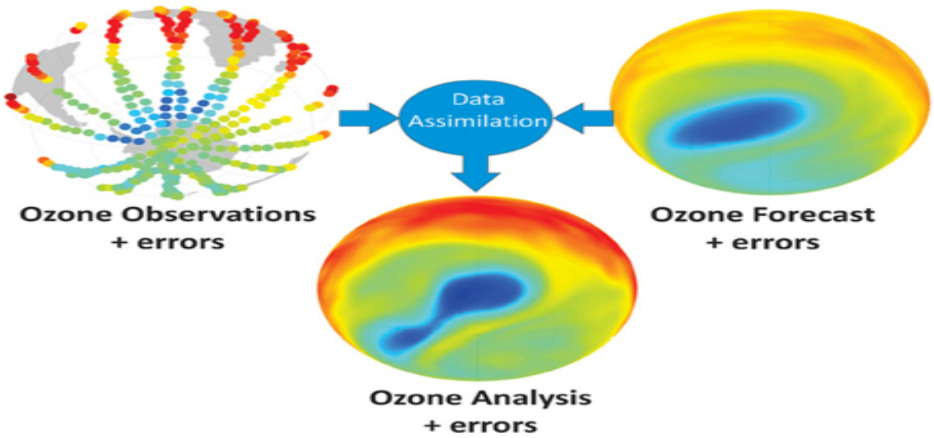
Modeling

Meteorological Modeling

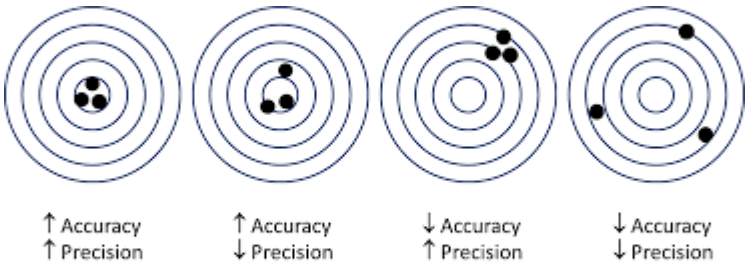


Modeling

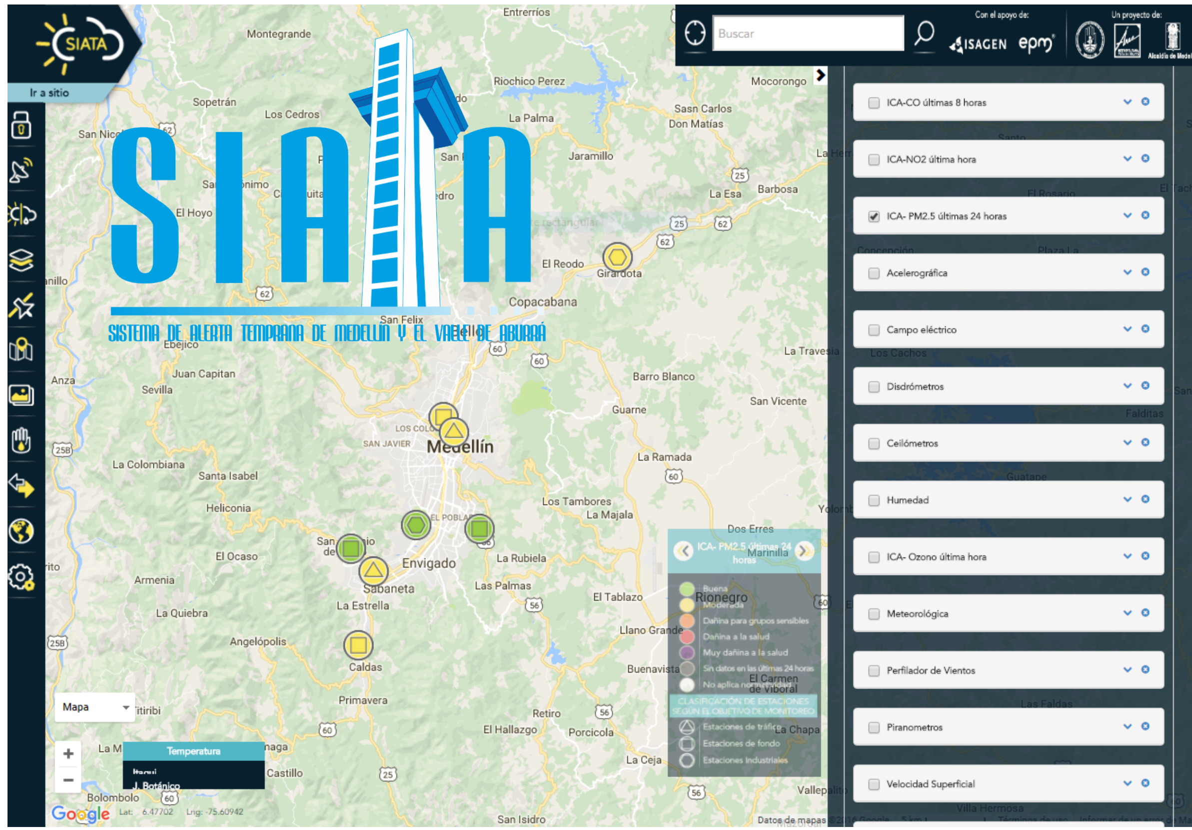
State Estimation – Parameter Estimation



Uncertainty Measurement

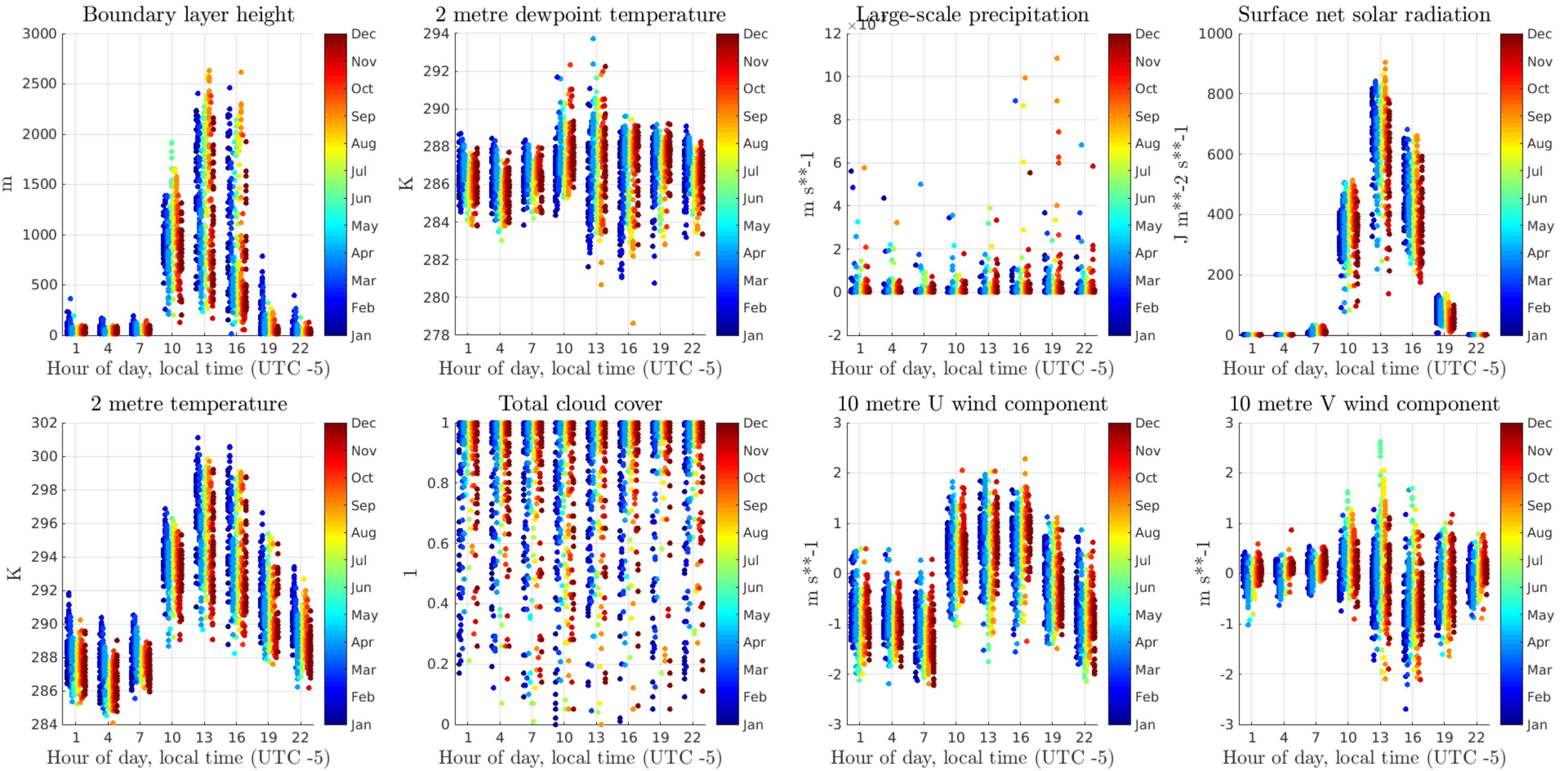


Instrumentation and Sensing



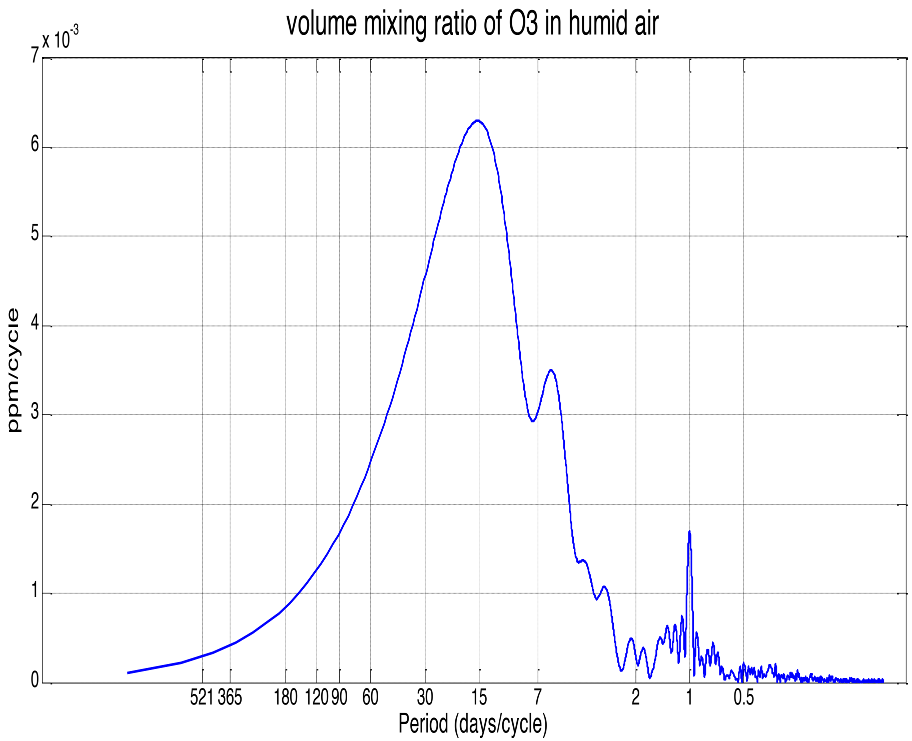
Instrumentation and Sensing

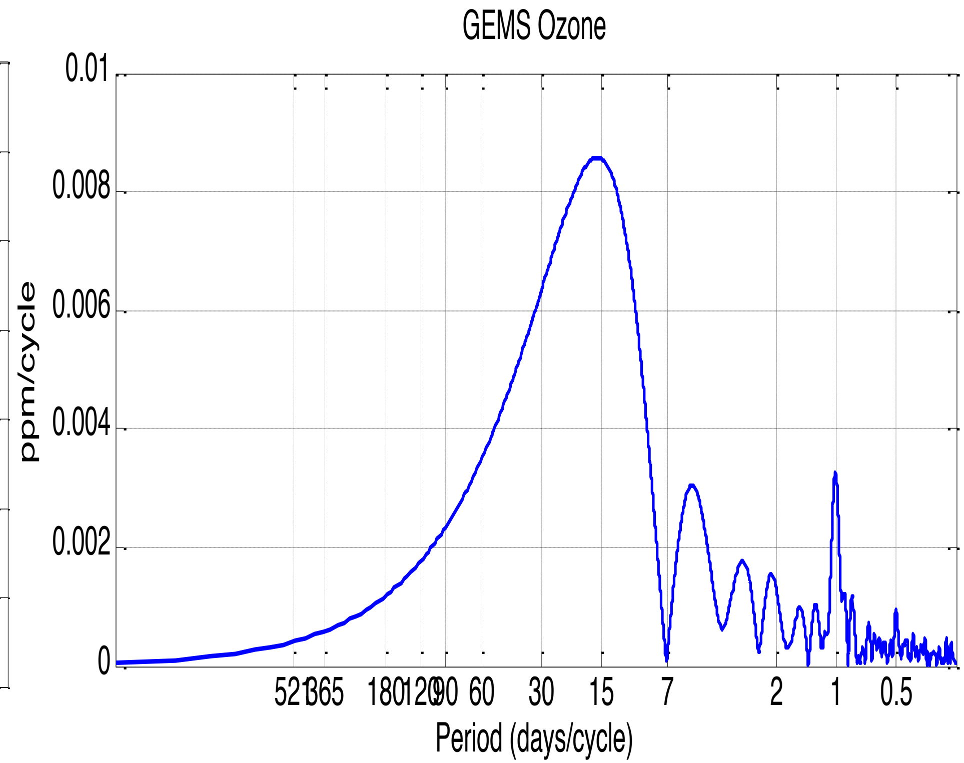
Preprocessing and analysis



Instrumentation and Sensing

Preprocessing and analysis

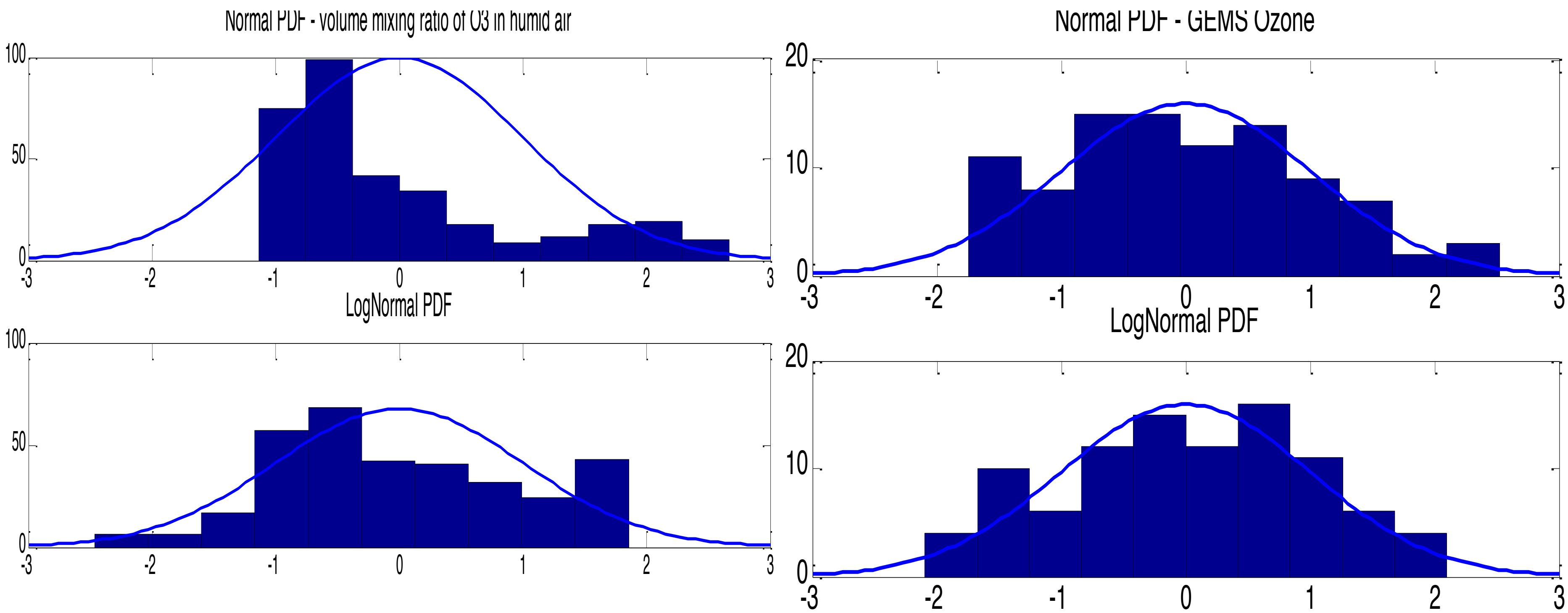




Comparison of frequency analysis between LOTOS-EUROS and MACC for O_3

Instrumentation and Sensing

Preprocessing and analysis



Comparison of distribution between LOTOS-EUROS and MACC for O_3

Instrumentation and Sensing- Model Evaluation

Statistical analysis

$$\text{ratio} = \frac{\sum_{s=1}^{S} \sum_{d=1}^{D} M_{s,d}}{\sum_{s=1}^{S} \sum_{d=1}^{D} O_{s,d}}$$

$$\text{residual} = \frac{1}{S} \sum_{s=1}^{S} \frac{1}{D} \sum_{d=1}^{D} \left| M_{s,d} - O_{s,d} \right|$$

$$\text{rms} = \frac{1}{S} \sum_{s=1}^{S} \sqrt{\frac{1}{D} \sum_{d=1}^{D} \left(M_{s,d} - O_{s,d} \right)^2}$$

$$\text{corr}_s = \frac{\sum_{d=1}^{D} \left(O_{s,d} - \overline{O}_s \right) \left(M_{s,d} - \overline{M}_s \right)}{\sigma_{s,O} \times \sigma_{s,M}}$$

$$\text{corr} = \frac{1}{S} \sum_{s=1}^{S} \text{corr}_s$$

Instrumentation and Sensing – Model Evaluation

Statistical measures features for all the domain

Variable	NO_2	O_3
Ratio	1.8	2.1
Residual	0.003	0.005
rms	0.053	0.183
Corr. Coef	0.62	0.65

Distributions and statistical measures of the comparison points. The red circle is the Aburrá Valley (Medellín) location.

Controller Design

Impossible, but it is posible to contribute to the decision-making process

Controller Design

Medellín **A**ir q**U**ality **I**nitiative

Challenges

LOTOS-EUROS Coupling with a meteorological model like WRF. The WRF model is currently implemented in the region for the GIGA Research Group of the Universidad de Antioquia.

WRF is able to do a representation of the meteorology in a higher resolution than the databases available for the region.

Data Assimilation and integration with Traffic models

erc
European Research Council
Established by the European Commission

Scale-FreeBack
Advanced Grant 2015
Scale-Free Control for Complex Physical Network Systems

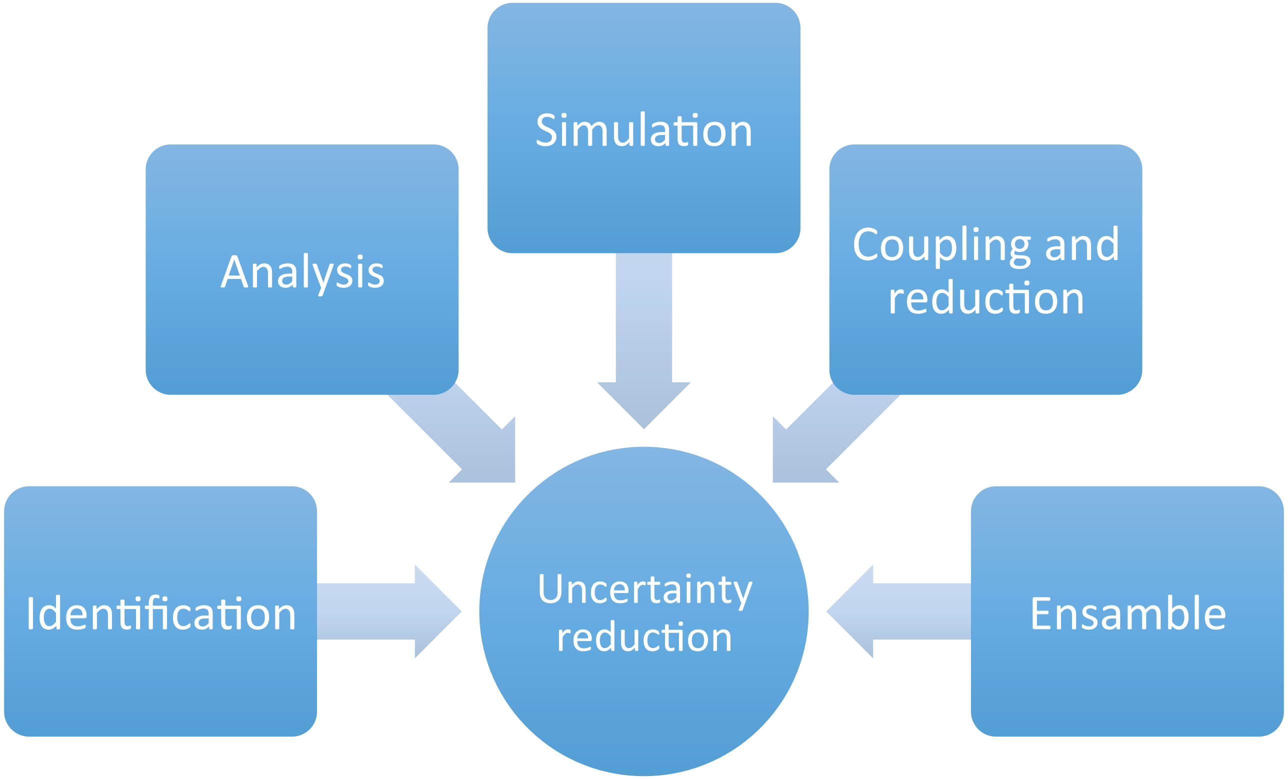
Research proposal – Main Objective

To develop a mathematical methodology to deal with significant sources of sensitivity and uncertainty in the short-term meteorological forecast with the numerical model WRF in the Aburrá river valley, discussing its mathematical and/or physical causes, and its implications for the air quality modeling.

Research proposal – Specific Objectives

- To identify significant sources of uncertainty in the WRF model for short-term meteorological forecast in the Aburrá river valley.
- To identify significant sources of sensitivity in the WRF model for short-term meteorological forecast in the Aburrá river valley.
- To discuss the implications of uncertainty and sensitivity in the WRF model on the forecast of air pollution transport mechanisms in the Aburrá river valley.
- To propose a methodology for uncertainty and sensitivity reduction for WRF model taking into account the magnification of errors in a coupling with a large scale model such as Lotos Euros.
- To evaluate the performance of the WRF model under extreme meteorological conditions in the Aburrá river valley

Research proposal - Methodology



Research proposal - Methodology

Phase 1: Identification of sources of uncertainty

- To identify sources of uncertainty, this study will involve similar techniques to the used in previous works such as Constantinescu et al. (2011).
- In these techniques, a current state of the atmosphere is obtained from data assimilation process, and model equations are integrated forward in time to produce a forecast.
- Different trajectories are calculated to obtain an estimation of the forecast covariance matrix, and uncertainty bounds are validated with observational meteorological data (Zavala et al. 2009).

Research proposal - Methodology

Phase 2: Analysis of uncertainty sources

- For the analysis of sources of sensitivity in the WRF model for short-term meteorological forecast in the Aburrá river valley, a process will be performed to evaluate the sensitivity of the model to distinct initial and boundary conditions, testing different sources of information.
- Furthermore, different configurations of the model at ~1 km resolution will be tested to obtain multi-ensembles of physical and/or numerical parameterizations. In this resolution some parameterizations would be deactivated to approach the gray zone paradigm.
- Similar approach to Borge et al. (2008), Carvalho et al. (2012) and Carvalho et al. (2014), will be used to evaluate the WRF performance under different numerical and physical options against to observational data seeking an adequate configuration for the Aburrá valley conditions.
- Through these methodologies different aspects related to uncertainty and sensitivity will be analyzed (initial-boundary conditions, physical and numerical parameters) to conclude around of model ability to perform short- term meteorological forecast in the Aburrá river valley.
- These uncertainty and sensitivity analyses will be used to discuss around the implications on the forecast of the mechanisms of air pollution transport in the Aburrá river valley. This information serves to contribute to strengthening between urban meteorology understanding and issues around urban planning.

Research proposal - Methodology

Phase 3: Model Simulation

- Simulations will be concentrated in the environmental contingency episode in Aburrá Valley between March 25 and April 4 of 2016, or any following extreme condition available, to evaluate the performance of the WRF model under extreme meteorological conditions.
- In all cases, different statistical criteria will be employed to compare the model results with different sources of information such as surface gauges, radiometer measures, global reconstructions, satellite data and other models results (Reanalysis).

Research proposal - Methodology

Phase 4: Model Coupling and reduction of uncertainty methodology

Model Coupling can briefly described in the following items:

- Coupling Modes: Subroutinized/Componentized
- Types of coupling: Sequential coupling /Concurrent coupling

Research proposal - Methodology

Phase 5: Model Ensemble

- Ensamble of the WRF model with Lotos Euros
- Ensamble of WRF Chem Model with Lotos Euros
- Analysis of global uncertainty and measurement of sensitivy of models ensemble.

Research proposal - Methodology

Research proposal – Student Plan

Student plan year 1

1. Theoretical foundations of Probability
2. Theoretical foundations of Systems and Control
3. Theoretical foundations of Data Assimilation
4. Theoretical foundations of Linear Algebra
5. High performance computing basics
6. Data retrieval from data sources: land cover, atmospheric, meteorological, emissions and boundary conditions
7. Setup of WRF model
8. Running WRF model for Colombia Domain
9. Analysis of the results for the WRF model for air quality in Colombia
10. Setup of WRF DA

Research proposal – Student Plan

Student plan Year 2

1. Implementing strategies of variance localization in WRF Data Assimilation in Colombia
2. Implementing WRF CHEM
3. Complete review of the state of the art in uncertainty measurement and formal sensitivity
4. Qualifying examination 1 and 2
5. Proposal definition for PhD Thesis
6. Thesis proposal defense

Research proposal – Student Plan

Student plan Year 3

1. Developing of mathematical methods and strategies of uncertainty reduction in WRF Data Assimilation in Colombia

2. Implementing WRF CHEM

3. Improvement of forecast METEO in Colombia

4. Data Assimilation/ uncertainty reduction improved schemes with CHEM model and high resolution

5. Developing the answers to research questions adressed in Thesis Proposal 6. Publication of preliminary results

Research proposal – Student Plan

Student plan Year 4

1. Developing the answers to research questions adressed in Thesis Proposal
2. Publication of preliminary results
3. Thesis Dissertation

Research proposal - Results

	Resultados
Tipo de Resultado	**Resultado**
Generación de Nuevo Conocimiento	Artículo de Investigación A1
Generación de Nuevo Conocimiento	Artículo de Investigación A1
Productos Resultados de Actividades de Investigación, Desarrollo e Innovación	Regulaciones, normas y reglamentos técnicos, basadas en resultados de investigación del grupo A
Productos de Apropiación Social del Conocimiento	Participación en Eventos Científicos (ponencia, poster, capítulo de memorias)
Productos de Apropiación Social del Conocimiento	Participación en Eventos Científicos (ponencia, poster, capítulo de memorias)
Productos de Formación de Recursos Humanos	Tesis de Doctorado A
Productos de Formación de Recursos Humanos	Apoyo a creación de curso de Doctorado
Productos de Formación de Recursos Humanos	Trabajo de Grado B
Productos de Formación de Recursos Humanos	Trabajo de Grado B
Productos de Formación de Recursos Humanos	Trabajo de Grado de Maestría A

Research proposal - Results

- A formal experiment design exploring different sources of uncertainty and sensitivity in the short-term meteorological forecast with the numerical model WRF in the Aburrá river valley.
- A set of simulations exploring the representation of extreme meteorological conditions in the Aburrá river valley.
- A comparative quantitative and qualitative analysis of the modeling results with different observational sources to assess the model capability to represent the atmospheric state in the Aburrá river Valley.
- A discussion of the implications on the forecast of air pollution transport mechanisms in the Aburrá river valley.
- An operational version of the WRF model for the Aburrá river valley.

Theoretical Framework

Data assimilation relies on the use of an extension for high dimensional systems of the classical approach for filtering called the Kalman Filter

$$\mathbf{x}_k = \mathcal{M}_{k,k-1}(\mathbf{x}_{k-1}) + \mathbf{u}_k ,$$

$$\mathbf{y}_k = \mathcal{H}_k(\mathbf{x}_k) + \mathbf{v}_k .$$

$\mathbf{x}_k \in \mathbb{R}^{m_x}$ $\mathbf{y}_k \in \mathbb{R}^{m_y}$ $\mathbf{u}_k \in \mathbb{R}^{m_x}$ $\mathbf{v}_k \in \mathbb{R}^{m_y}$

$\mathcal{M}_{k,k-1}\colon \mathbb{R}^{m_x} \to \mathbb{R}^{m_x}$ $\mathcal{H}_k\colon \mathbb{R}^{m_x} \to \mathbb{R}^{m_y}$

[Evensen, 2009]

$\mathbf{u}_k$ and $\mathbf{v}_k$ are independent white noise

The EnKF is a modification that uses Monte Carlo approach to estimate the minimum variance solution to the state estimation problem.

At the analysis step in the EnKF, an ensemble of the system state, is generated with sample mean ans covariance as the analysis state and error covariance matrix with the ensemble n typically much smaller than the dimension mx in large scale applications.

$$\mathbf{X}_{k-1}^{a} = \{\mathbf{x}_{k-1,i}^{a}: i = 1, 2, \ldots, n\}$$

By propagating the analysis ensemble through the transition operator, we obtain forecast ensemble at the next data assimilation cycle.

$$\mathbf{X}_k^f = \{\mathbf{x}_{k,i}^f : \mathbf{x}_{k,i}^f = \mathcal{M}_{k-1,k}(\mathbf{x}_{k-1,i}^a) + \mathbf{u}_{k,i}, i = 1, 2, \ldots, n\}$$

When a new observation is available, the analysis step is used to compute the analysis ensemble from its forecast counterpart based on the sample covariance matrix of the forecast ensemble.

Two types of data assimilation:

- Related to the Ensemble Kalman filter for state estimation

$$\mathbf{x}^a_{k,i} = \mathbf{x}^f_{k,i} + \mathbf{K}_k[\mathbf{y}^s_{k,i} - \mathcal{H}_k(\mathbf{x}^f_{k,i})], \quad \text{for} \quad i = 1, 2, \ldots, n,$$

$$\mathbf{K}_k = \hat{\mathbf{P}}^{xy}_k (\hat{\mathbf{P}}^{yy}_k + \mathbf{R}_k)^{-1},$$

$$\hat{\mathbf{S}}^f_k = \frac{1}{\sqrt{n-1}}[\mathbf{x}^f_{k,1} - \hat{\mathbf{x}}^f_k, \ldots, \mathbf{x}^f_{k,n} - \hat{\mathbf{x}}^f_k],$$

$$\hat{\mathbf{S}}^{yy}_k = \frac{1}{\sqrt{n-1}}[\mathbf{y}^f_{k,1} - \hat{\mathbf{y}}^f_k, \ldots, \mathbf{y}^f_{k,n} - \hat{\mathbf{y}}^f_k],$$

$$\mathbf{x}^a_{k,i} = \hat{\mathbf{x}}^a_k + \sqrt{n}(\mathbf{L}_k \mathbf{C}_k \mathbf{\Xi}_k)_i, \quad \text{for} \quad i = 1, \ldots, n$$

$$(\delta \mathbf{x}_{k,i})_j = (\hat{p}^j_{xy,k} / \hat{p}^f_{yy,k}) \delta y_{k,i}, \quad j = 1, \ldots, m_x,$$

- Variational methods for the parameter estimation

$$X(t_{i+1}) = M_i X(t_i), \quad i = 1, \ldots, m-1, \; X(t_{i+1}) \in \Re^n$$

$$Y(t_i) = H(X(t_i)) + \eta(t_i), \qquad H : \Re^n \to \Re^q$$

$$J(X_0) = \frac{1}{2}(X^b - X_0)^T B_0^{-1} (X^b - X_0) + \frac{1}{2}\sum_i (Y(t_i) - H(X(t_i)))^T R_i^{-1} (Y(t_i) - H(X(t_i))),$$

[Barbu 2010, Krymskaya, 2013, Sebacher, 2014, Altaf 2015, Fu et al, 2015, Lu et al, 2015, Krymskaya, 2013, Tijana et al, 2014 Verlaan and Sumihar, 2016]

Instrumentation and Sensing

Impact of Data on Models
To answer the question: is it possible, under lineality and stationarity assumptions, to use the observation impact analysis methods developed by Verlaan and Sumihar, 2016 to improve the Data Assimilation Schemes over LOTOS-EUROS model forecasting?.

This will be held by studying the impact of the observations at the most recent analysis update under Ensemble based schemes in LOTOS EUROS model for volcanic ash.

$$\tilde{\mathbf{x}}(k|k-1) = \begin{bmatrix} \hat{\mathbf{x}}(k+m|k-1) \\ \hat{\mathbf{x}}(k|k-1) \end{bmatrix} \qquad \begin{aligned} \tilde{H}_a &= [\mathbf{0} \;\; H] \\ \tilde{H}_v &= [H \;\; \mathbf{0}] \end{aligned}$$

$$\tilde{\mathbf{x}}(k|k) = \tilde{\mathbf{x}}(k|k-1) + \tilde{\mathbf{K}}_c\left(\mathbf{y}(k) - \tilde{H}_a\tilde{\mathbf{x}}(k|k-1)\right)$$

$$H\hat{\mathbf{x}}(k+m|k) = \tilde{H}_v\tilde{\mathbf{x}}(k|k-1) + \tilde{H}_v\tilde{\mathbf{K}}_c\left(\mathbf{y}(k) - \tilde{H}_a\tilde{\mathbf{x}}(k|k-1)\right)$$

Measuring the impact of observations (data) over the performance of a Data Assimilation Scheme in the enhancement of a model

$$\begin{aligned}\Delta J(k,m) \approx\ & [(\mathbf{y}(k+m) - H\hat{\mathbf{x}}(k+m|k)) + (\mathbf{y}(k+m) - H\hat{\mathbf{x}}(k+m|k-1))]' \\ & \mathbf{R}(k+m)^{-1}\mathbf{D}(k+m|k-1)\mathbf{D}(k|k-1)' \\ & \left(\mathbf{D}(k|k-1)\mathbf{D}(k|k-1)' + \mathbf{R}(k)\right)^{-1}(\mathbf{y}(k) - H\hat{\mathbf{x}}(k|k-1))\end{aligned}$$

[Barbu 2010, Krymskaya, 2013, Sebacher, 2014, Altaf 2015, Fu et al, 2015, Lu et al, 2015, Krymskaya, 2013, Tijana et al, 2014, Verlaan and Sumihar, 2016]

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