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The Variational approach on the road to Data Assimilation (DA) for Chemical Transport Models (CTM).

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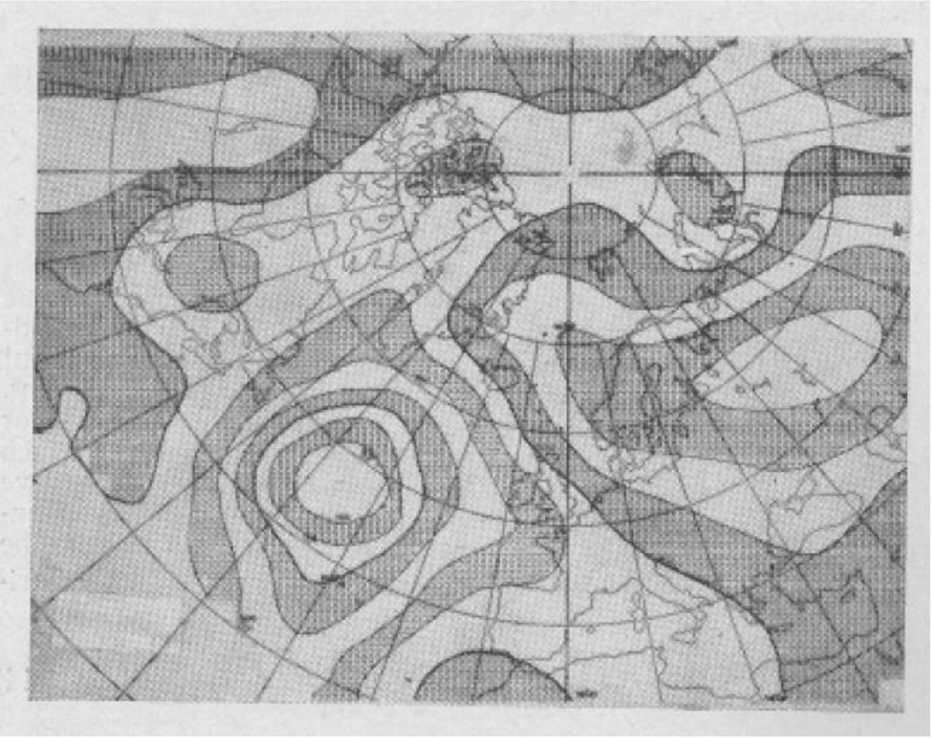
Outline

- Motivation
- Introduction
- Data assimilation fundamentals
- Variational approach
- Previous results

    TU Delft theses

- Current research questions and future work
- References

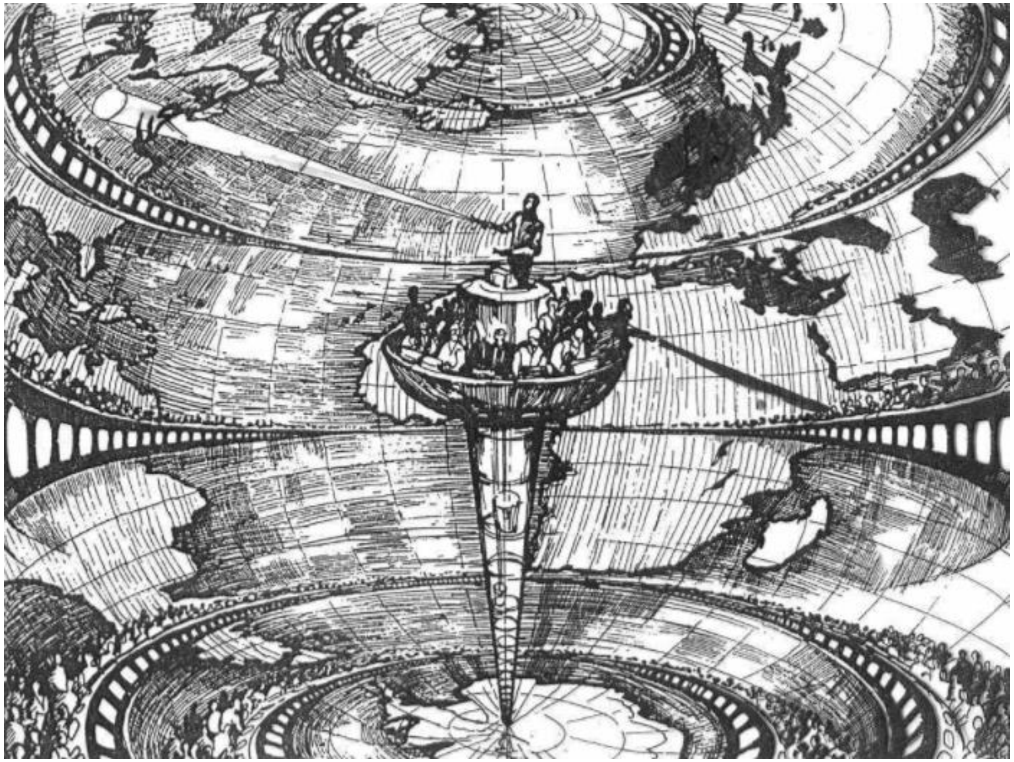
Motivation



For Bergeron, weather map analysis was rather a fine art than applied science.

(Persson, 2004)

Motivation



https://celebrating200years.noaa.gov/foundations/numerical_wx_pred/theater.html

This illustration depicts Richardson's "forecast factory." *Image courtesy of L. Bengtsson.*

1922

Motivation

The Cray supercomputer used for weather analysis at the European Centre for Medium Range Weather Forecasts (Cray)

https://www.seattletimes.com/business/technology/crays-supercomputers-advance-weather-forecasts/

Introduction

Chemical Transport Model (CTM)

Compute numerical model which simulates the atmospheric chemistry and transport

$$\frac{\partial C}{\partial t} = -\nabla \cdot (\mathbf{u} \cdot \mathbf{C}) + \frac{\partial}{\partial \mathbf{v}}\left(K_{\mathbf{v}} \frac{\partial C}{\partial \mathbf{v}}\right) + E + R + Q - D - W$$

Change in concentration with time

Grid resolved transport (Advection)

Diffusion process

Entrainment and detrainment

Generation/Consumption chemical reactions

Emissions

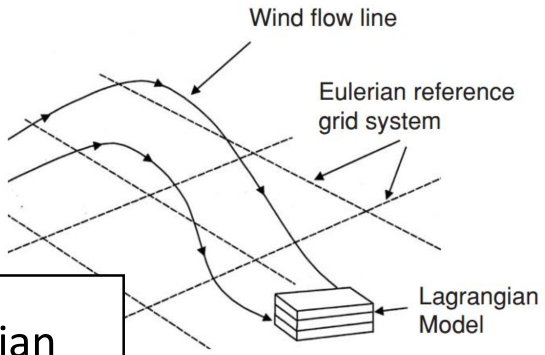
Dry and wet deposition procce

Introduction

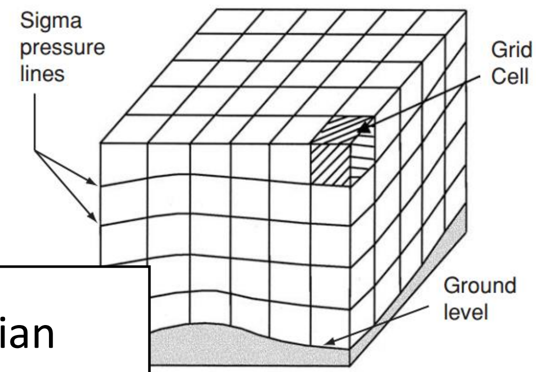
Chemical Transport Model (CTM)

Compute numerical model which simulates the atmospheric chemistry and transport

$$\frac{\partial C}{\partial t} = -\nabla \cdot (\mathbf{u} \cdot \mathbf{C}) + \frac{\partial}{\partial \mathbf{v}}(K_{\mathbf{v}} \frac{\partial C}{\partial \mathbf{v}}) + E + R + Q - D - W$$

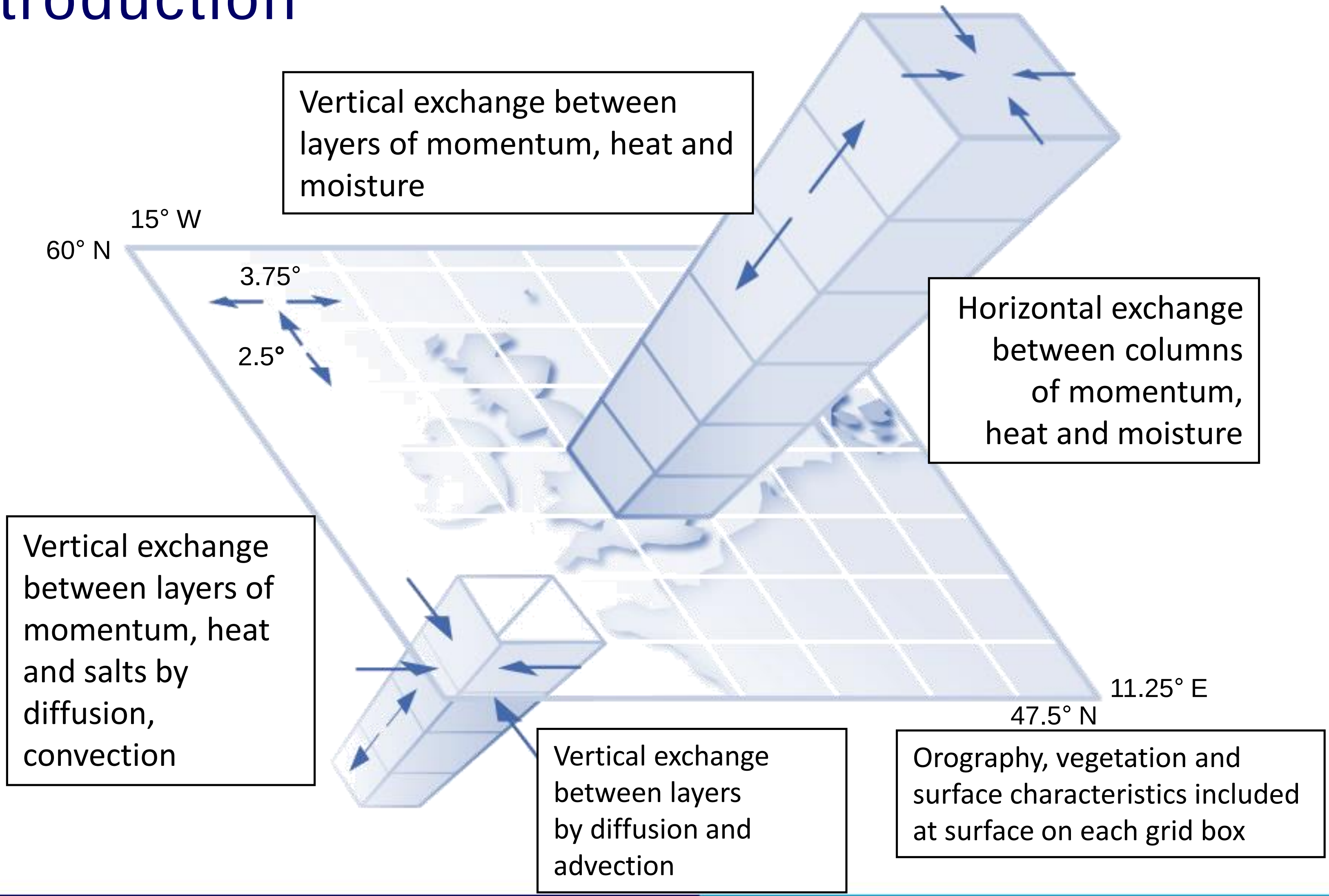


Lagrangian



Eulerian

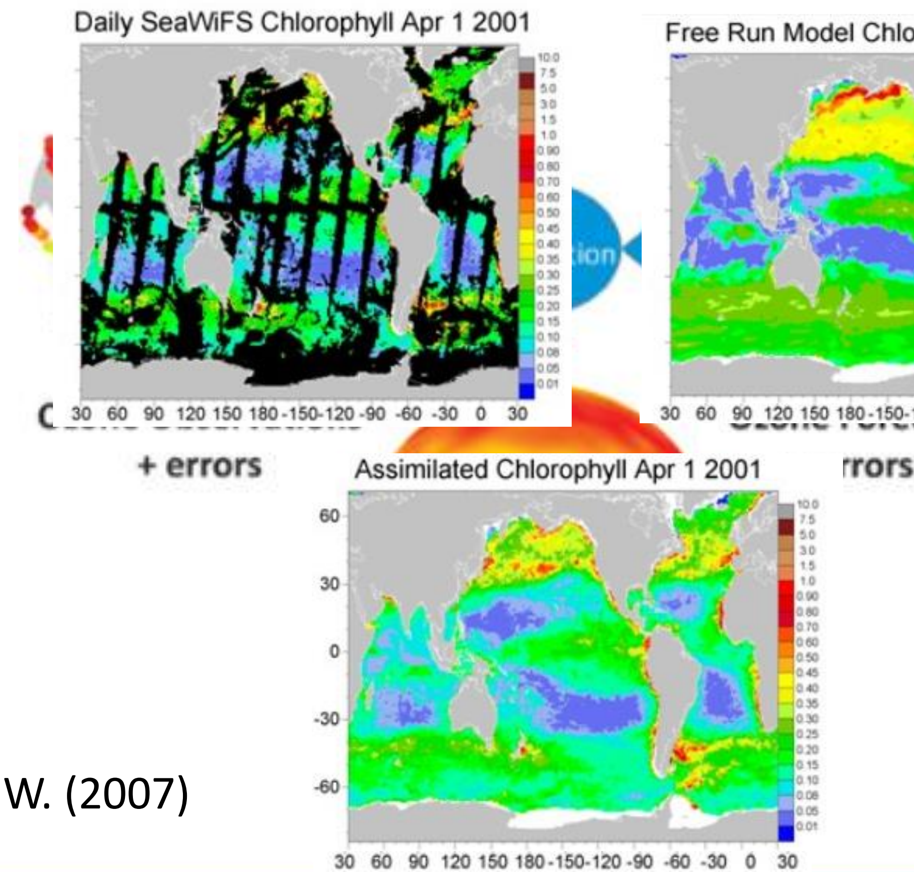
Introduction



Introduction

Data Assimilation is the process of absorbing (incorporate) observed information to improve a dynamical prognostic numerical model results

Information from **Observations**



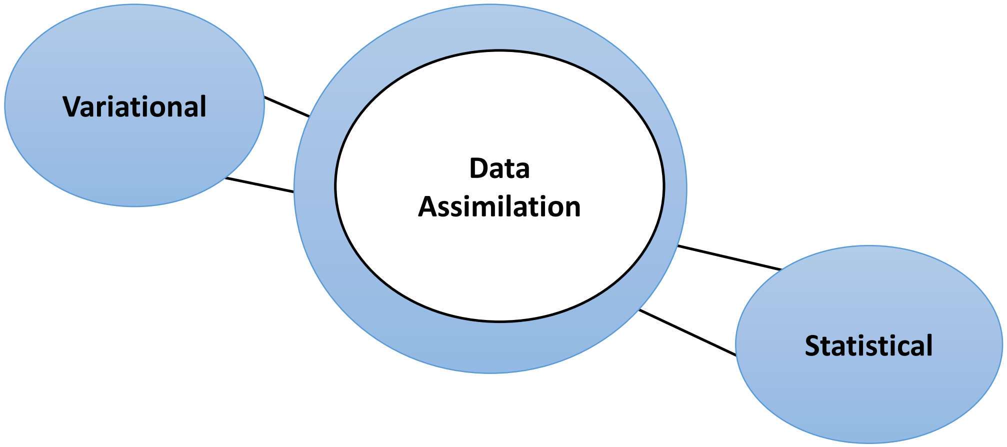
Information from the **model**

Combination of information through Data Assimilation

Improved analysis and forecast. example: Water temperatura, Ice coverage, wind velocity…

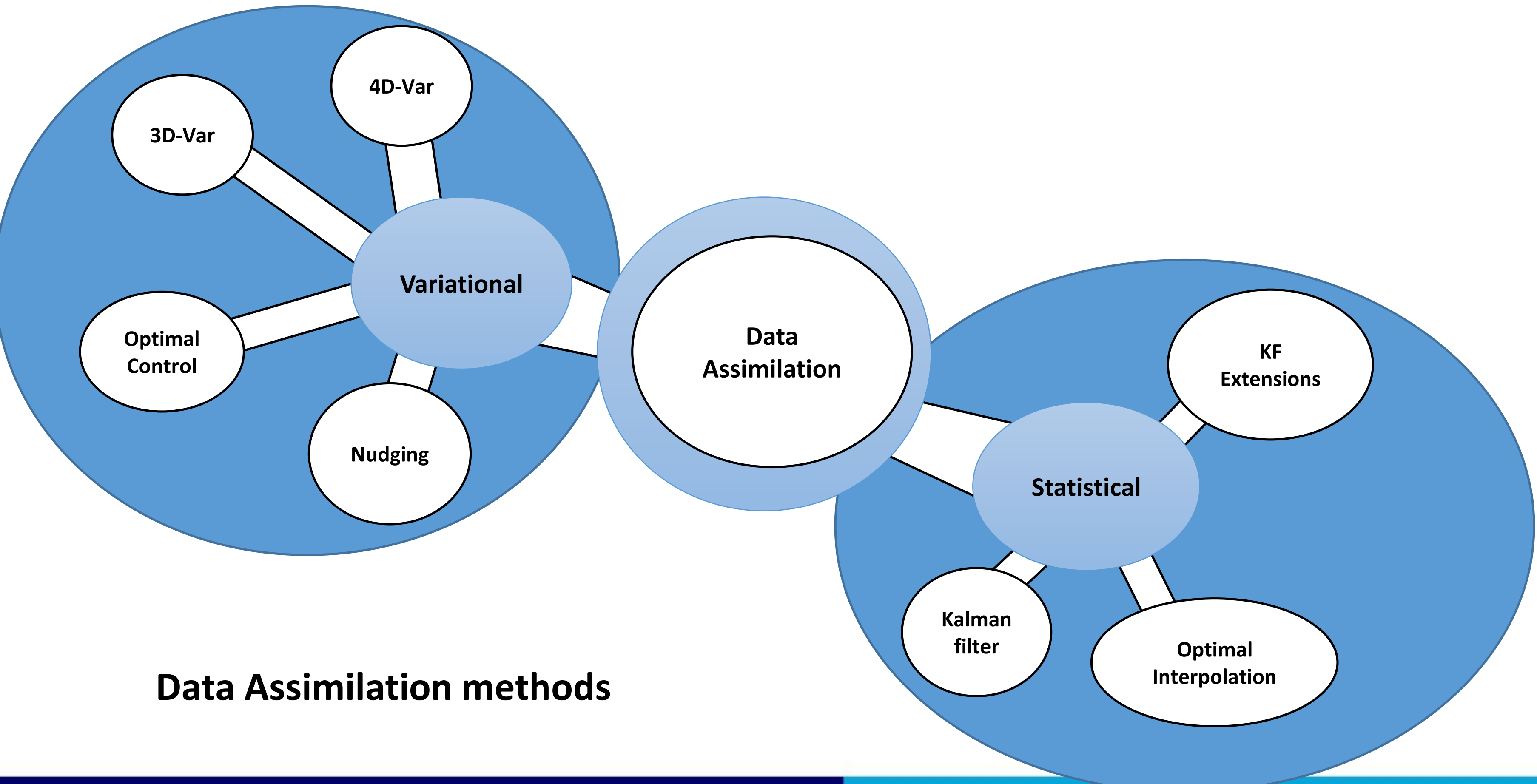
Gregg, W. (2007)

Data Assimilation fundamentals



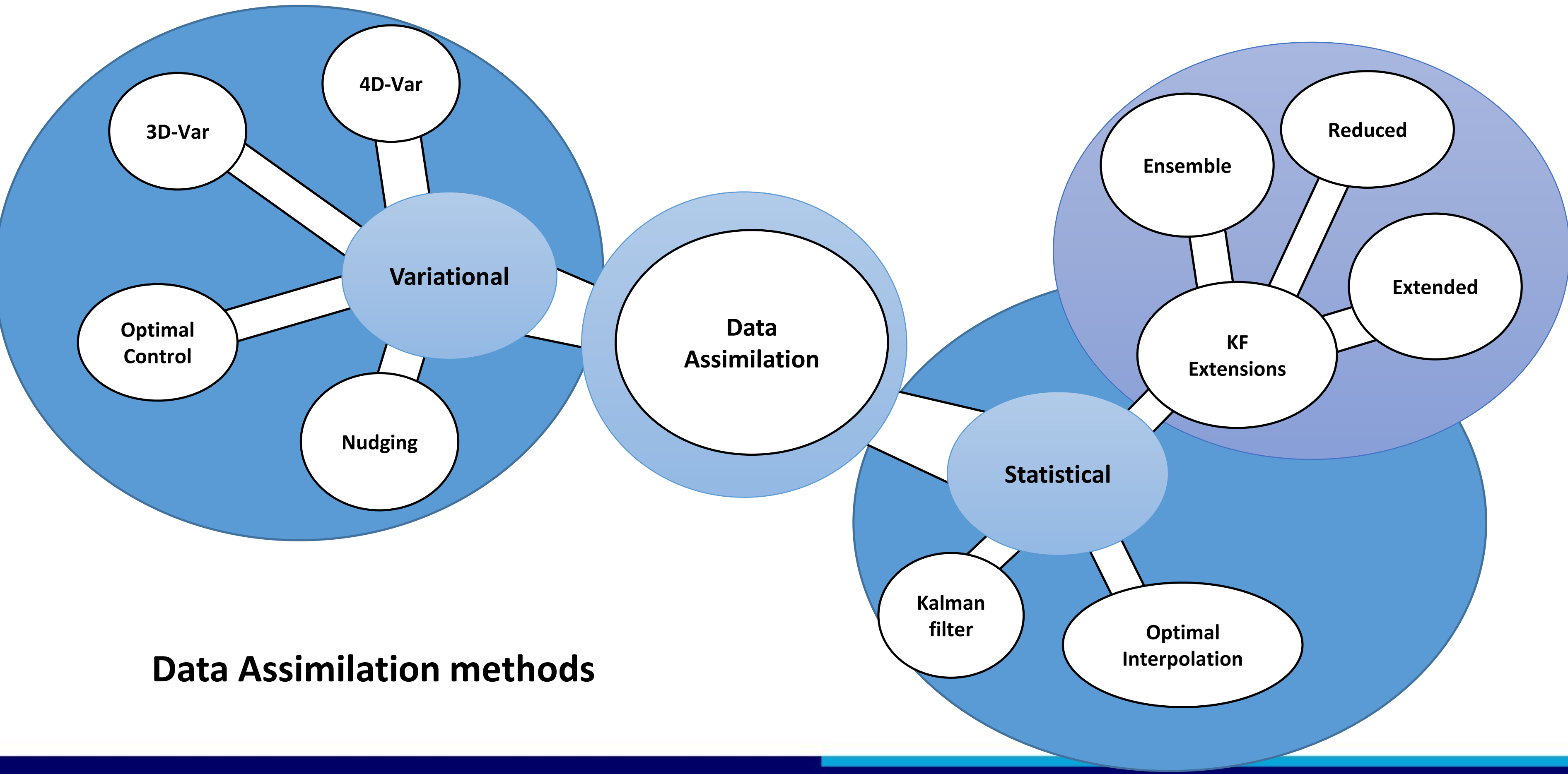
Data Assimilation methods

Data Assimilation fundamentals



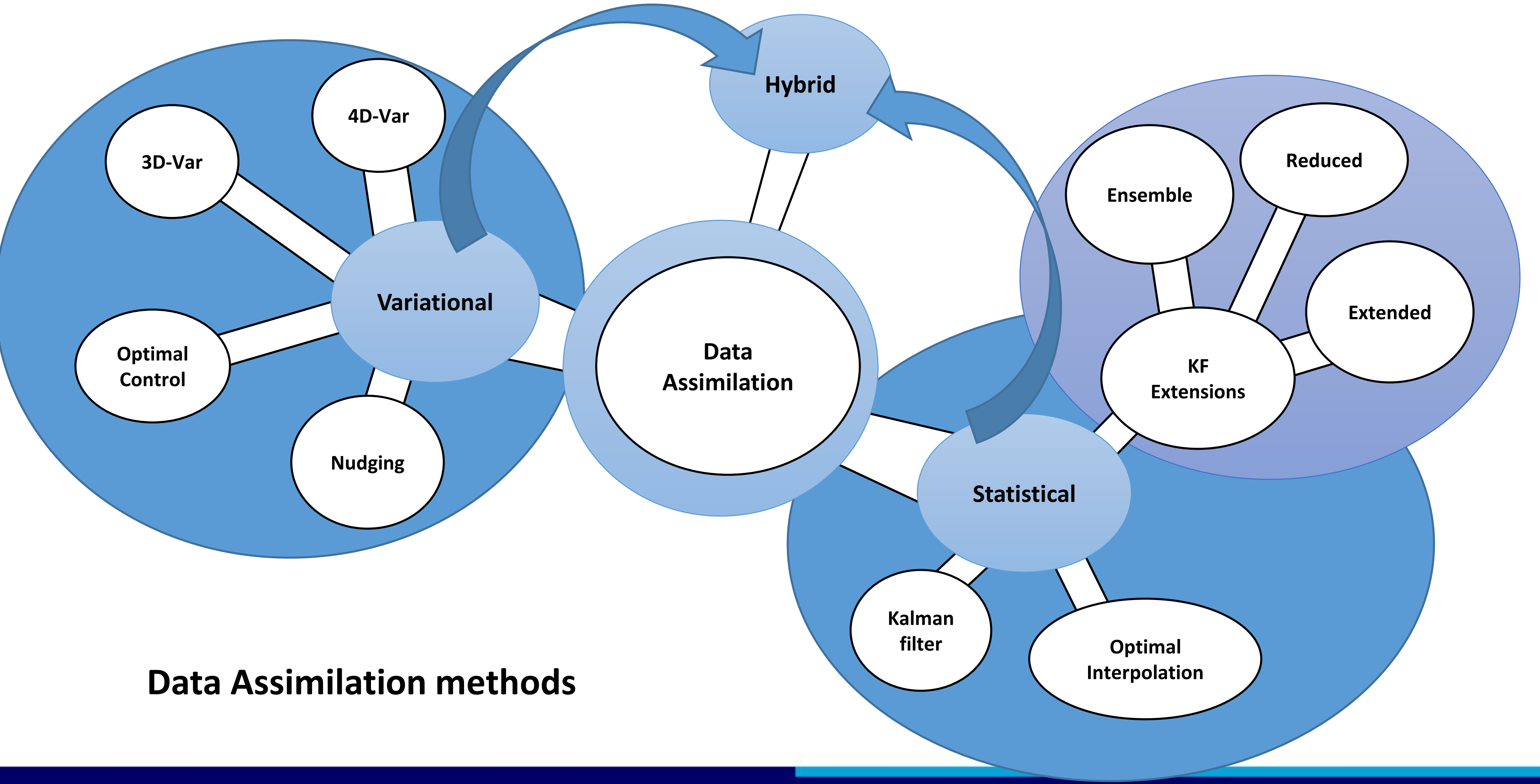
Data Assimilation methods

Data Assimilation fundamentals

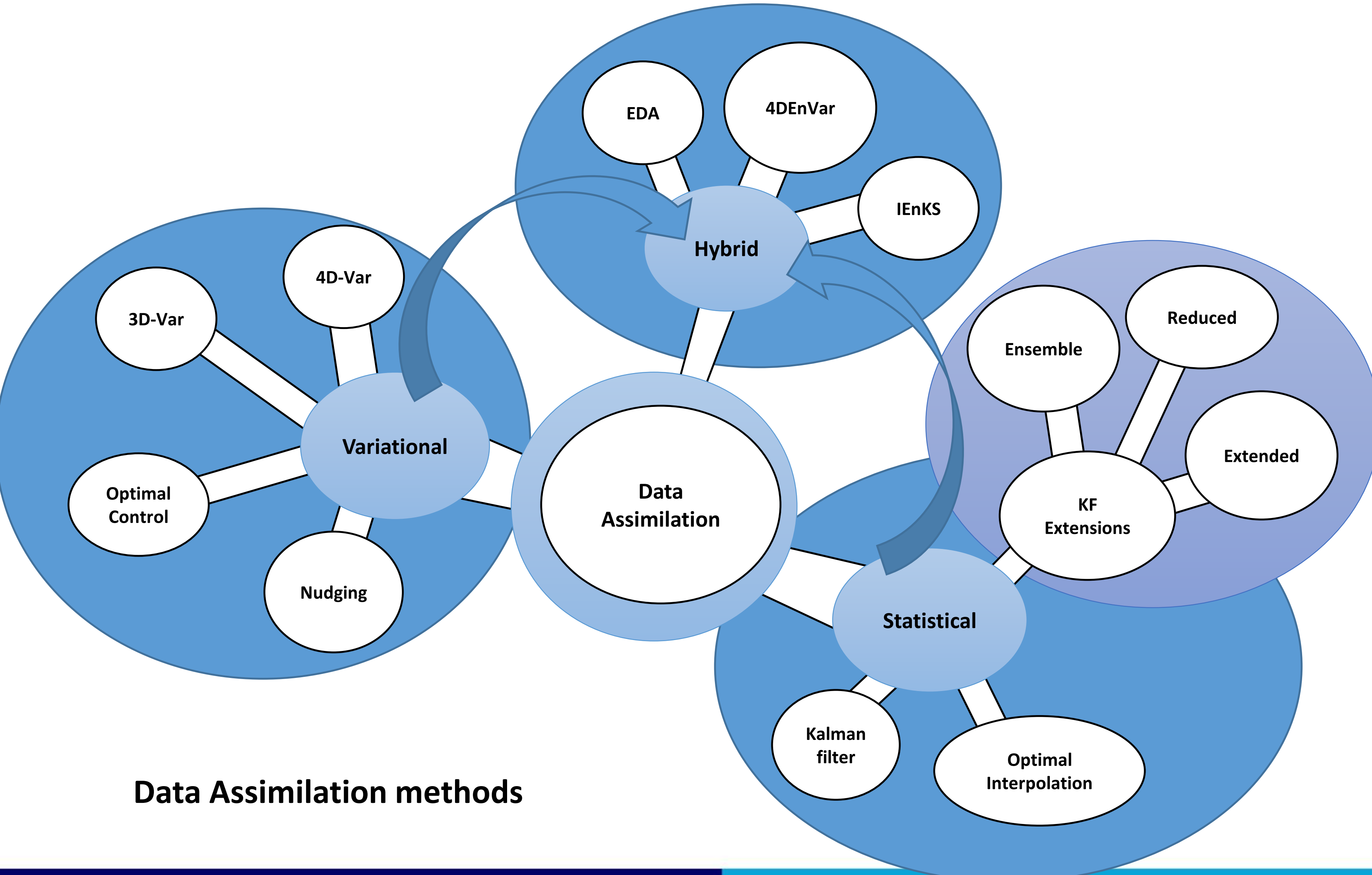


Data Assimilation methods

Data Assimilation fundamentals



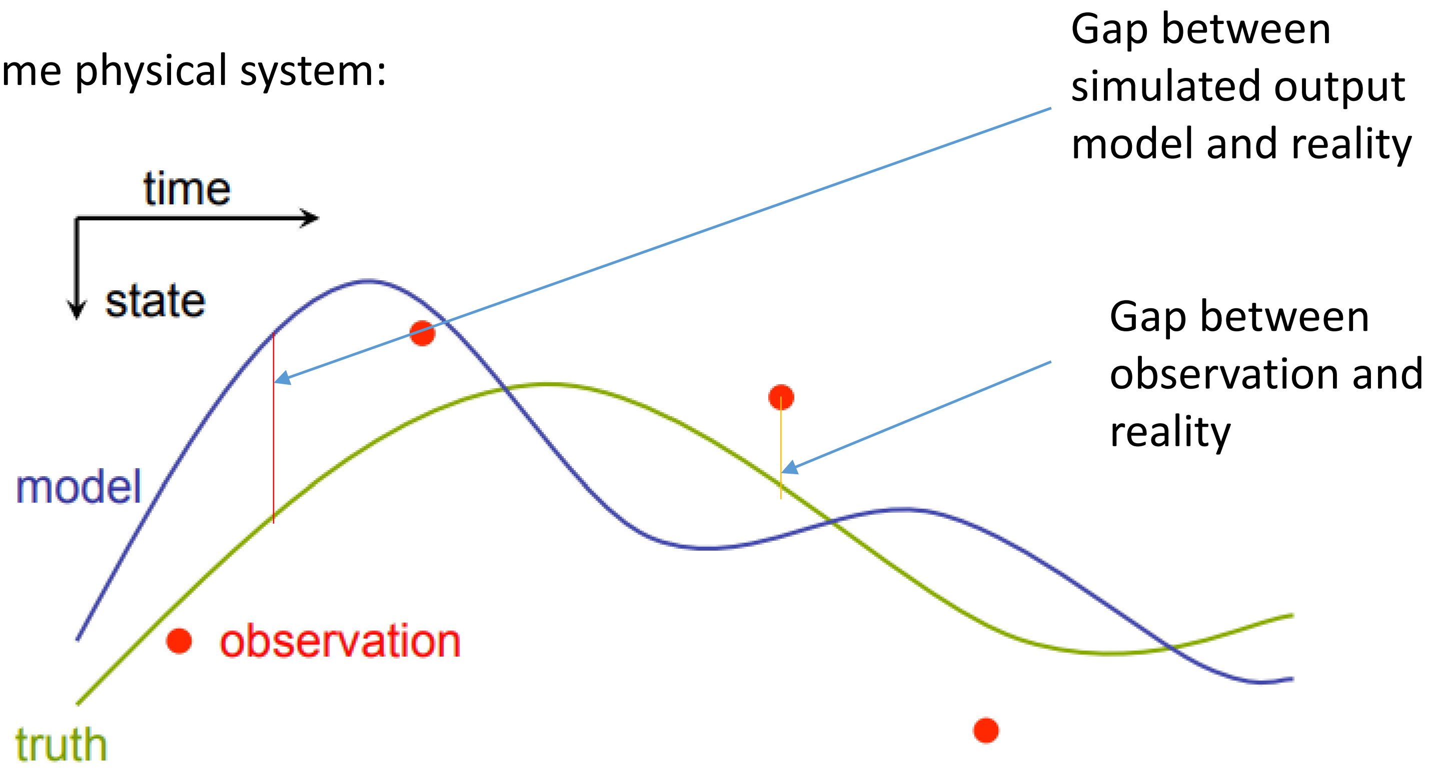
Data Assimilation methods



Data Assimilation methods

Data Assimilation approaches

Consider some physical system:



Sequential Assimilation

Variational Assimilation

Data Assimilation approaches

Basic idea of Data assimilation

True state of the variable of interest: X_t

Model gives a predicted state X_b with an error

Make a series of observations of some function $H(X_t)$ of the true state

Combine the prediction with the observations

Do it again

Variational approach

Data Assimilation techniques

Filter Techniques

Statistical optimization

Kalman filter approach: **Sequential** method that search to improve the model predictions **reducing the covariance error** between observations and model outputs

Variational methods

Least squares error minimization

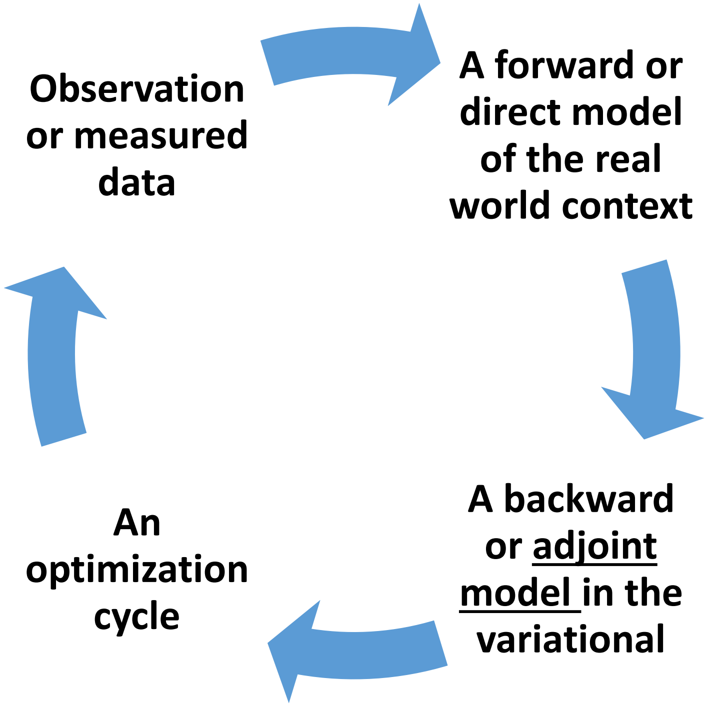
Adjoint of the forward model: Looks for the set of optimal states that **minimize cost functions** between observations made and model outputs

Data Assimilation approaches

Inverse modelling:

The inverse modelling problem consists of using the actual result of some measurements **to infer** the values of the parameters that characterize the system. A. Tarantola (2005)

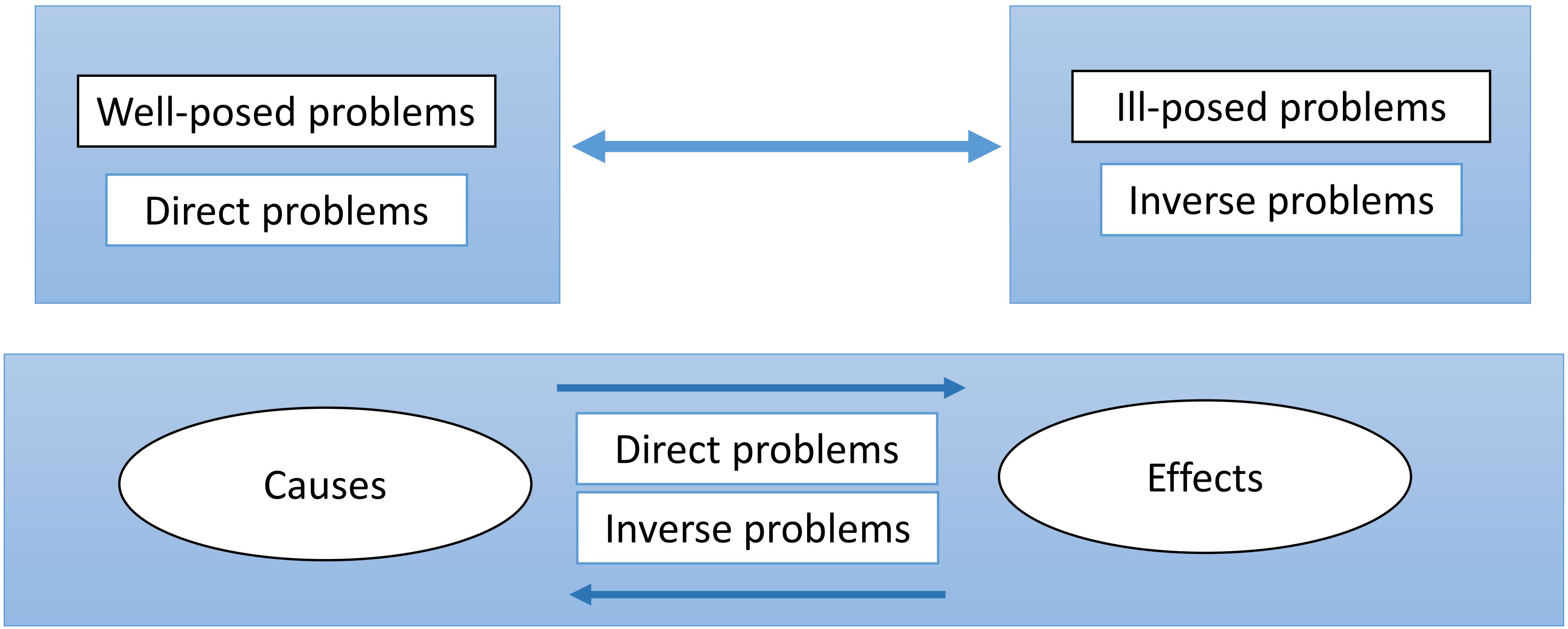
Four basic ingredients in any inverse or DA problem:



“Two problems are inverse to each other if the formulation of each involves all or part of the solution of the other” J.B.Keller (1966)

Variational approach

Variational assimilation is based on **optimal control theory**



Direct problem: the computation of the trajectories of bodies from the knowledge of the forces.
Inverse problem: determination of the forces from the knowledge of the trajectories

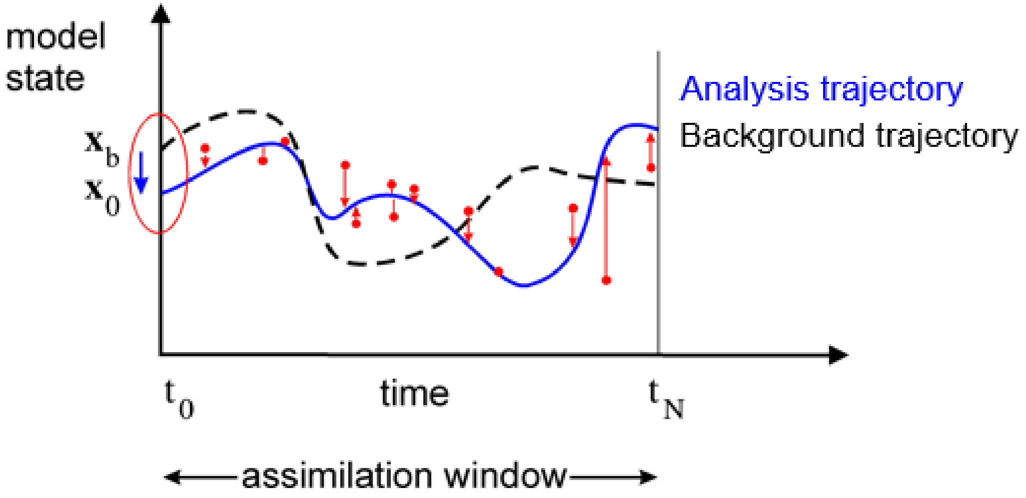
Variational approach

Theory of **maximization** and **minimization.**

***Weiertrass* theorem**: Every continuous function in a bounded domain attains a *maximal* and a *minimal* value inside the domain or on its boundary.

Variational Data Assimilation

$$J(\boldsymbol{x}_0) = \frac{1}{2}(\boldsymbol{x}_0 - \boldsymbol{x}_b)^T \boldsymbol{B}^{-1}(\boldsymbol{x}_0 - \boldsymbol{x}_b) + \frac{1}{2}(H(\boldsymbol{x}_0) - \boldsymbol{y})^T \boldsymbol{R}^{-1}(H(\boldsymbol{x}_0) - \boldsymbol{y})$$



The **calculus of variations** deals with the following problema:

Find the *maximum* or *minimum* of a functional, over the given domain of admisible functions, for which the functional attains the **extremum** with respect to all argument functions in a small neighborhood of the extremal argument function.

Variational approach

Cost function $\boldsymbol{J}(\boldsymbol{m})$ as an **energy functional**

3D-Var

$$J = min\frac{1}{2}[(\boldsymbol{x}_0 - \boldsymbol{x}_b)^T\boldsymbol{B}^{-1}(\boldsymbol{x}_0 - \boldsymbol{x}_b) + (H(\boldsymbol{x}_0) - \boldsymbol{y})^T\boldsymbol{R}^{-1}(H(\boldsymbol{x}_0) - \boldsymbol{y})]$$

Distance to forecast — Distance to observations

4D-Var

$$J = min\frac{1}{2}[(\boldsymbol{x}_0 - \boldsymbol{x}_b)^T\boldsymbol{B}^{-1}(\boldsymbol{x}_0 - \boldsymbol{x}_b) + \sum_i^s(H(\boldsymbol{x}_i) - \boldsymbol{y}_i)^T\boldsymbol{R}^{-1}(H(\boldsymbol{x}_i) - \boldsymbol{y}_i)]$$

Distance to forecast — Distance to observations

A misfit **functional** that quantifies the distance between the observation and the model prediction.

Variational approach

Which approach, Kalman filtering or variational assimilation, is better?

Previous Results

TU Delft

Prof.dr.ir. A.W. Heemink

Delft Institute of Applied Mathematics DIAM

Fu, G. (2016). Improving volcanic ash forecast with ensembled-based data assimilation (doctoral dissertation). Technische Universiteit Delft, Delft, The Netherlands.

Lu, S. (2016). *Variational data assimilation of satellite observations to estimate volcanic ash emission* (doctoral dissertation). Technische Universiteit Delft, Delft, The Netherlands.

Previous Results

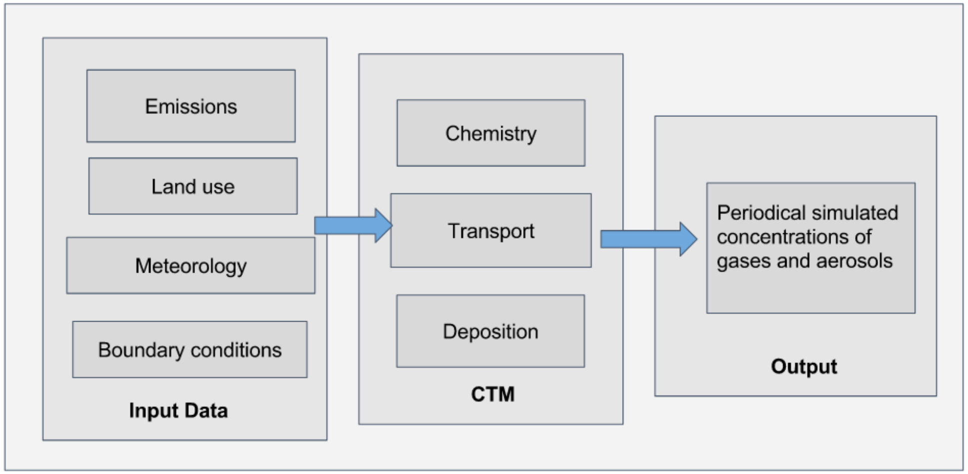
TuDelft PhD Theses

Eyjafjallajokull volcano eruption plume

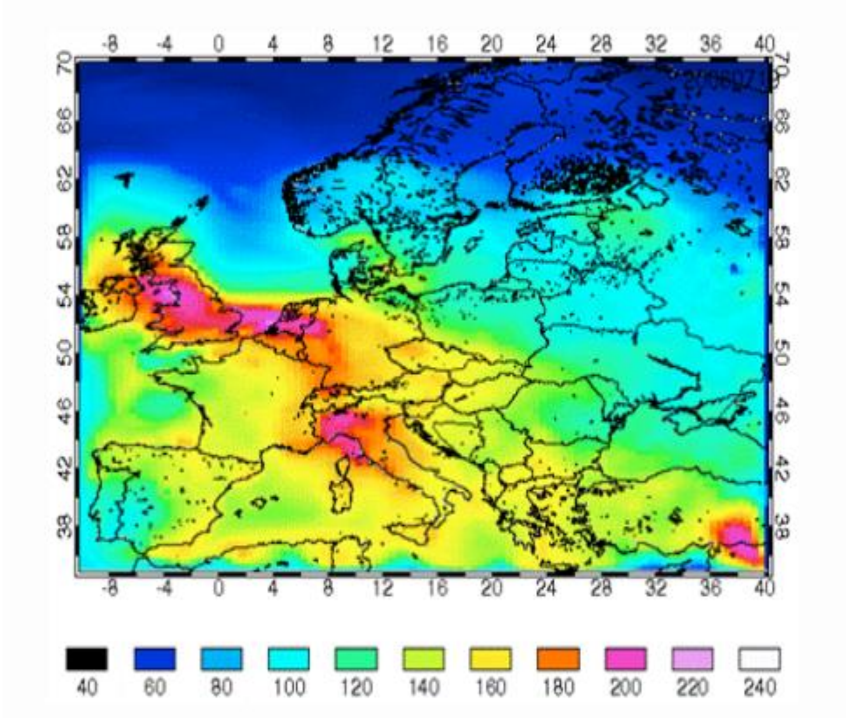
The **April-May 2010** eruption of Eyjafjallajokull volcano (Iceland) caused an unprecedent closure of the European and North Atlantic airspace with global economic losses of **5 billion US dollars**

Oxford-Economics (2010)

Previous Results



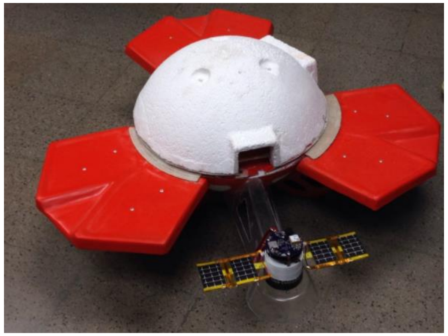
Chemical Transport Model (CTM)



LOTOS EUROS Output for NO2

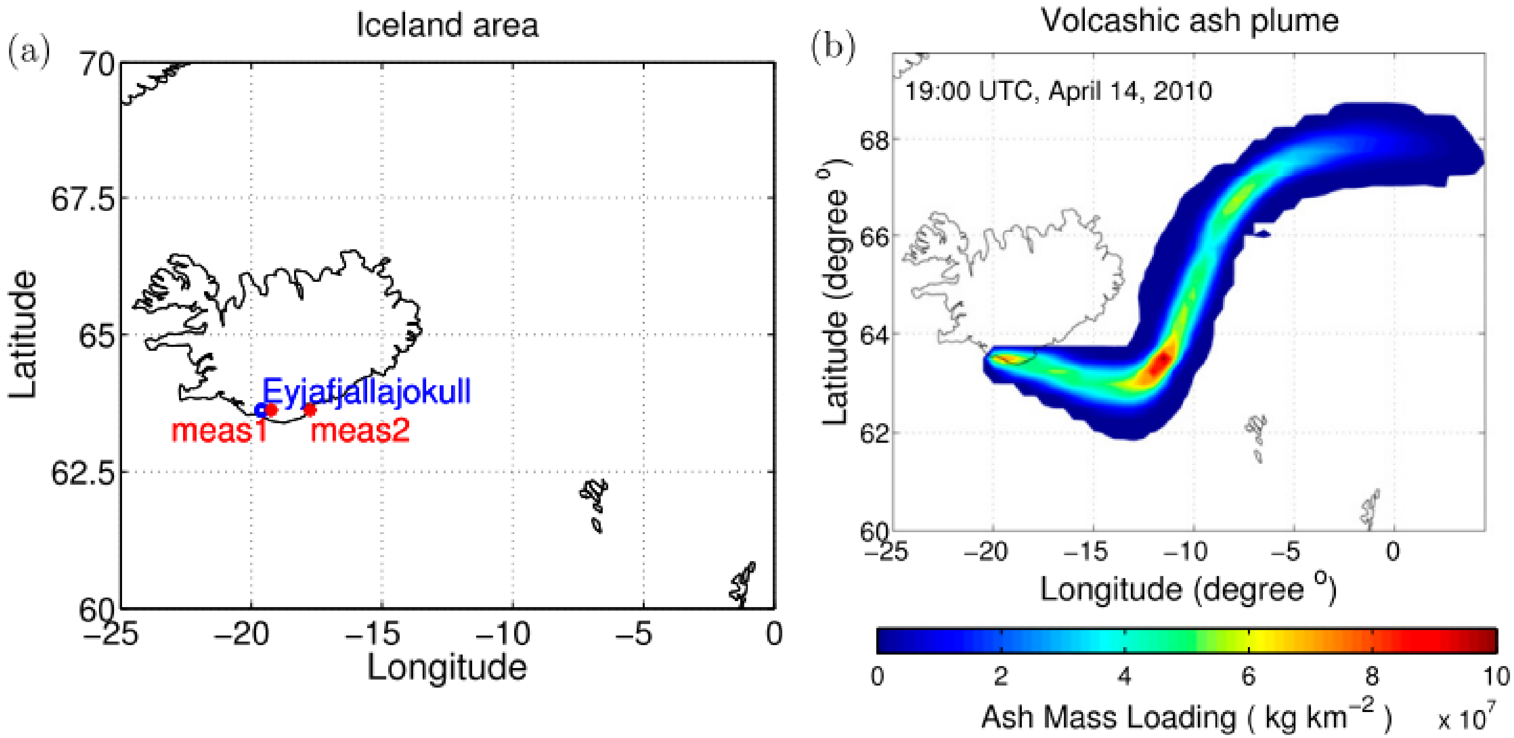
Previous Results

Image extracted from https://www.youtube.com/watch?v=bjAOqMf3DUY&t=119s



Previous Results

TU Delft Doctoral dissertations

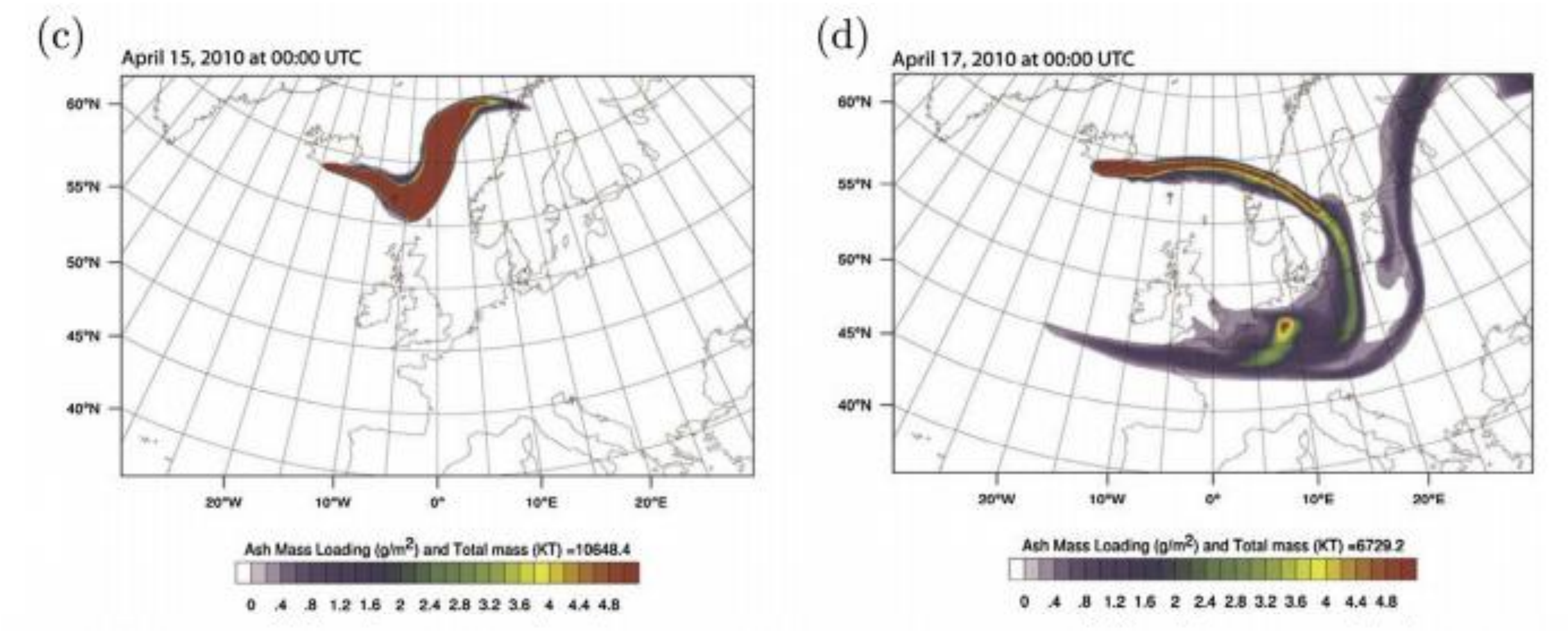


(Lu. S. (2016). Fu. S (2016).)

Previous Results

April 14-18, 2010

TU Delft Doctoral dissertations

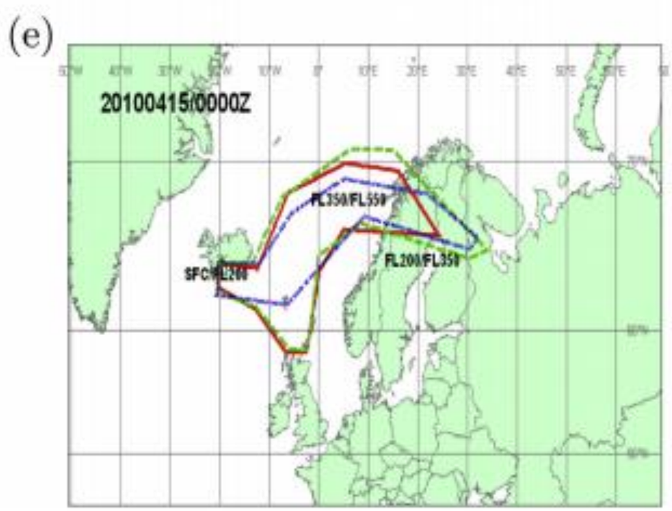


<u>April 15, 2010</u> <u>April 17, 2010</u>

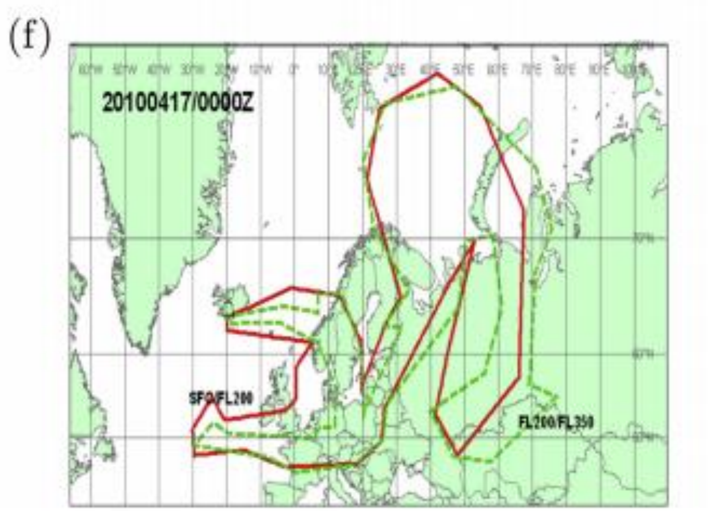
LOTOS-EUROS

Previous Results

TU Delft Doctoral dissertations



April 15, 2010



April 17, 2010

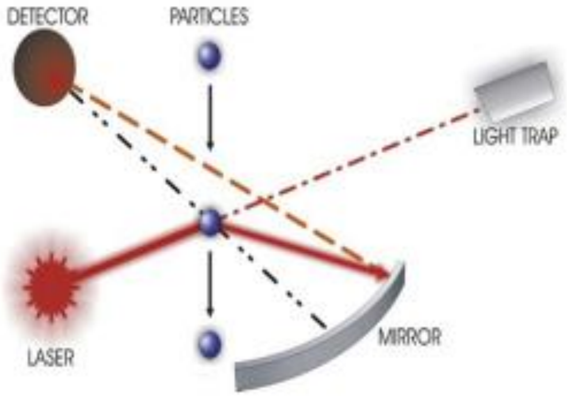
Volcanic Ash Advisory Center (VAAC) based on the **NAME** model

Previous Results

TU Delft Doctoral dissertations

(a)

(b)



OPC Optical Particle Counter

Previous Results

TU Delft Doctoral dissertations

Variations of the proposed DA methods

Lu, S. (2016).

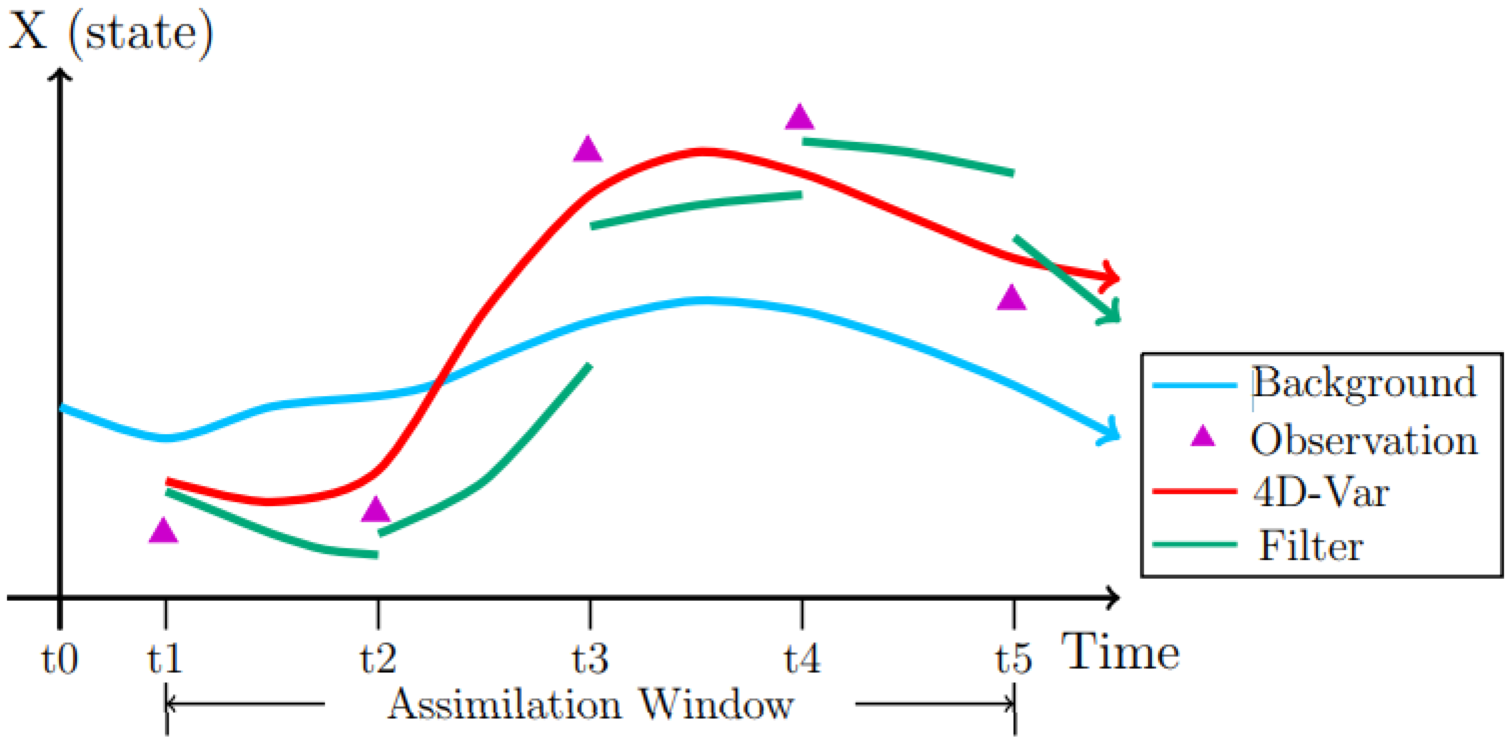
Trajectory 4D-Var

Fu, G. (2016).

Two-way-tracking
Localized EnKF (TL-EnKF)

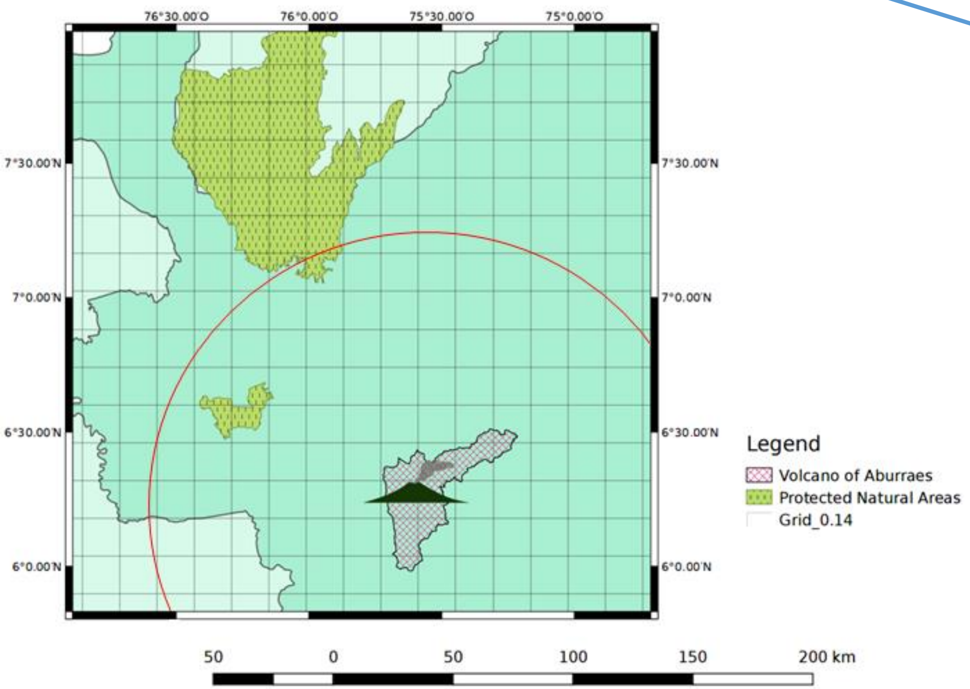
Previous Results

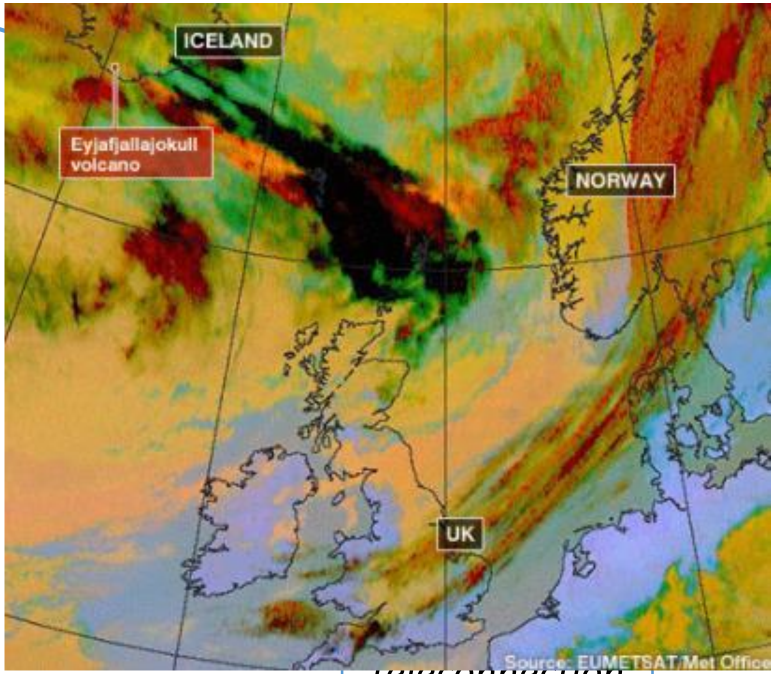
TuDelft PhD Theses



Current and future work

"The Volcano of the Aburraes"





teleconnection

Analogy of the **volcano of the Aburraes** with the volcano of Iceland

Current research questions

How to generalize and formalize, through the help of Control Systems formalism, the answers to the Data Assimilation questions regarding the **volcano of Aburraes**.

How can we try or propose a **hybrid scheme** for the ill-conditioned problem in order to deal with reduced **observational noise.**

How to develop further evidence and formalize the postulate of accuracy of the method for a physical-related window of assimilation, regarding the demonstrated accuracy in assimilation windows that does not compromise the constant concentration of particles in atmosphere (Lu et al, 2016 under review).

Current research questions

Is it possible to use a formal sensitivity analysis to analyze the perturbation of the inputs to the two experience based modifications in order to the penalty term to develop a generalized method and probe the stability of the solution for the **trj-4DVar**?

Verify the feasibility for the development of an extension for the **trj-4DVar** in LOTOS-EUROS Volcanic ash problem to bigger systems and mathematically feasible solutions to solve the modified cost function in a new or improved approach **adjoint free** for the case of the Aburrá Valley

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