Inspire Create Transform

Vigilada Mineducación

TU Delft Delft University of Technology

UNIVERSIDAD EAFIT®

Seminar 3 of the PhD in Mathematical Engineering

Conciliating models with reality: The Variational data assimilation technique

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Advisors

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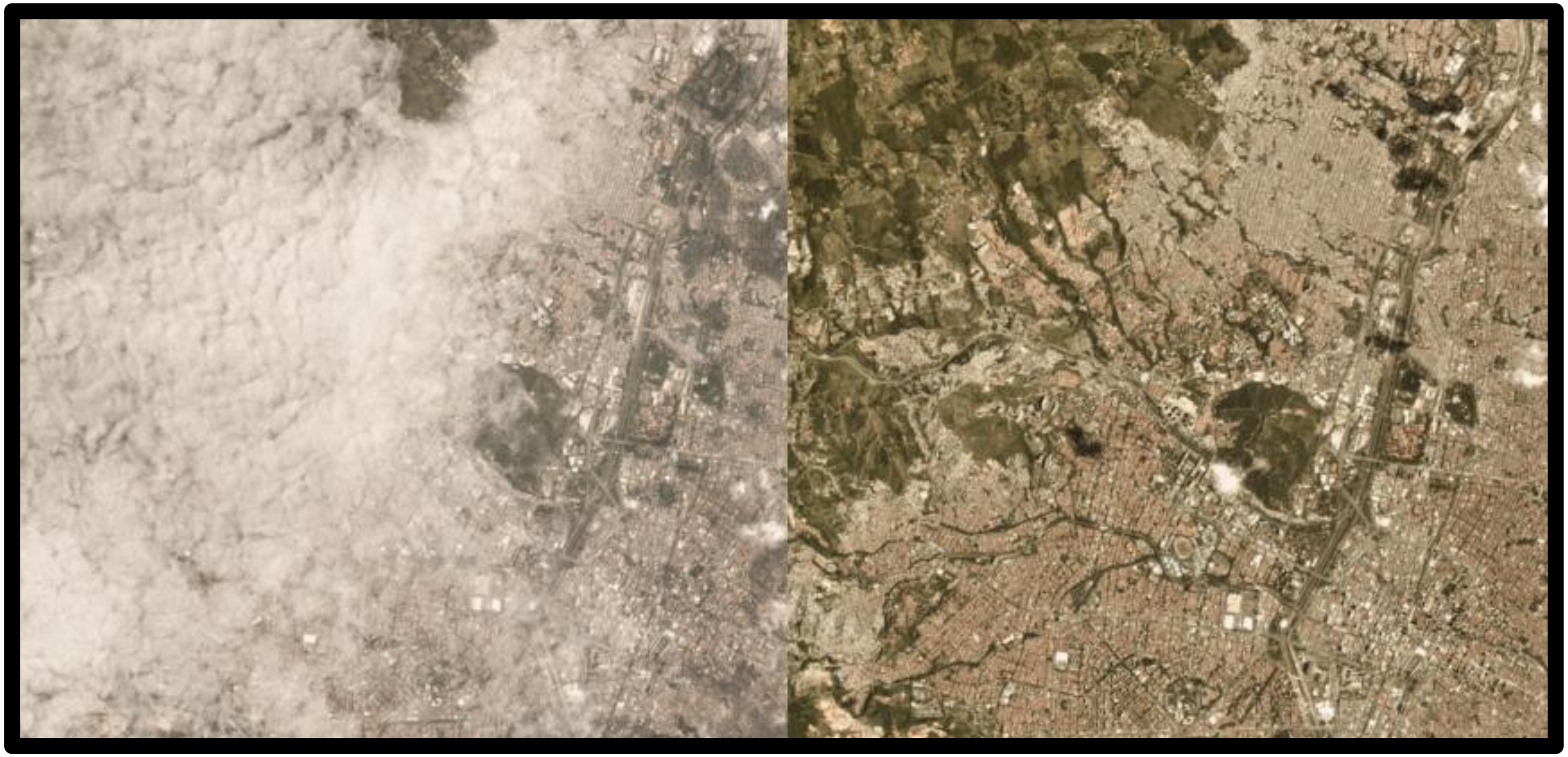
1/06/18

Outline

- Motivation
- Introduction: Inverse modelling
- Data assimilation: Variational Data assimilation
- 4D-Var model example: The Lorenz 63 model
- Current and future work
- References

Motivation



March 6 2018   9:52 am

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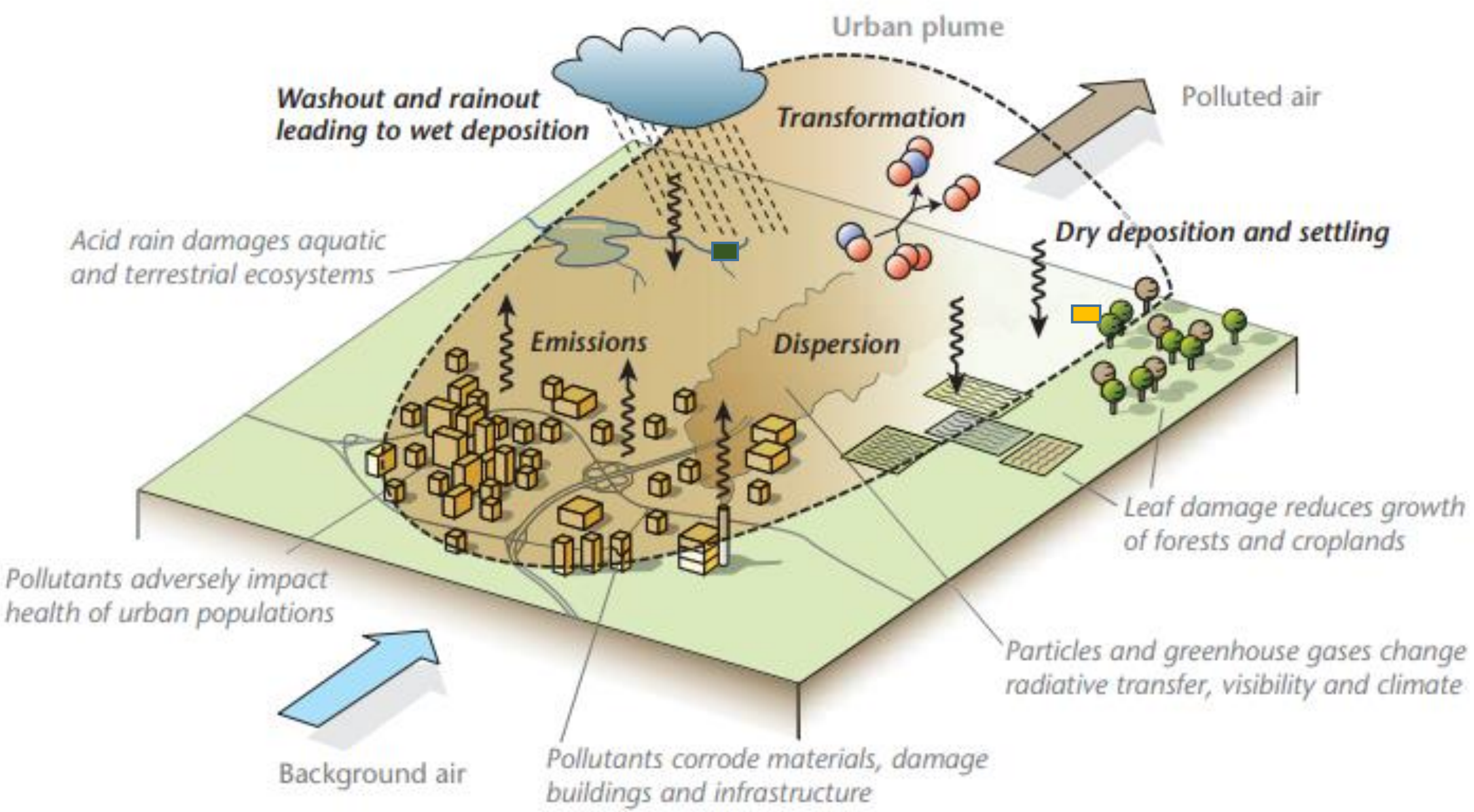
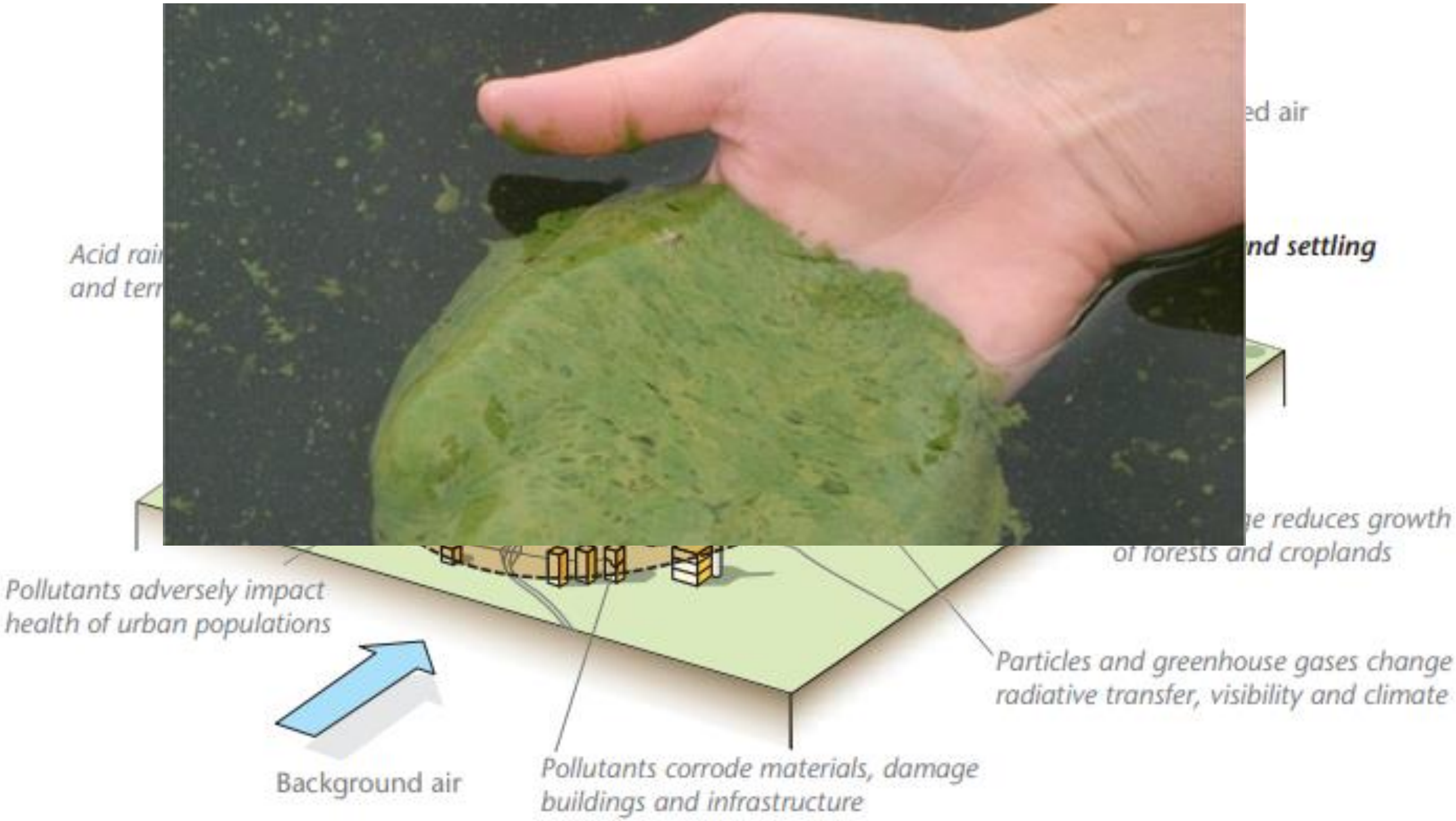
planet.

Motivation



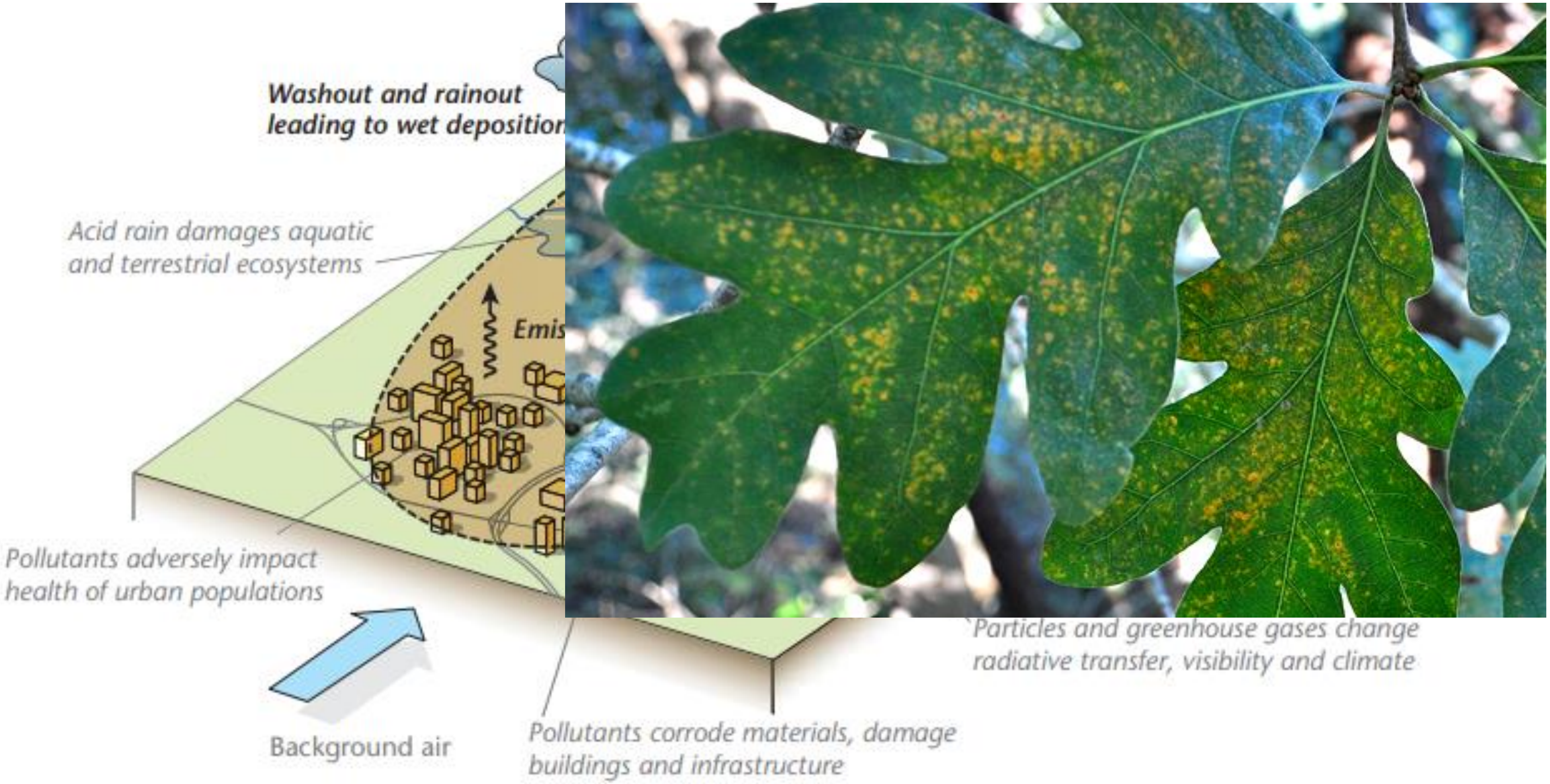
(Oke, T et. al (2017))

Motivation



(Oke, T et. al (2017))

Motivation



(Oke, T et. al (2017))

What, how much, and whence is being emitted if we know how much is being deposited in different protected natural areas?

Motivation

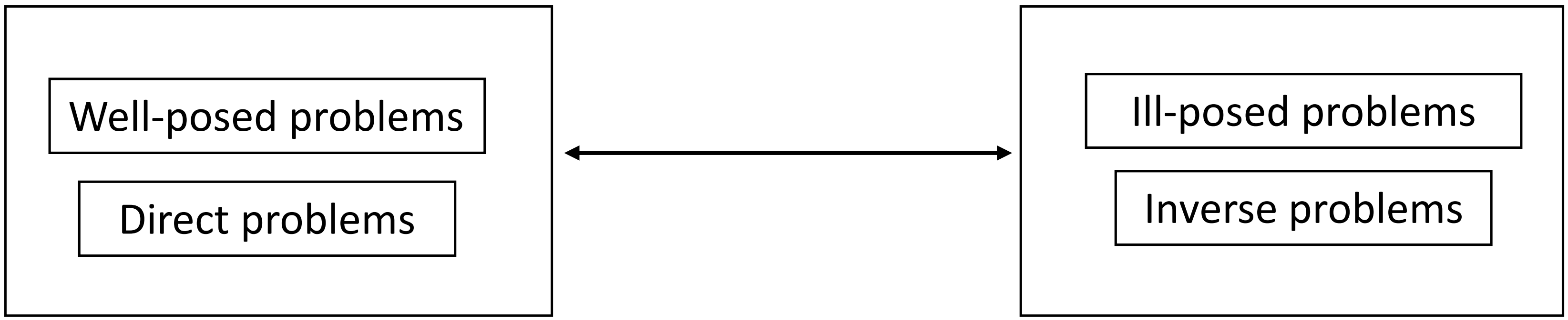
Inverse modelling

… Most people, if you describe a train of events to them Will tell you what the result Will be. There are few people, however that if you told them a result, would be able to evolve from their own inner consciousness what the steps were that led to that result. This power is what I mean when I talk of reasoning backward

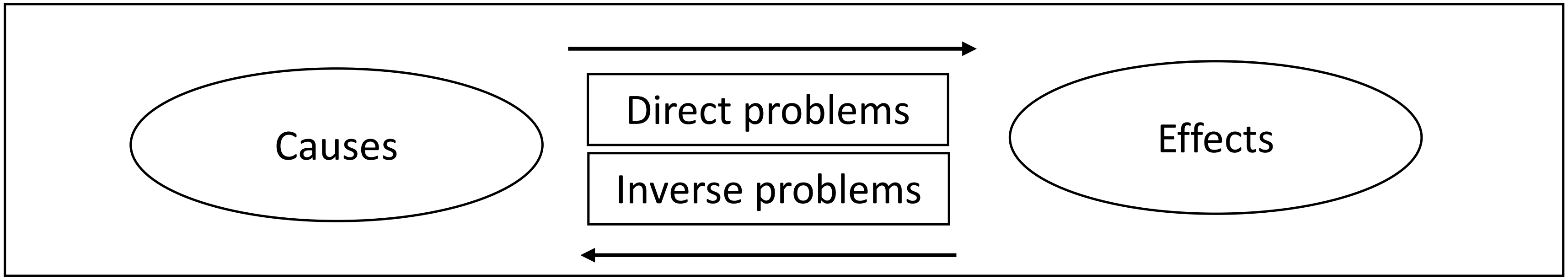
Sherlock Holmes
A Study in Scarlet
Sir Arthur Conan Doyle (1887)

Motivation

Inverse modelling



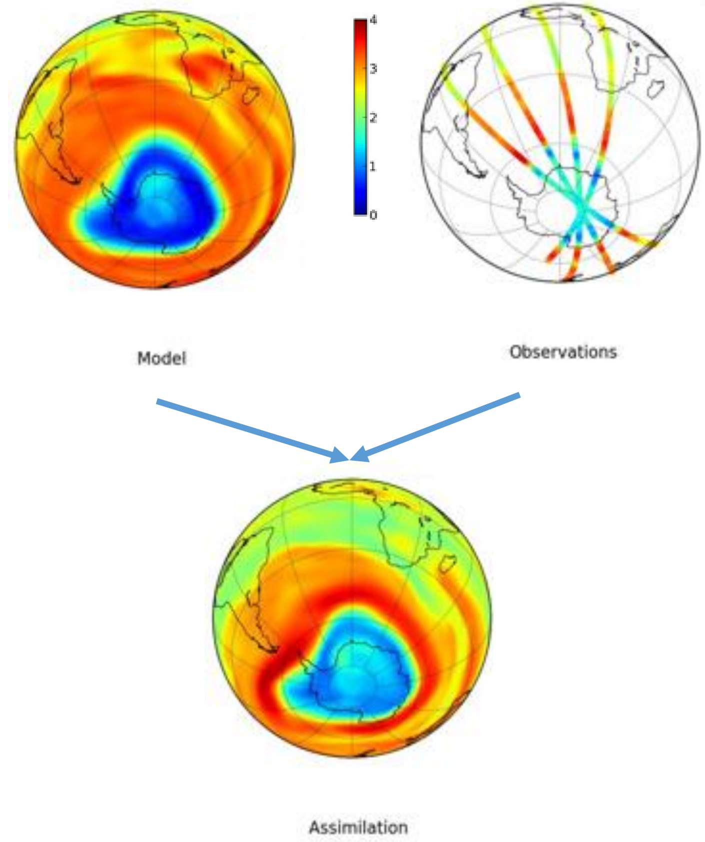
"Two problems are inverse to each other if the formulation of each involves all or part of the solution of the other" J. B. Keller (1976)



Tarantola A. et al. (2005).

Data assimilation methods

First I need a model ☑



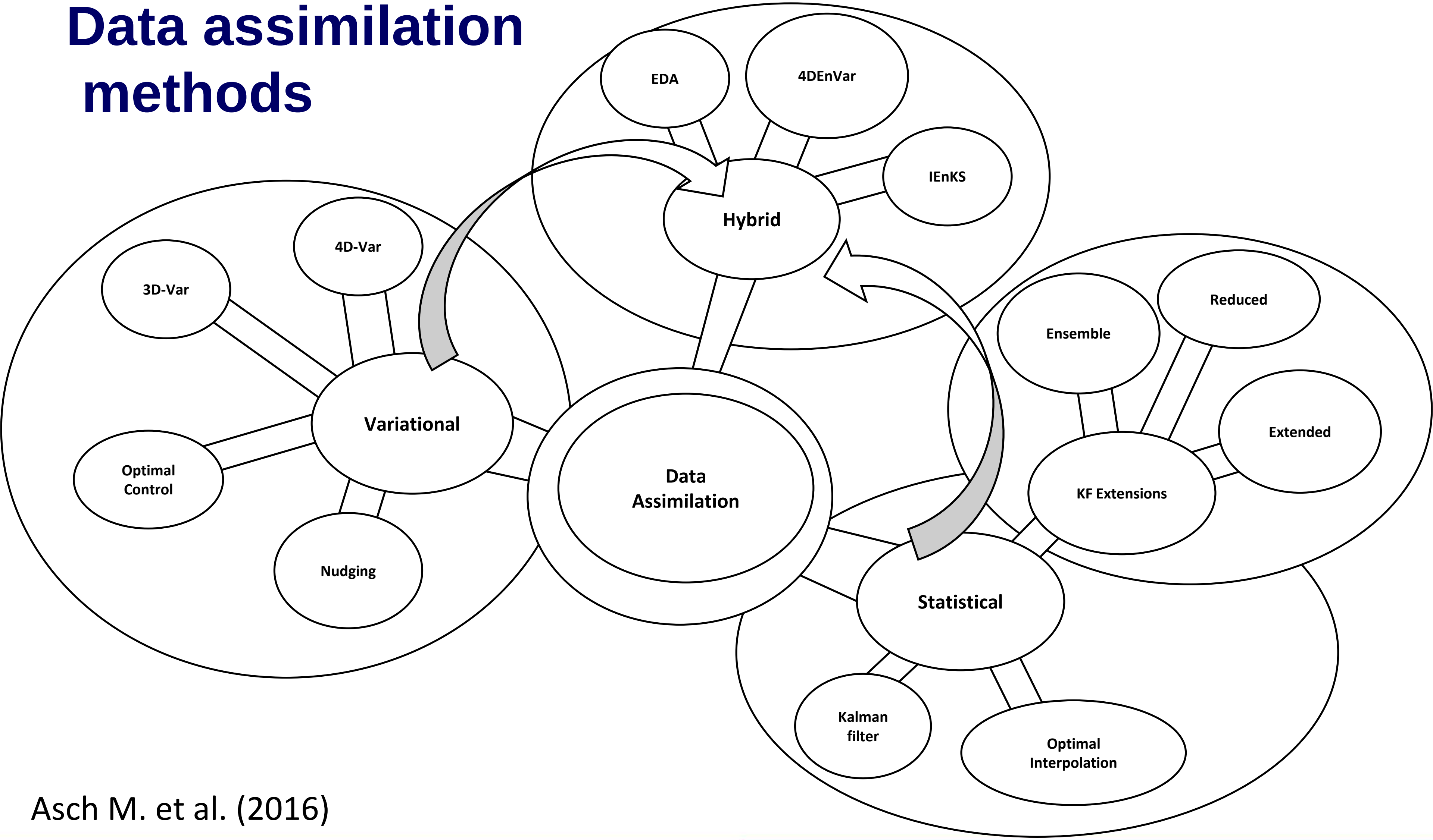
My model is not accurate

But,

I have mesurements of the reality

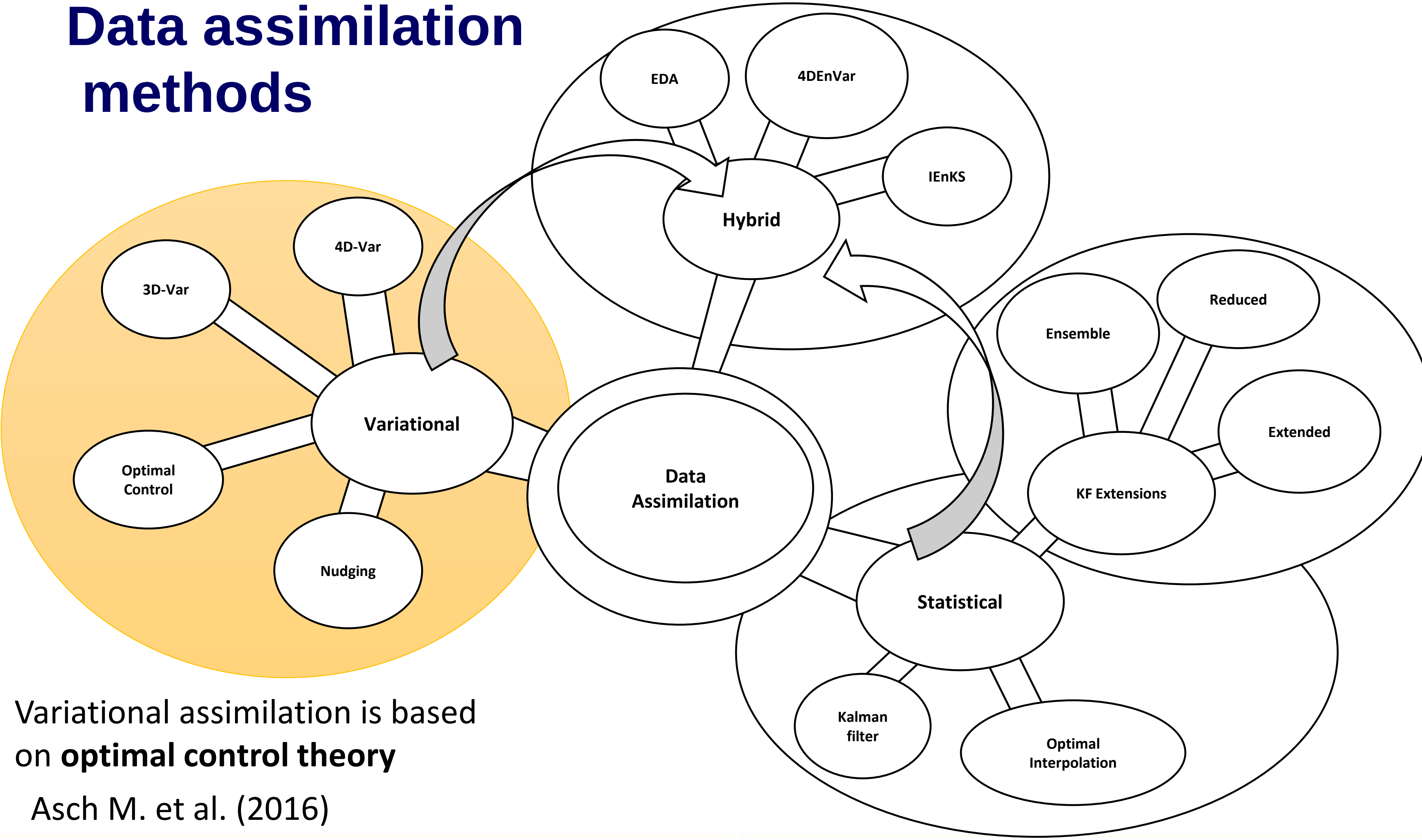
Data assimilation

Data assimilation methods



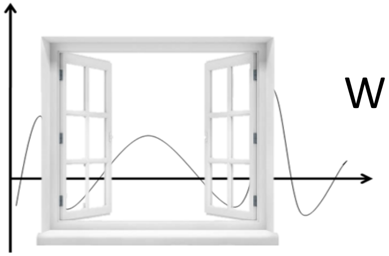
Asch M. et al. (2016)

Data assimilation methods

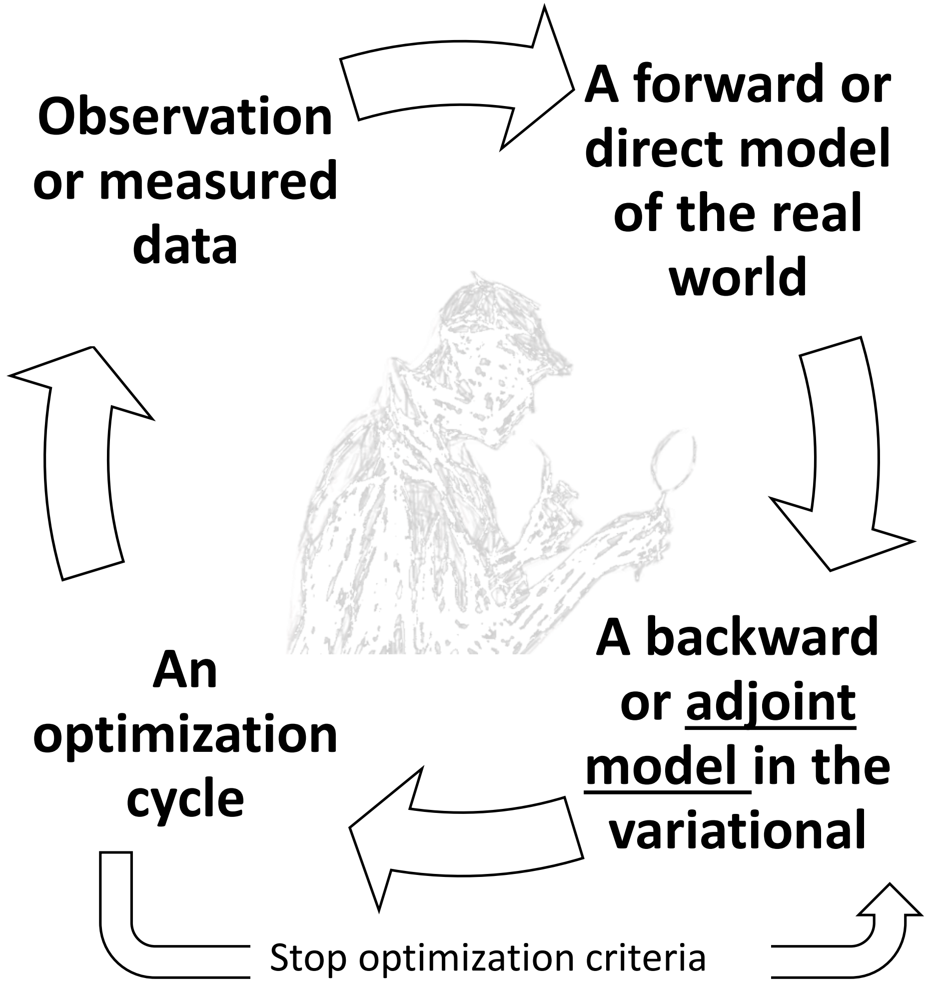


Variational assimilation is based on **optimal control theory**

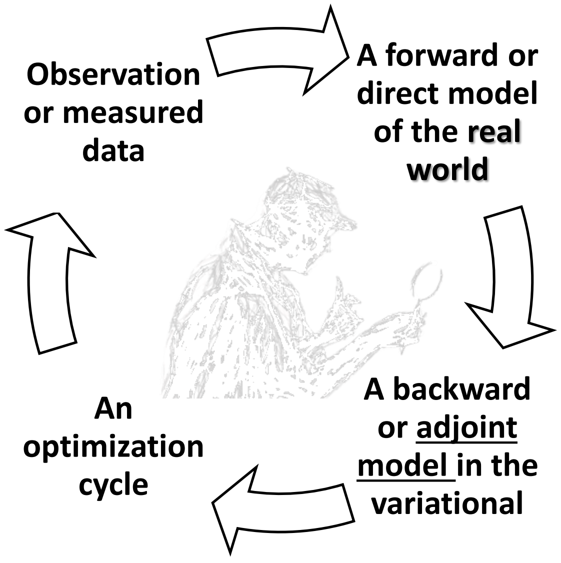
Asch M. et al. (2016)



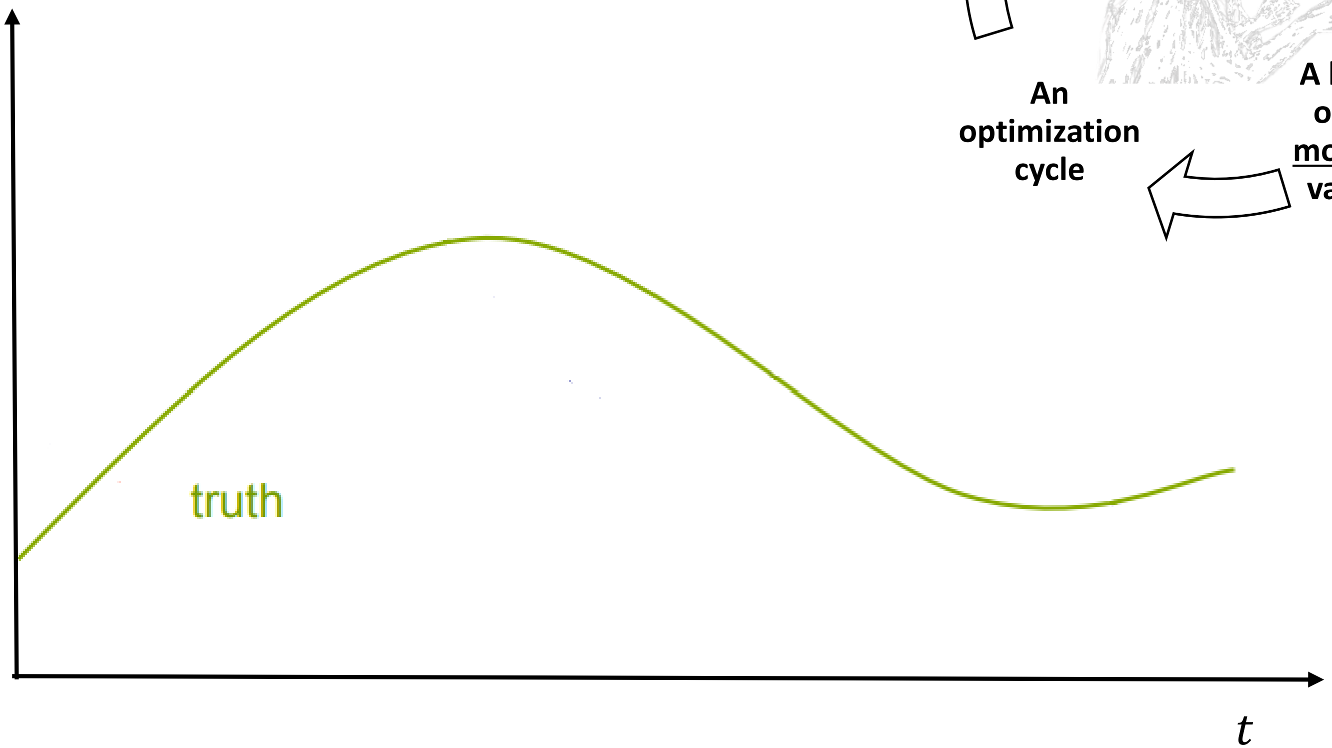
Windowing step



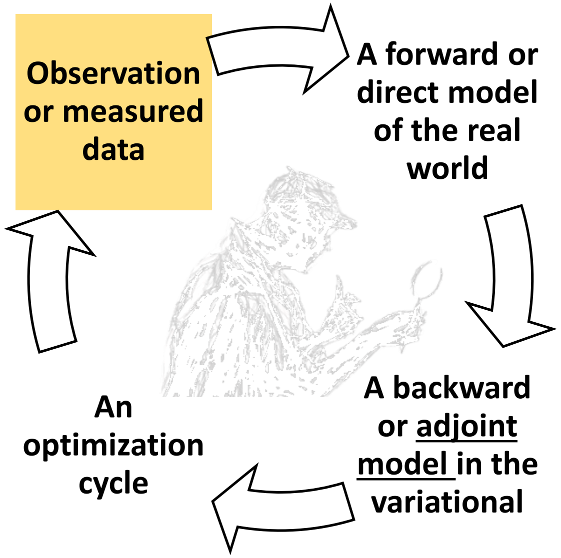
Variational Data assimilation

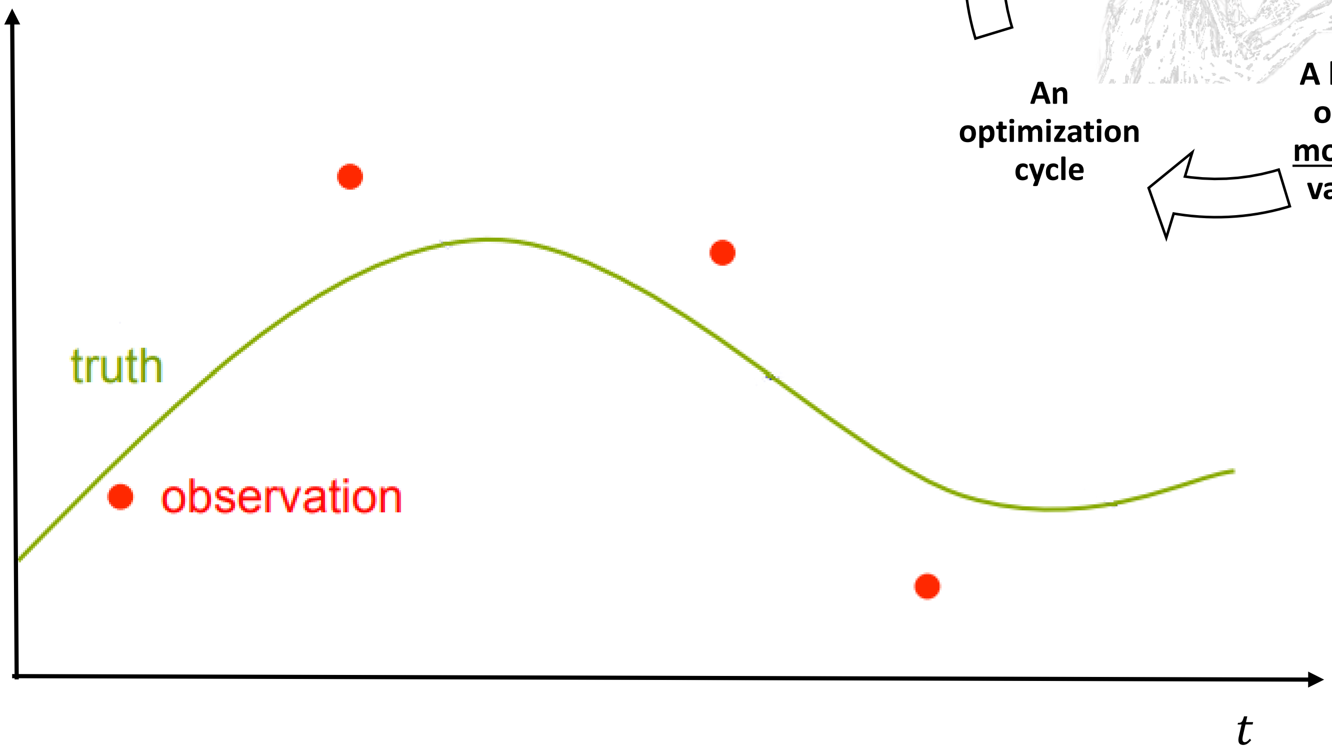


Consider some physical system:



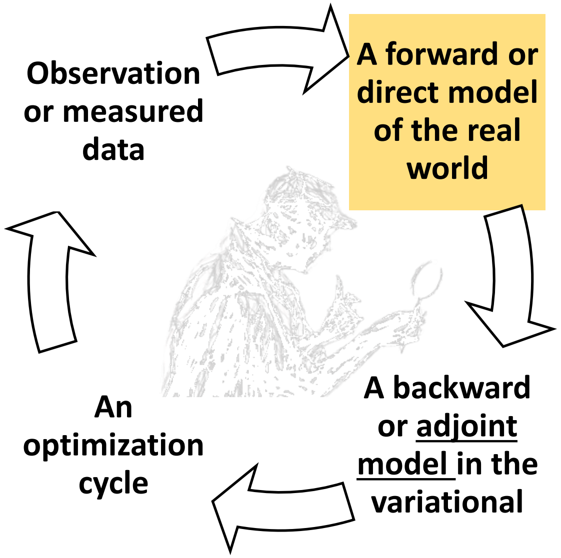
Variational Data assimilation

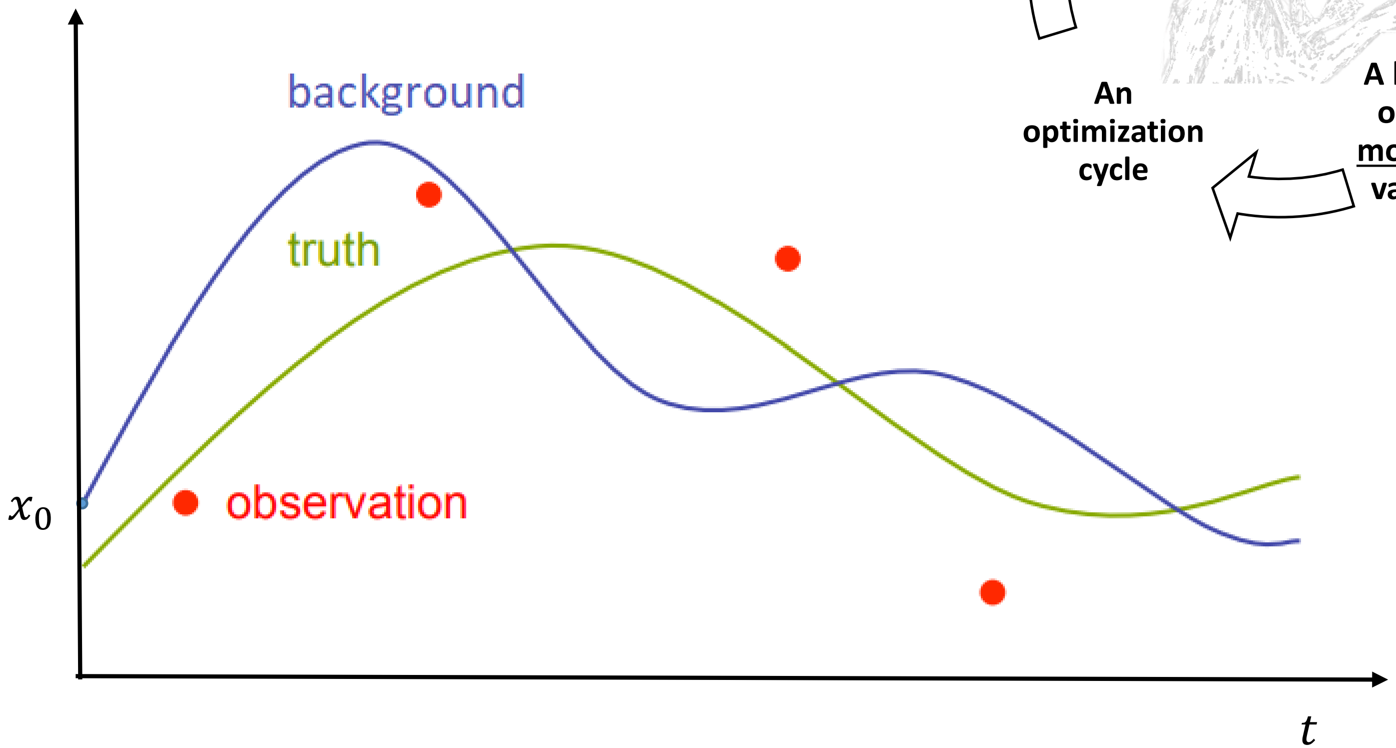




$$y_k = \mathcal{M}_k x_k + v_k \qquad v_k \sim N(0, \boldsymbol{R})$$

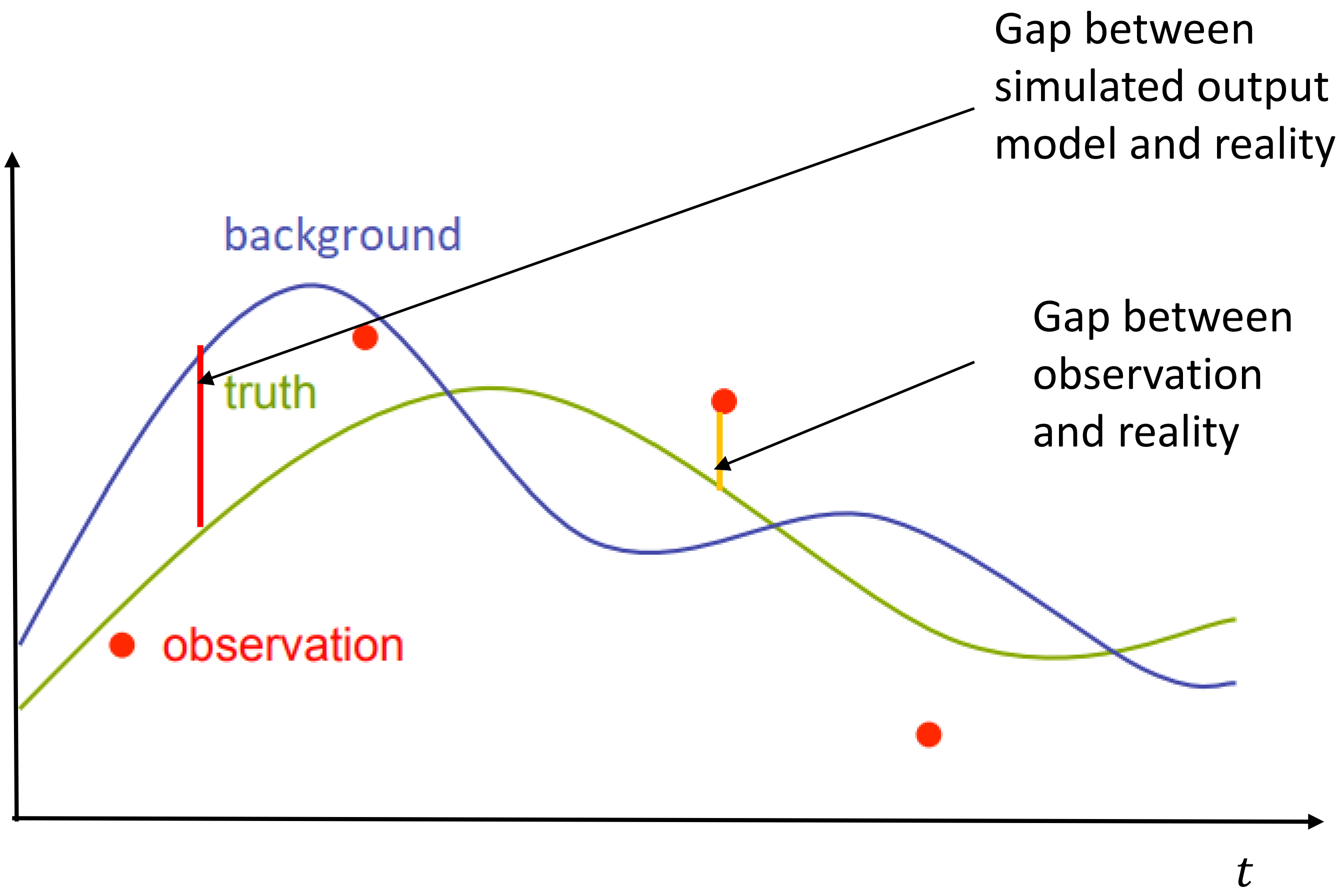
Variational Data assimilation



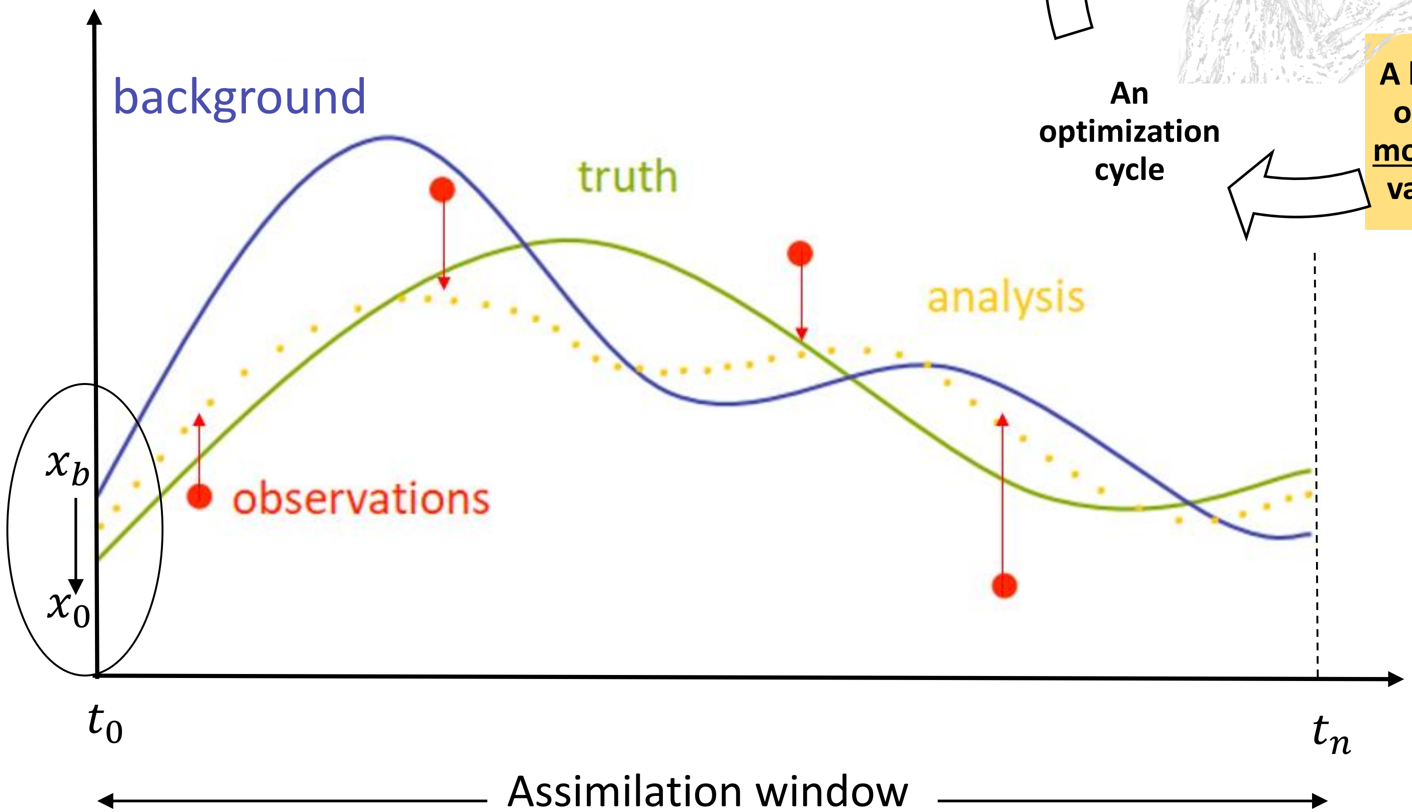


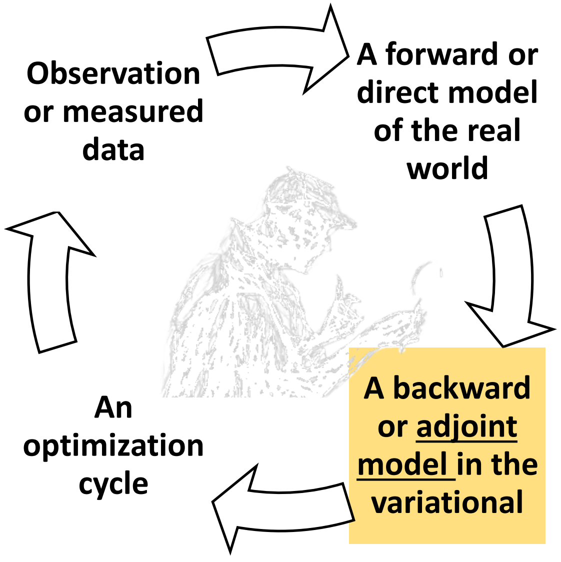
$$x_{k+1} = \mathcal{F}_k(x_k, p)$$

Variational Data assimilation

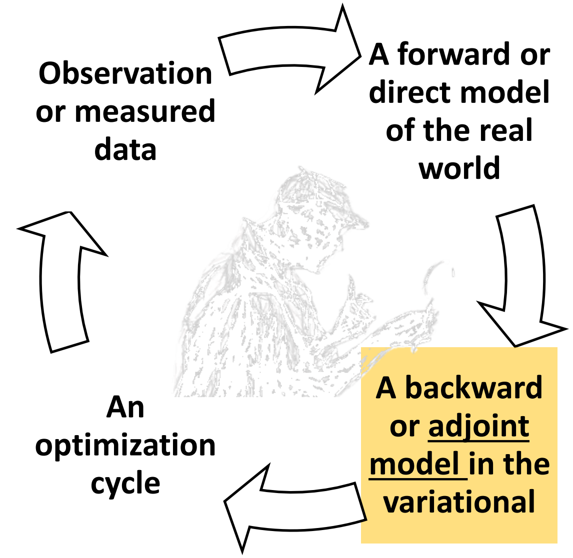


Variational Data Assimilation

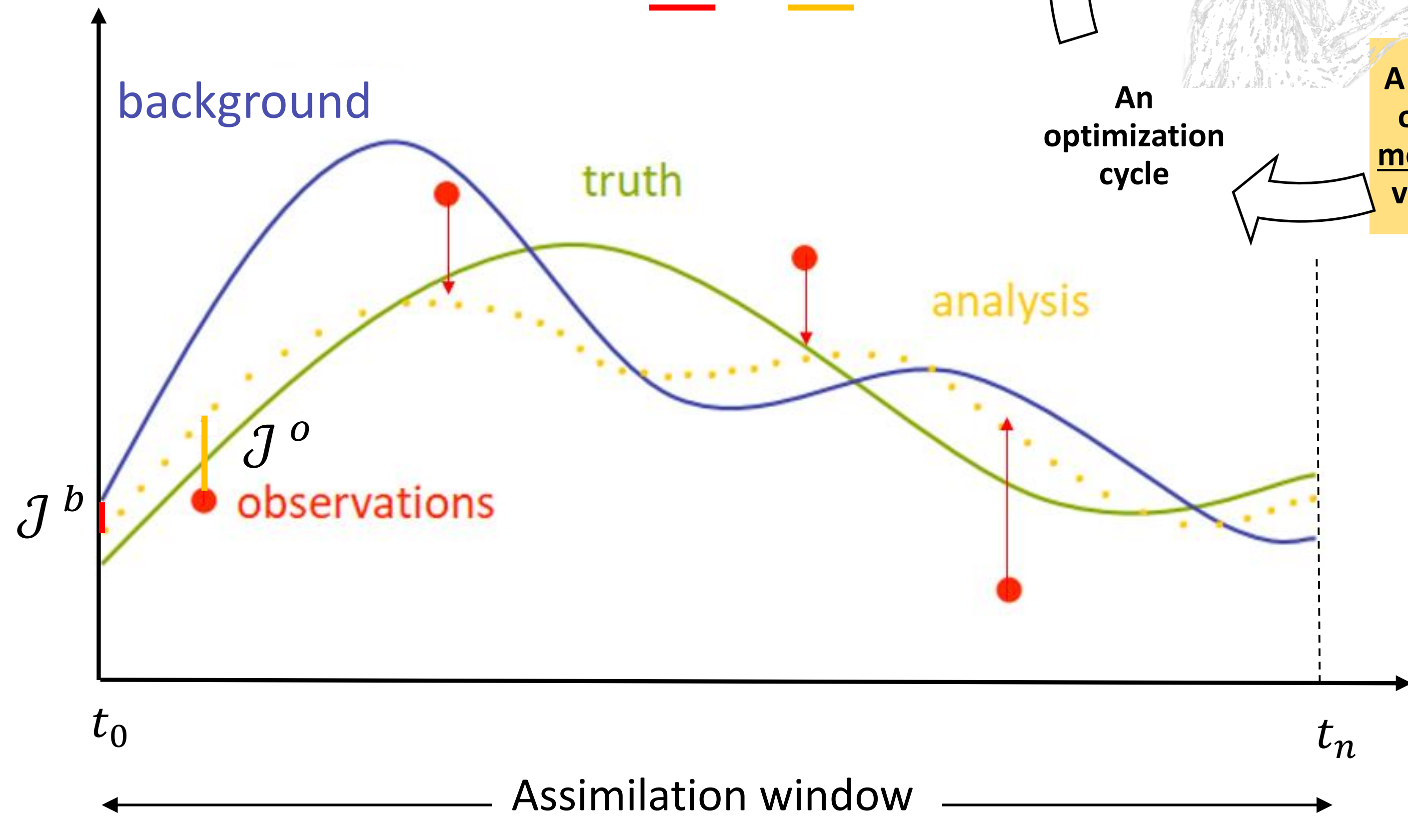




Variational Data Assimilation



$$\mathcal{J} = \mathcal{J}^{b} + \mathcal{J}^{o}$$



Variational Data Assimilation

3D-Var

$$\mathcal{J} = \mathcal{J}^{b} + \mathcal{J}^{o}$$

A priori (background) state

Observation operator

Observations

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

Background error covariance matrix

Observation error covariance matrix

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

Distance to forecast

Distance to observations

Variational Data Assimilation

4D-Var

$$\mathcal{J}(x_o) = \frac{1}{2}\left[(\boldsymbol{x}_0 - \boldsymbol{x}_b)^T \boldsymbol{B}^{-1}(\boldsymbol{x}_0 - \boldsymbol{x}_b) + \sum_{i=0}^{s} (H(\boldsymbol{x}_i) - \boldsymbol{y}_i)^T \boldsymbol{R}^{-1}(H(\boldsymbol{x}_i) - \boldsymbol{y}_i)\right]$$

$$= \frac{1}{2}\|\boldsymbol{x}_0 - \boldsymbol{x}_b\|_{\boldsymbol{B}}^2 + \frac{1}{2}\sum_{i=0}^{s} \|HM(\boldsymbol{x}) - \boldsymbol{y}_i\|_{\boldsymbol{R}}^2$$

Distance to background   Distance to observations

Variational Data Assimilation

$$x_k = \mathcal{F}\, x_{k-1} \qquad y_k = \mathcal{M} x_s + v_s \qquad v_s \sim N(0, \boldsymbol{R})$$

$$\mathcal{J}(\boldsymbol{x}_0) = \frac{1}{2}(\mathcal{M} x_s - y_s)^T \boldsymbol{R}^{-1}(\mathcal{M} x_s - y_s)$$

$$x_1 = \mathcal{F}\, x_0 \qquad x_2 = \mathcal{F}\, x_1 = \mathcal{F}\mathcal{F} x_1 \qquad \ldots \qquad x_s = \mathcal{F}\, x_{s-1} = \mathcal{F}^s\, x_0$$

$$\mathcal{J}(\boldsymbol{x}_0) = \frac{1}{2}(\mathcal{M}\mathcal{F}^s x_0 - y_s)^T \boldsymbol{R}^{-1}(\mathcal{M}\mathcal{F}^s x_0 - y_s)$$

$$\delta\mathcal{J} = -(\mathcal{M}\mathcal{F}^s x_0 - y_0)^T \boldsymbol{R}^{-1}\mathcal{M}\frac{\partial \mathcal{F}^s}{\partial x}\delta\, x_0$$

Variational Data Assimilation

$$\delta\mathcal{J} = \left\langle \mathcal{M}^T \boldsymbol{R}^{-1} (\mathcal{M}\mathcal{F}^s x_0 - y_0)^T, \frac{\partial \mathcal{F}^s}{\partial x} \delta\, x_0 \right\rangle$$

$$\langle x, Ay \rangle = \langle A^T x, t \rangle$$

The adjoint trick

$$\delta\mathcal{J}(\boldsymbol{x}_0) = \left\langle \left[\frac{\partial \mathcal{F}^s}{\partial x}\right]^T \mathcal{M}^T \boldsymbol{R}^{-1} (\mathcal{M}\mathcal{F}^s x_0 - y_0)^T, \delta x_0 \right\rangle$$

$$\delta\mathcal{J}(\boldsymbol{x}_0) = \left\langle \nabla_{\delta(\boldsymbol{x}_0)} \mathcal{J}, \delta \boldsymbol{x}_0 \right\rangle$$

$$\nabla_{\delta(\boldsymbol{x}_0)} \mathcal{J} = \left[\frac{\partial \mathcal{F}^s}{\partial x}\right]^T \mathcal{M}^T \boldsymbol{R}^{-1} (\mathcal{M}\mathcal{F}^s x_0 - y_0)^T$$

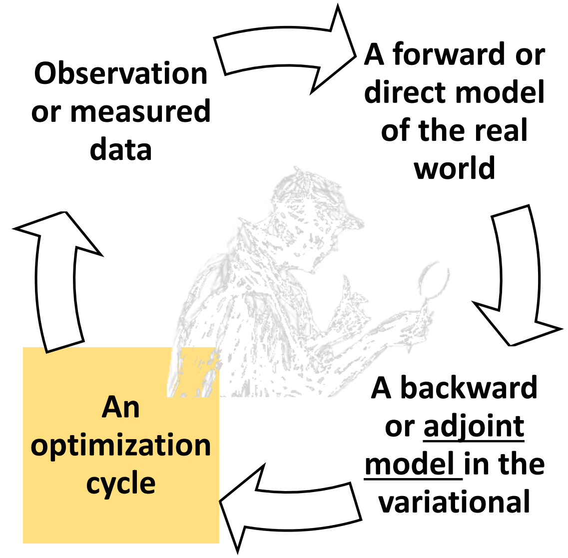
Variational Data Assimilation

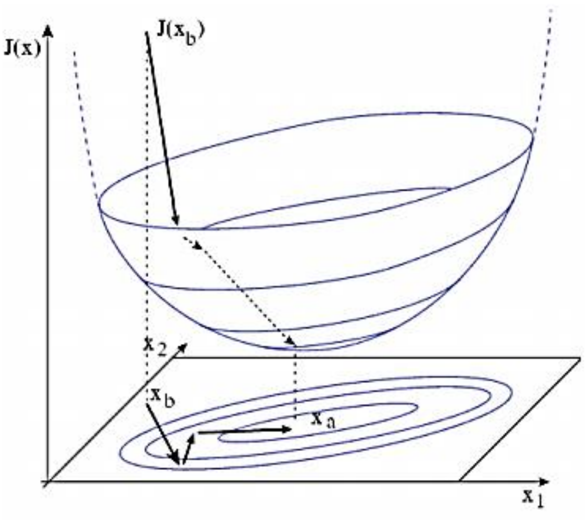
$$\nabla_{\delta(x_0)}\mathcal{J} = \left[\frac{\partial \mathcal{F}^s}{\partial p}\right]^T \mathcal{M}^T \boldsymbol{R}^{-1}(\mathcal{M}\mathcal{F}^s x_0 - y_0)^T$$

$$\begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \frac{\partial f_3}{\partial x_1} & \frac{\partial f_3}{\partial x_2} & \frac{\partial f_3}{\partial x_3} & \cdots & \frac{\partial f_3}{\partial x_n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \frac{\partial f_n}{\partial x_3} & \cdots & \frac{\partial f_n}{\partial x_n} \end{bmatrix}$$

Atmospheric Chemical Transport Model: High-dimensional numerical model $\sim \mathbf{10^6} - \mathbf{10^7}$ states

Variational Data Assimilation





Gradient $\nabla\mathcal{J}(\boldsymbol{x}_0)$

of the distance function

find $x_{k+1} = x_k + \alpha_k \boldsymbol{d}_{Ck}$

Such that

$$\nabla\mathcal{J}(x^{n+1}(\boldsymbol{t}_0)) < \nabla\mathcal{J}(x^{n}(\boldsymbol{t}_0))$$

With $\boldsymbol{d}_k = \begin{cases} -\nabla\mathcal{J}(\boldsymbol{x}_k) \\ -[\text{Hess}(\mathcal{J}(\boldsymbol{x}_k))]^{-1}\nabla\mathcal{J}(\boldsymbol{x}_k) \\ -\nabla\mathcal{J}(\boldsymbol{x}_k) + \frac{\|\nabla\mathcal{J}(\boldsymbol{x}_k)\|^2}{\|\nabla\mathcal{J}(\boldsymbol{x}_{k-1})\|^2} \\ \ldots \end{cases}$

Gradient method

Quasi(Newton method)

Conjugate gradient

...

Repeat until $\mathcal{J}$ become smaller than treshold value

4DVar model example: the Lorenz 63 model

Intensity of convection

$$\frac{dx}{dt} = f_1(x, y) = \sigma(y - x)$$

Maximum temperature difference

$$\frac{dy}{dt} = f_2(x, y, z) = x(\rho - z) - y$$

$$\frac{dz}{dt} = f_3(x, y, z) = xy - \beta z$$

Stratification change due to convection

Similitudes with the non linear atmospheric system, simple in structure, rich in solution patterns

4DVar model example: the Lorenz 63 model

Prandtl number

$$\frac{dx}{dt} = f_1(x, y) = \sigma(y - x)$$

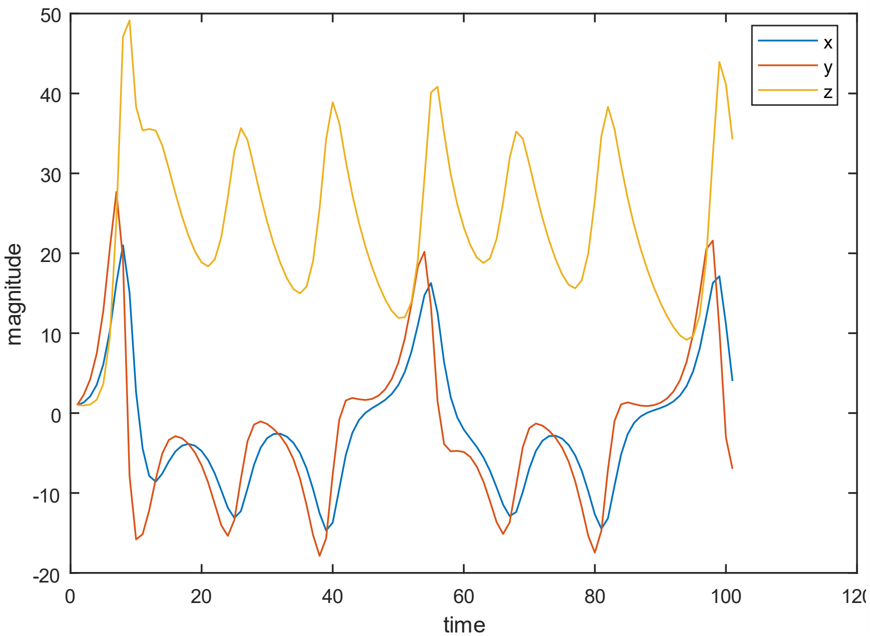
$$\frac{dy}{dt} = f_2(x, y, z) = x(\rho - z) - y$$

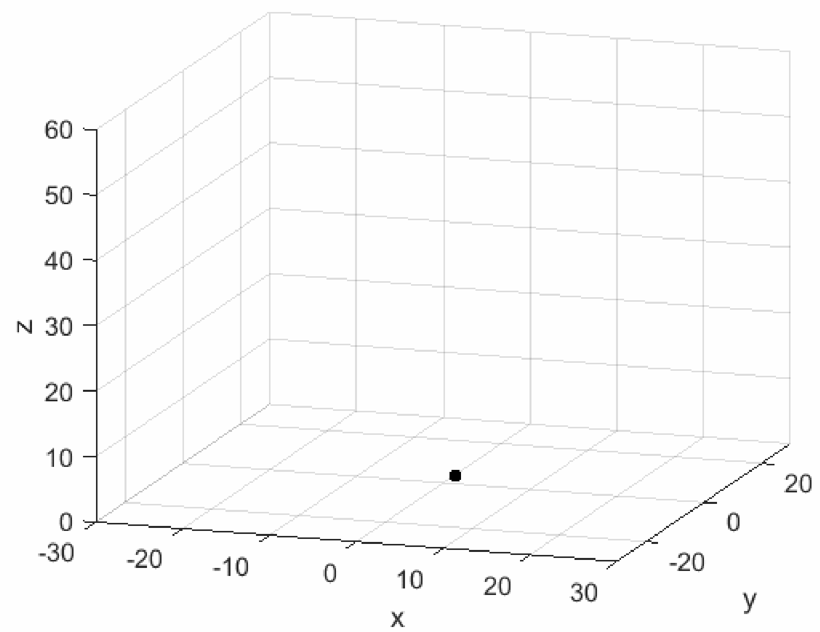
$$\frac{dz}{dt} = f_3(x, y, z) = xy - \beta z$$

Modified Rayleigh number

Aspect ratio

4DVar model example: the Lorenz 63 model





Deterministic, chaotic model in which the future evolution trajectory is uniquely determined by initial conditions

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(2002)  Data Assimilation Research Centre (http://www.met.reading.ac.uk/~darc/)
Original Fortran program by Marek Wlasak
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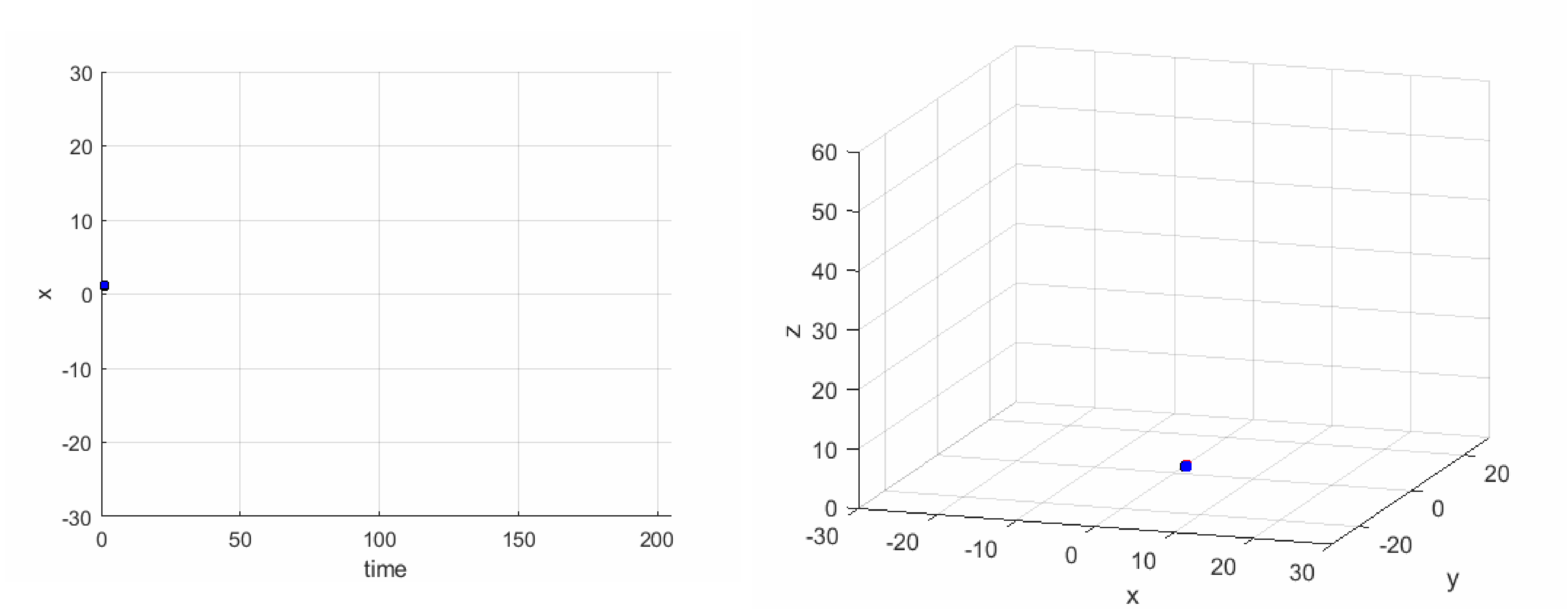
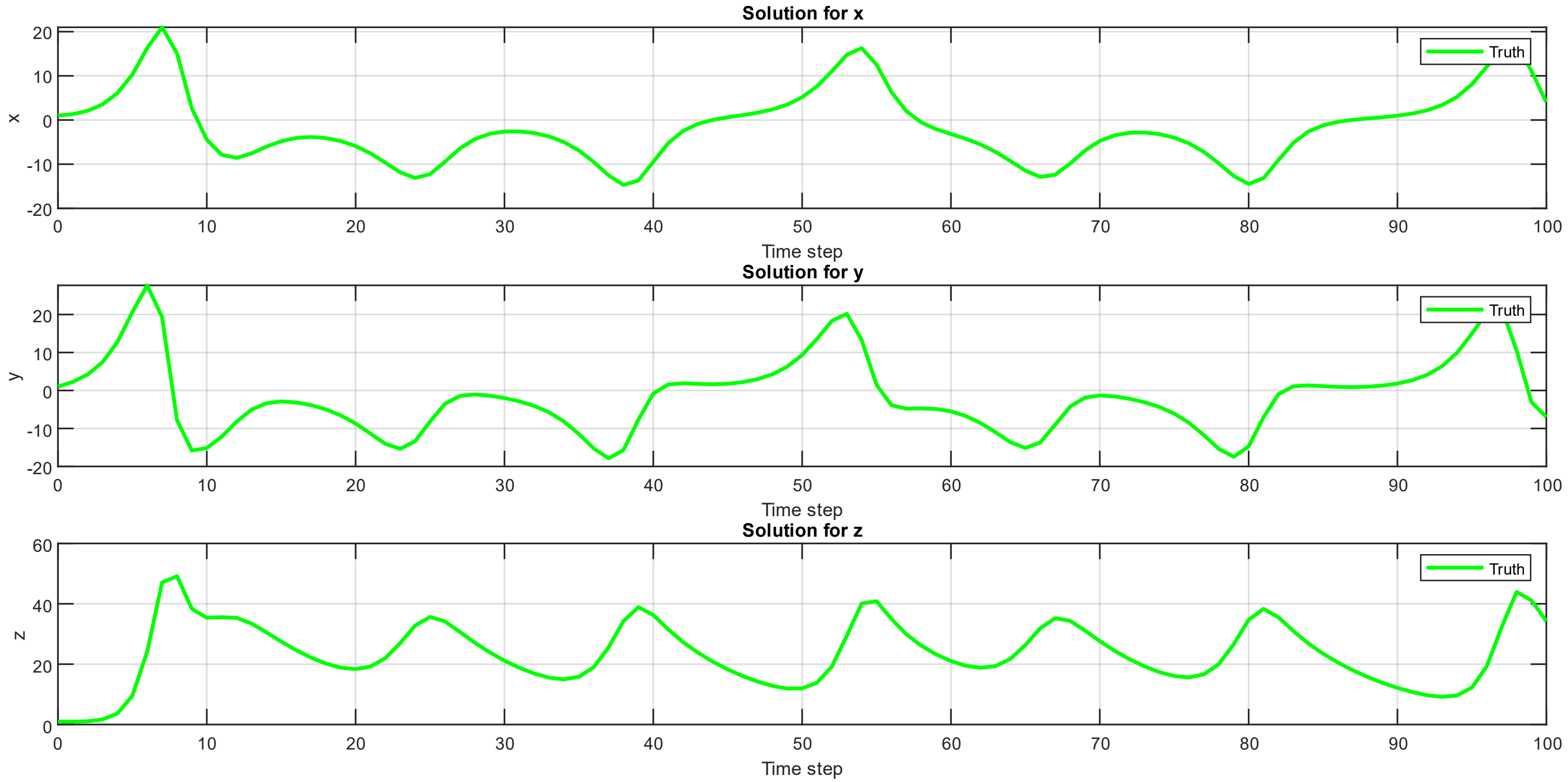
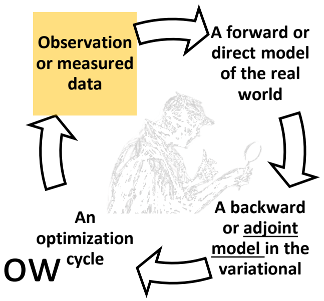
4DVar model example: the Lorenz 63 model



4DVar model example: the Lorenz 63 model



4DVar model example: the Lorenz 63 model

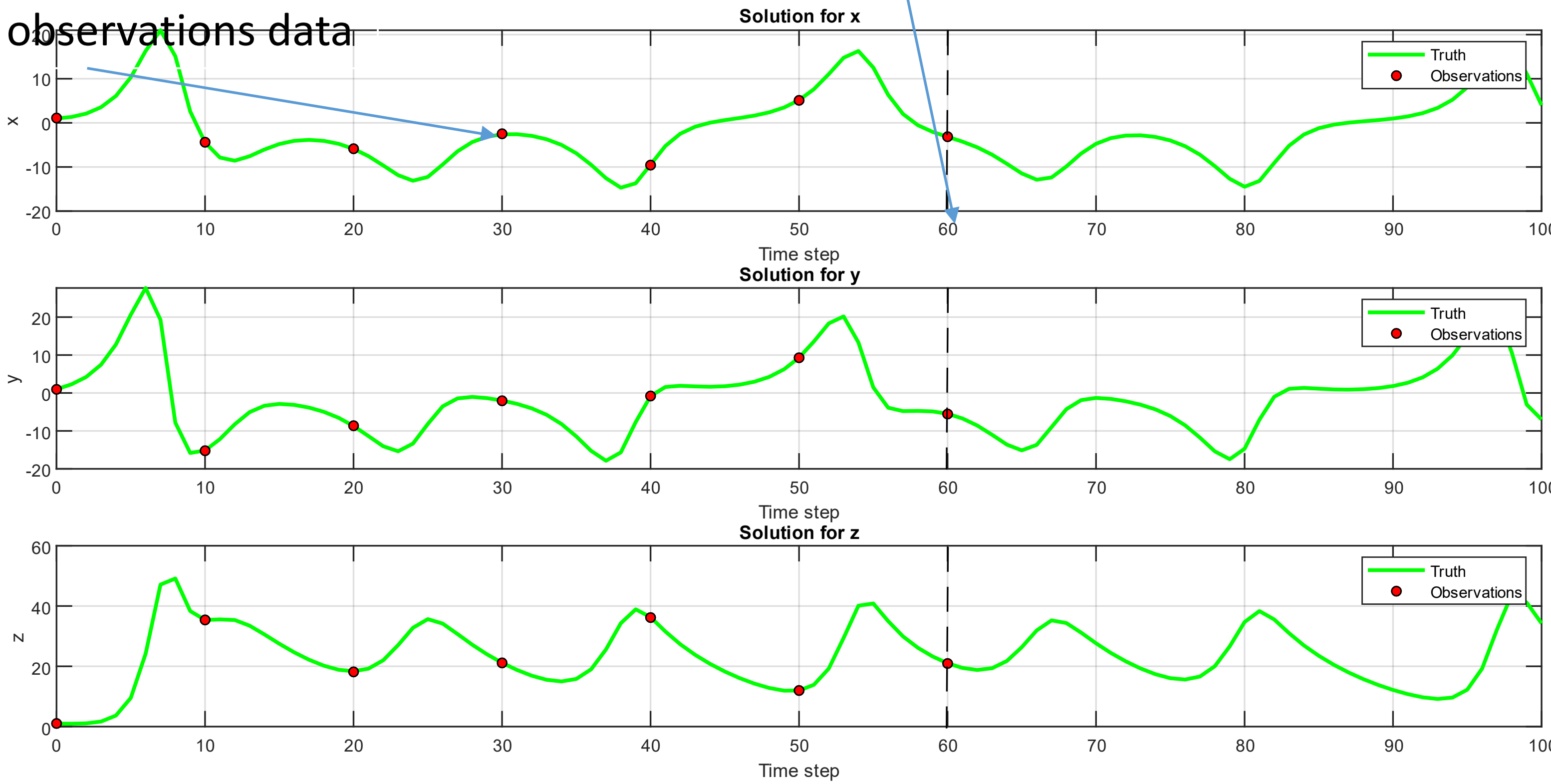


Analysis window

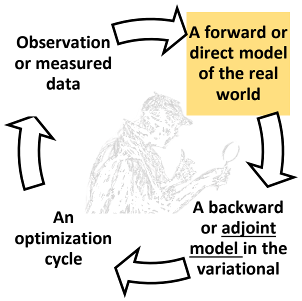
Analysis time

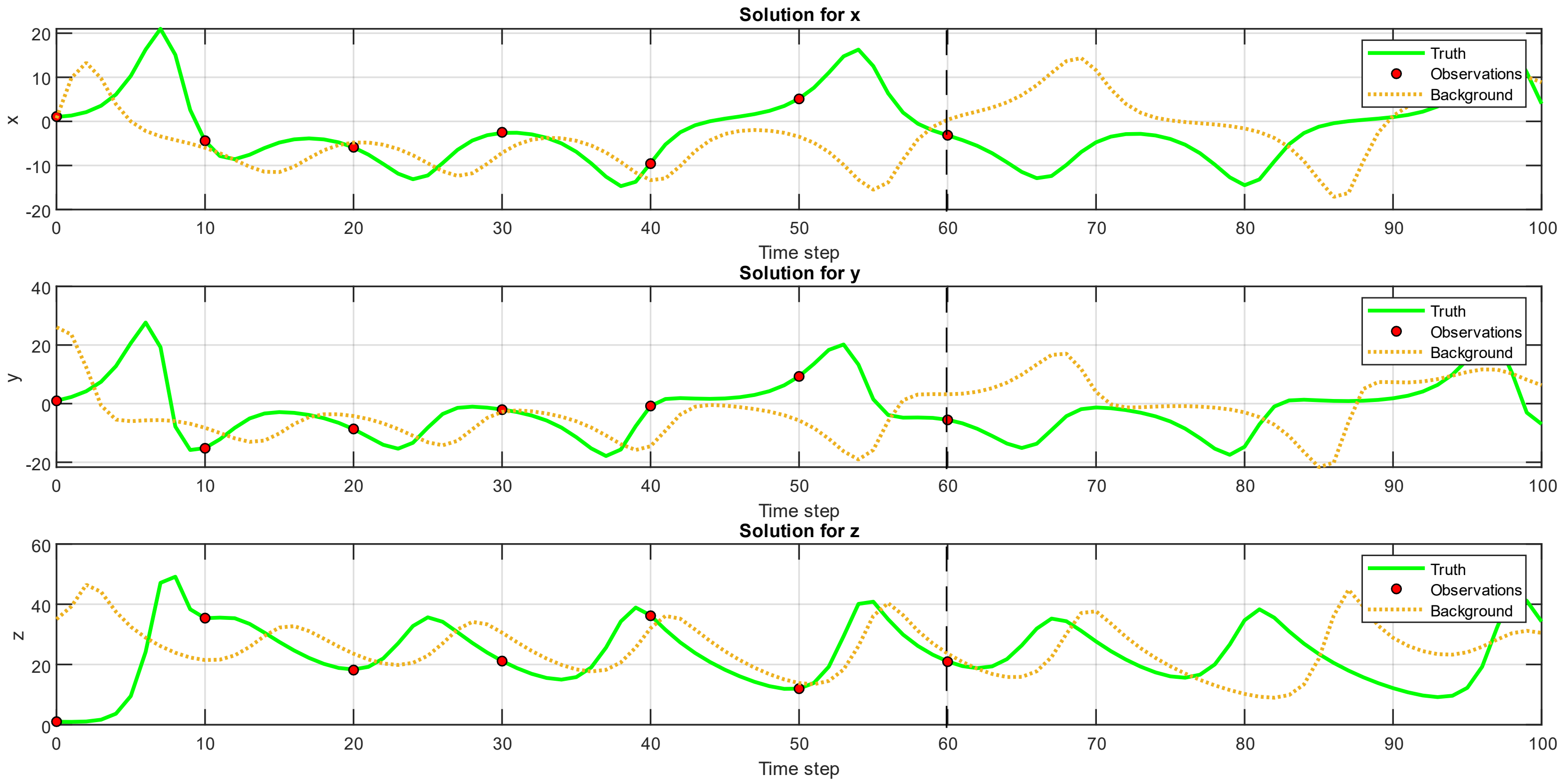
Forecast window

Synthetic observations data

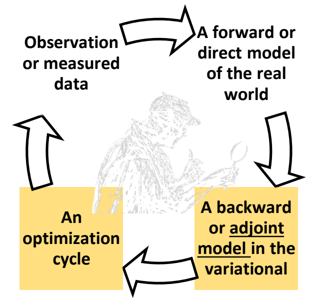


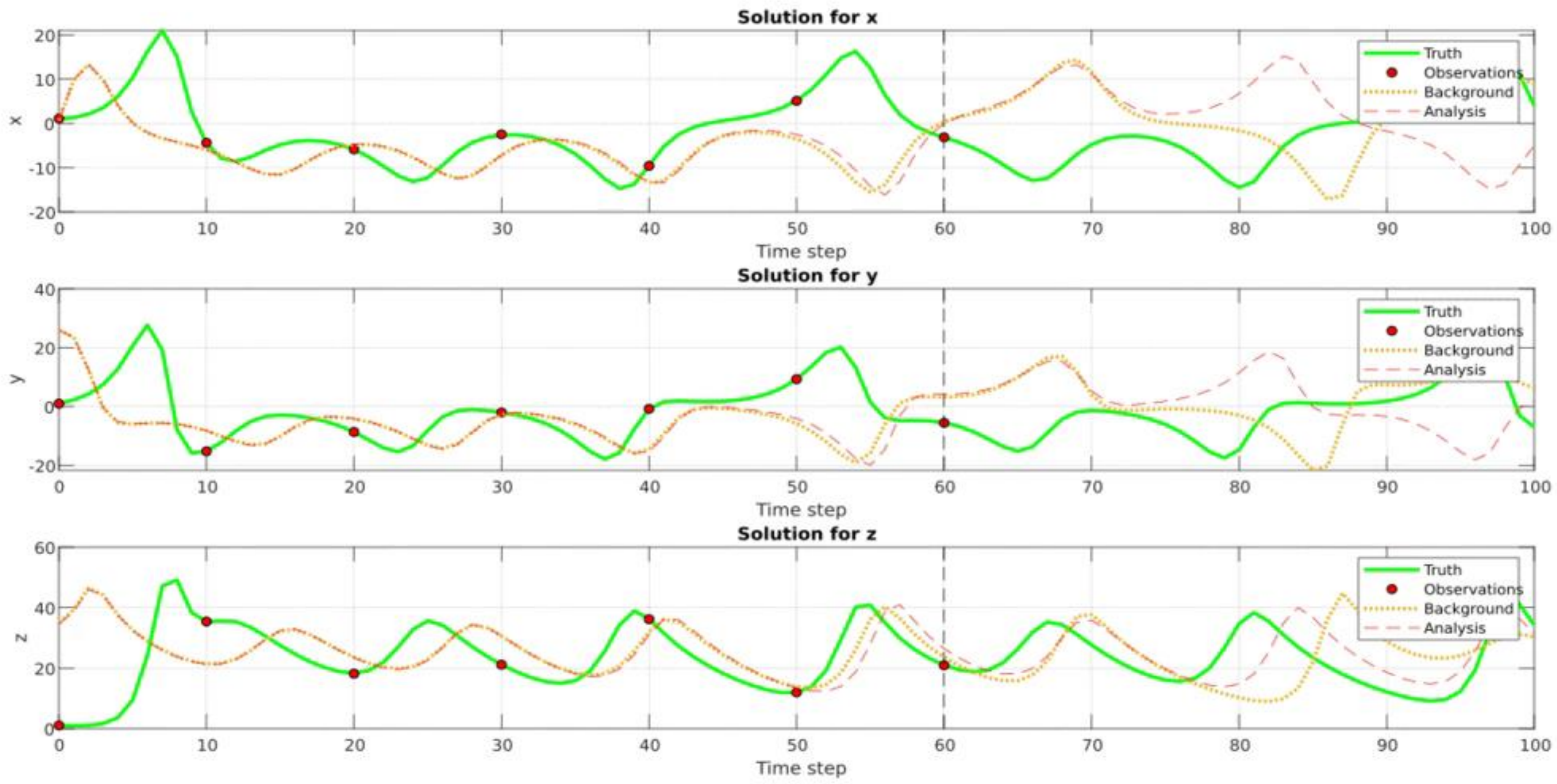
4DVar model example: the Lorenz 63 model



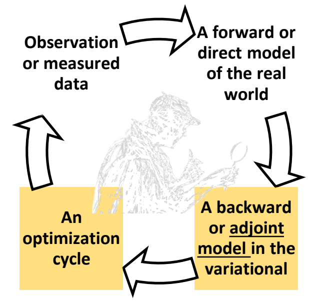


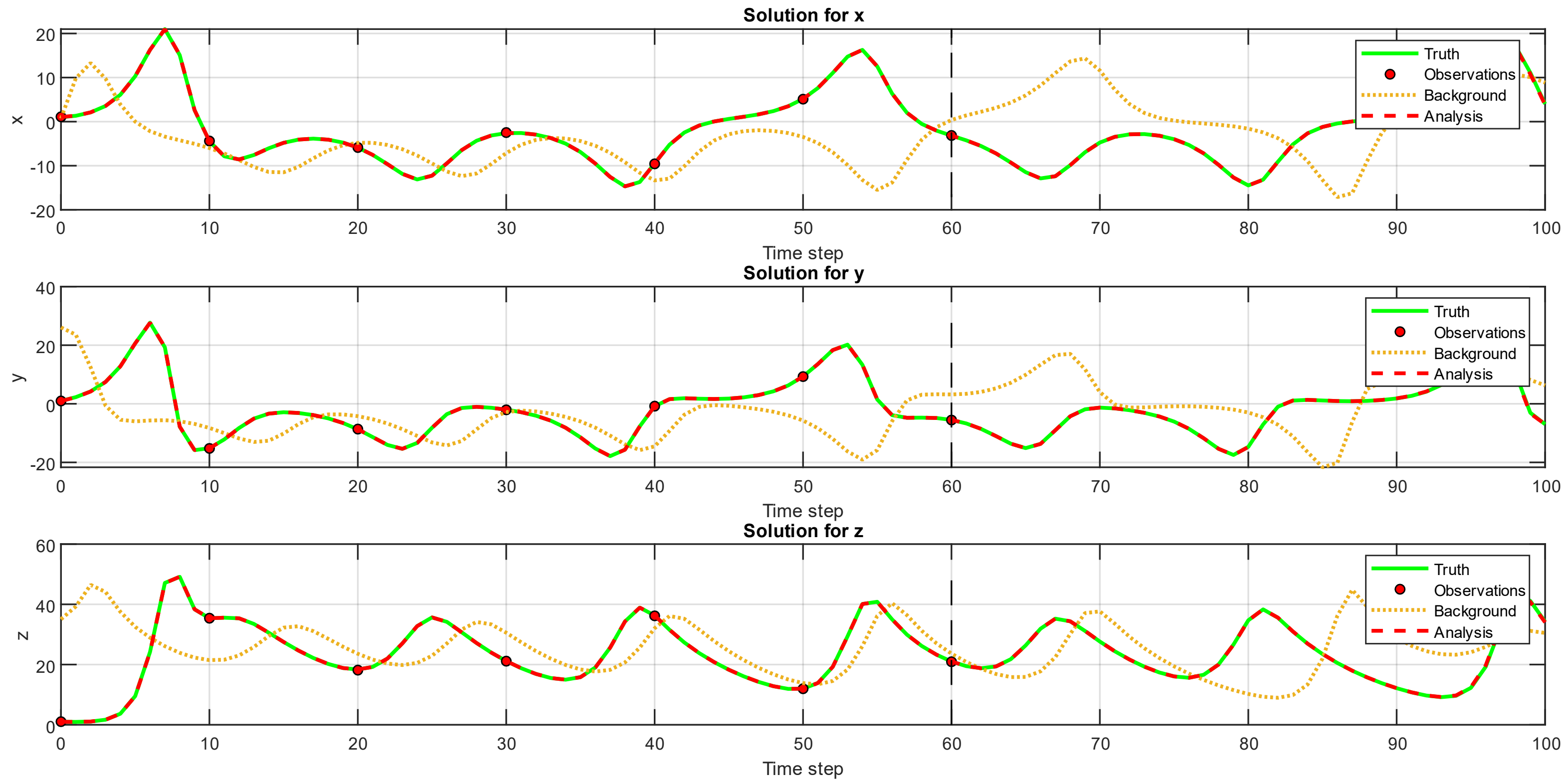
4DVar model example: the Lorenz 63 model





4DVar model example: the Lorenz 63 model





How to conciliate model with reality

$$\mathcal{J} = \frac{1}{2}\left[(\boldsymbol{x}_0 - \boldsymbol{x}_b)^T \boldsymbol{B}^{-1} (\boldsymbol{x}_0 - \boldsymbol{x}_b) + \sum_{i=0}^{s} (H(\boldsymbol{x}_i) - \boldsymbol{y}_i)^T \boldsymbol{R}^{-1} (H(\boldsymbol{x}_i) - \boldsymbol{y}_i)\right]$$

MODEL

ANALYSIS

OBSERVATIONS

How to conciliate model with reality

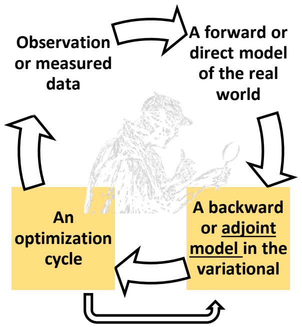
$$\mathcal{J} = \frac{1}{2}\left[(\boldsymbol{x}_0 - \boldsymbol{x}_b)^T \boldsymbol{B}^{-1}(\boldsymbol{x}_0 - \boldsymbol{x}_b) + \sum_{i=0}^{s}(H(\boldsymbol{x}_i) - \boldsymbol{y}_i)^T \boldsymbol{R}^{-1}(H(\boldsymbol{x}_i) - \boldsymbol{y}_i)\right]$$

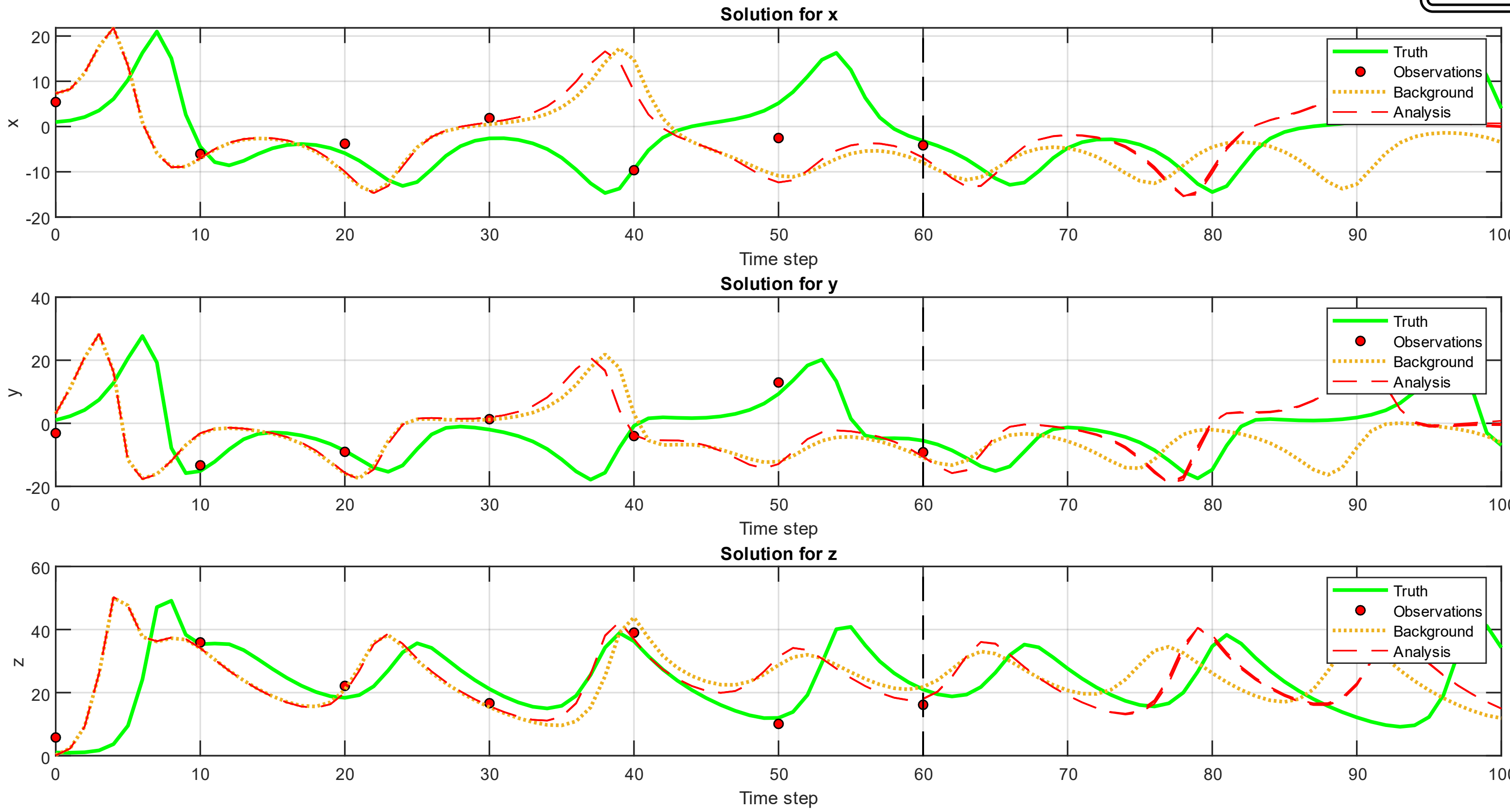
MODEL

ANALYSIS

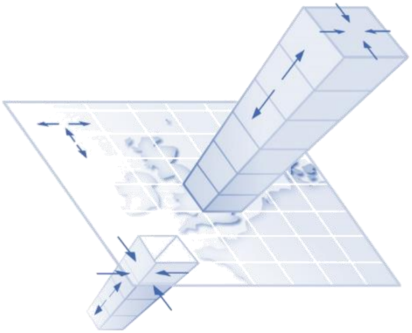
OBSERVATIONS

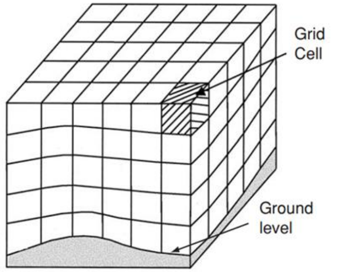
Adjoint approach toy model example: the Lorenz 63 model





Current and future work





Chemical Transport Model (CTM)

LOTOS EUROS

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

Change in concentration with time

Grid resolved transport (Advection)

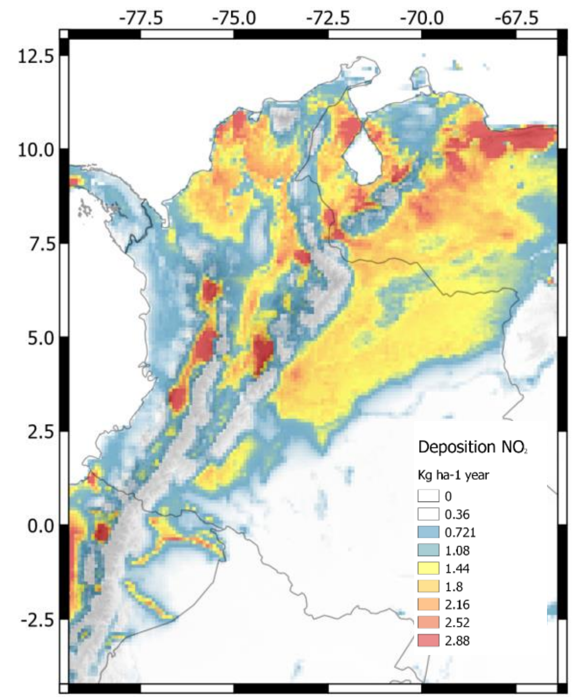
Diffusion process

Entrainment and detrainment

Generation/Consumption chemical reactions

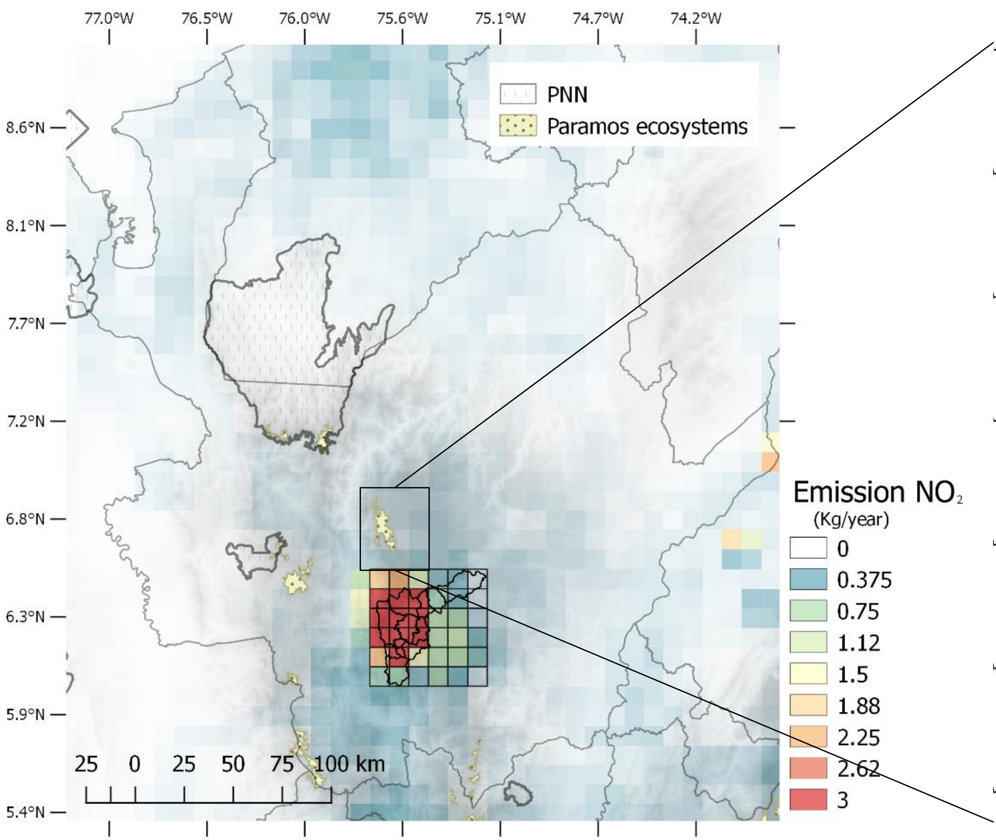
Emissions

Dry and wet deposition proccess

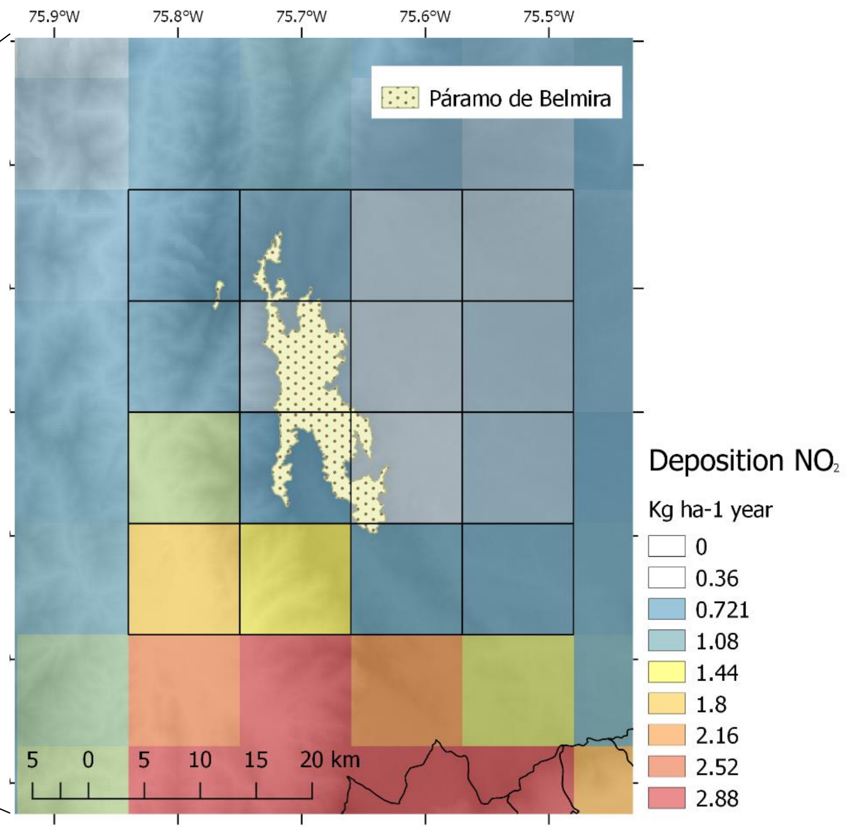


NO_2 Dry deposition new land use

Current and future work



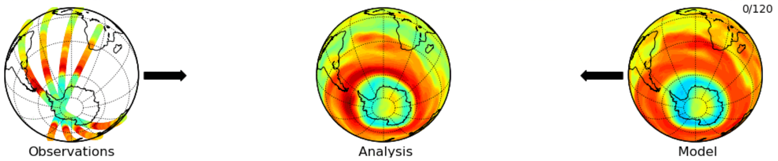
CAUSES

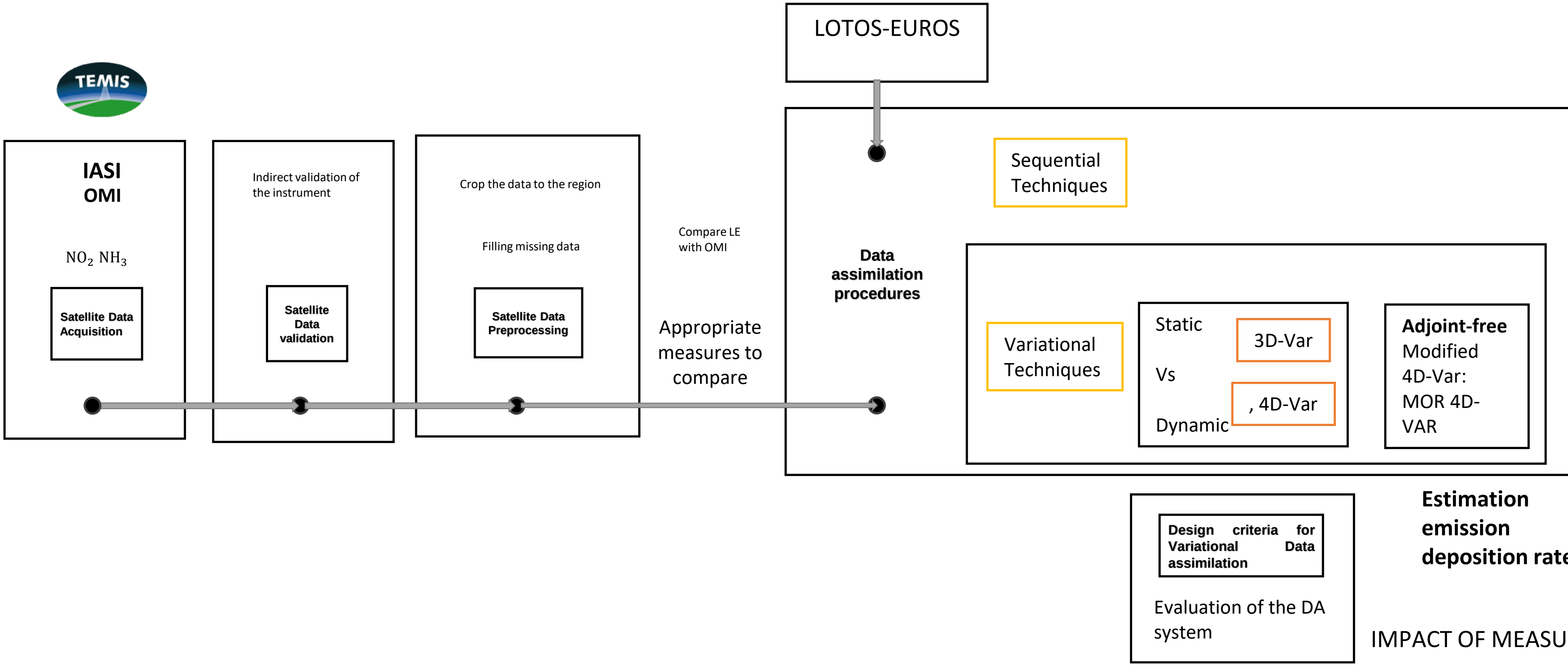


EFFECTS

Current and future work

Operational schematic Variational Approach system for satellite data assimilation





Lu S. et al. (2017).

Estimation emission deposition rates

IMPACT OF MEASURES

Baier F. et al. (2013).

Modified standard 4D-Var methods and future work

Model Order Reduction MOR-4D-Var

Adjoint free perpectives to address the disadvantage of not having an adjoint for a model such the LOTOS-EUROS

Ensemble 4D-Var

Fu S. et al. (2016).

References

Asch M. et al. (2016). Data Assimilation methods, algorithms and applications.SIAM. Society for Industrial and Applied Mathematics Philadelphia. ISBN: 9781611974546.

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