Data Assimilation

1 March 2023

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CONTENT

- Uncertainty quantification, backward error analysis and propagation of errors in data-driven models

- Data Assimilation for uncertainty minimization and data learning for effectively merging heterogeneous data

What is AI?

Artificial Intelligence (AI), the ability of a digital computer or computer-controlled robot to perform tasks commonly associated with intelligent beings.

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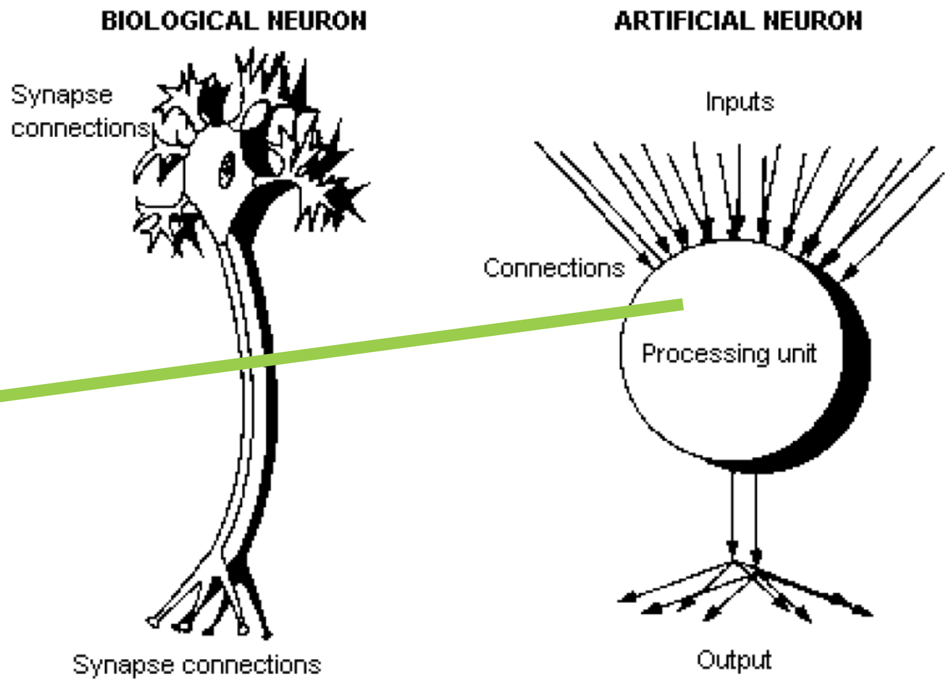
ARTIFICIAL NEURAL NETWORK



What is AI?

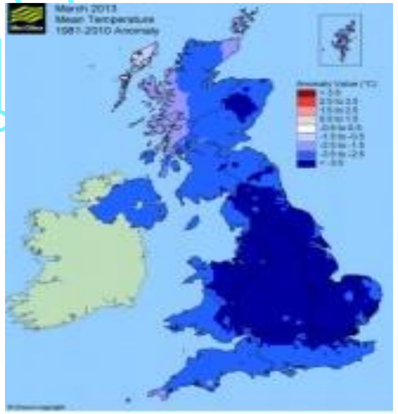
Artificial Intelligence (AI), the ability of a digital computer or computer-controlled robot to perform tasks commonly associated with intelligent beings.

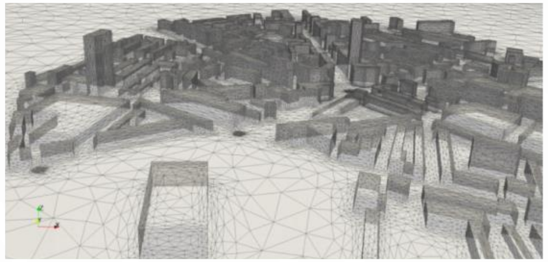
DATA

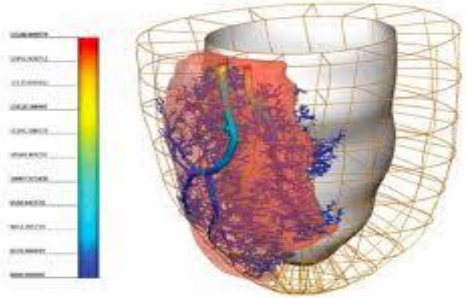
SYNONYMS
facts, figures, statistics, details, particulars, specifics, features
information, evidence, intelligence, material, background, input
proof, fuel, ammunition
statement, report, return, dossier, file, documentation, archive, archives

… the era of the data!

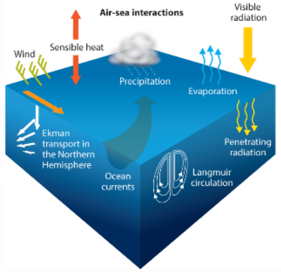
High resolution Models…

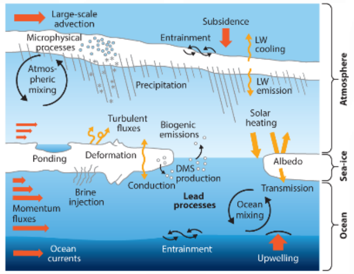


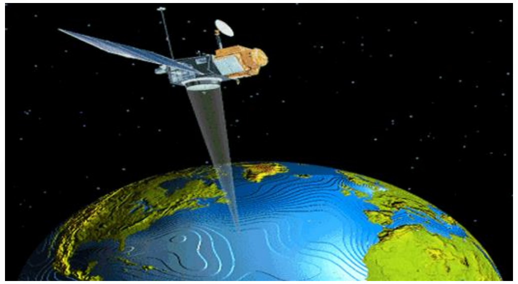


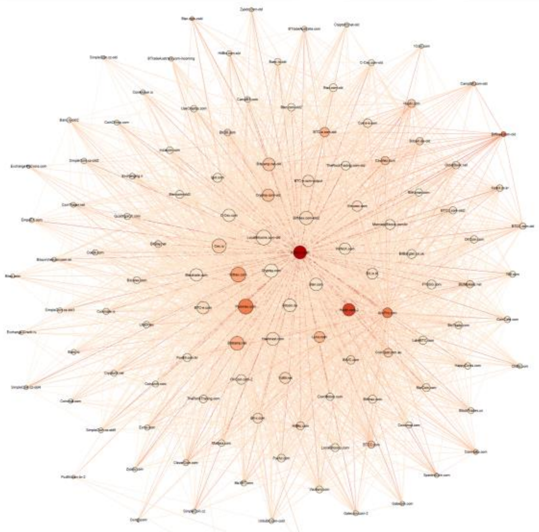


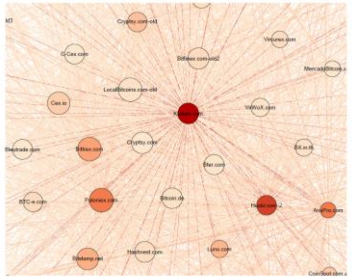
Real observations…

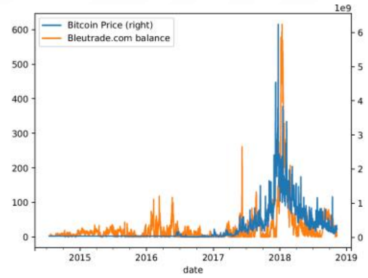












TYPE OF DATA ANALYSIS

Descriptive analytics	: What happened?
Diagnostic analytics	: Why did it happen?
Predictive analytics	: What is likely to happen in the future?
Prescriptive analytics	: What is the best course of action to take?

SOME EFFECTS OF THE ERRORS

Input data
(initial conditions)

M(P):

$$\begin{cases} L(u(t))=f \\ u(t_0)=u_0 \end{cases}$$

Solution
(forecast)

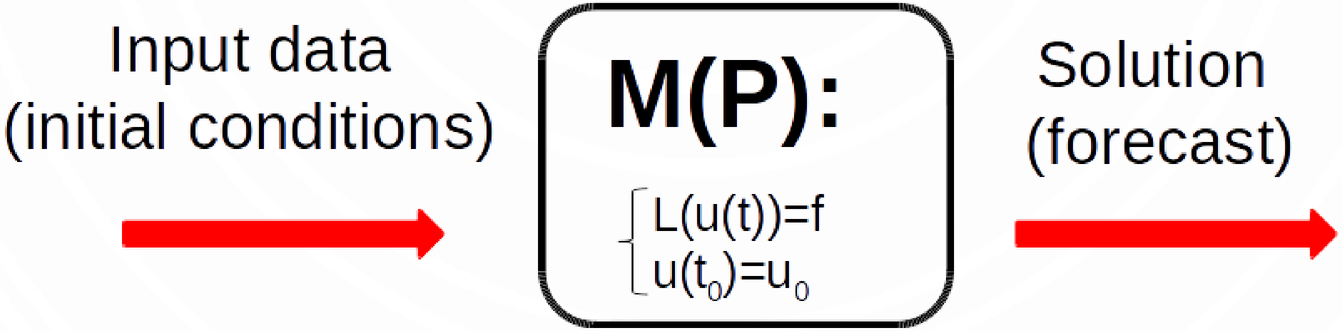
The numerical solution (the prediction of the system) is affected by errors:

- Simplifications of the model
- Discretization of the model
- Implementation by finite precision computations

- Model's approximation errors
- Discretization erros
- Round-off errors

errors on data

SOME EFFECTS OF THE ERRORS

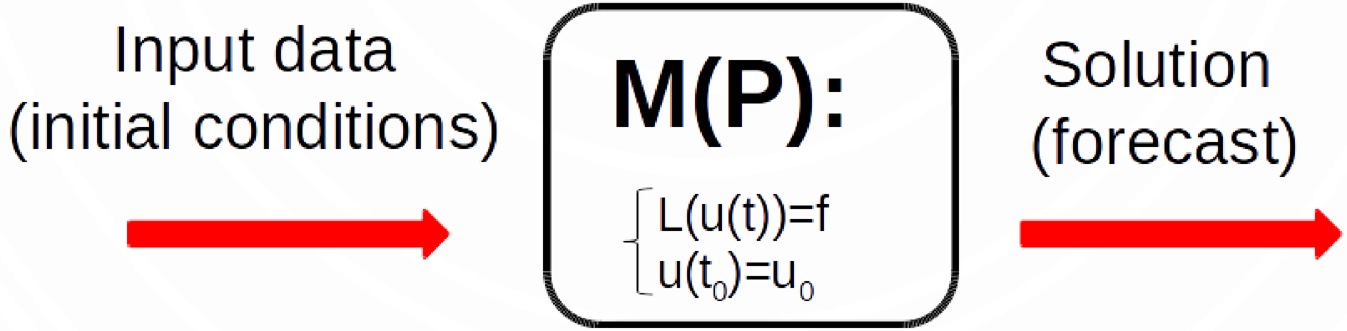


The numerical solution (the prediction of the system) is affected by errors:

$$\text{(absolute error)} = \text{(approximate value)} - \text{(true value)}$$

$$\text{(relative error)} = \frac{\text{(absolute error)}}{\text{(true value)}} = \frac{\text{(approximate value)}}{\text{(true value)}} - 1$$

SOME EFFECTS OF THE ERRORS



The numerical solution (the prediction of the system) is affected by errors:

Fundamental difficulty with measuring error: for many problems we cannot compute the exact answer, we can only approximate it!

Often, the best we can do is *estimate* the error!

SOME EFFECTS OF THE ERRORS

backward error analysis:

Input data
(initial conditions)

M(P):

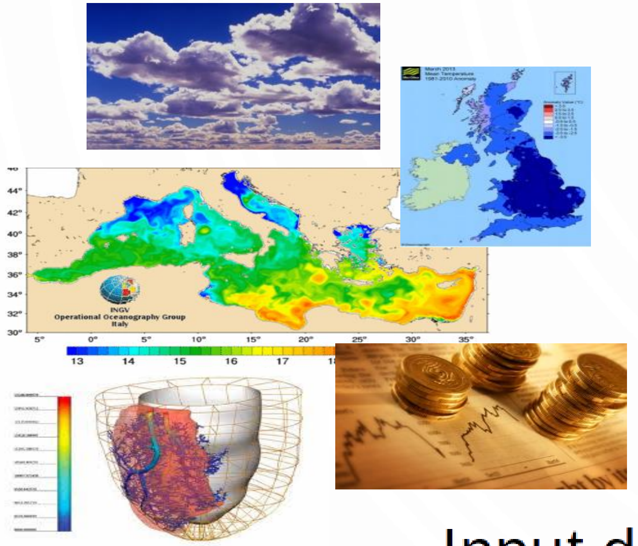
$$\begin{cases} L(u(t))=f \\ u(t_0)=u_0 \end{cases}$$

Solution
(forecast)

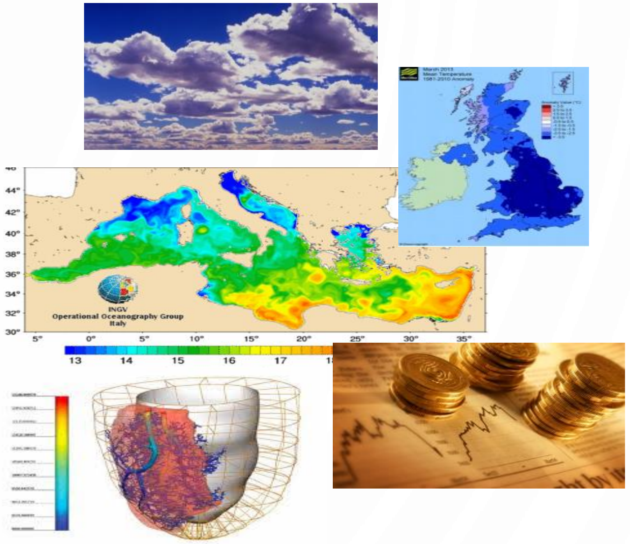
any perturbation on the data (**δ**) propagates on the solution (**σ**) by an amplification factor given by **c** = a parameter that depends on the algorithm and **μ** = the Condition number of the problem

Error on the solution: $\sigma=\mu c \delta$

data at t=0 (initial condition)



data at t=t+k



Input data
(initial conditions)

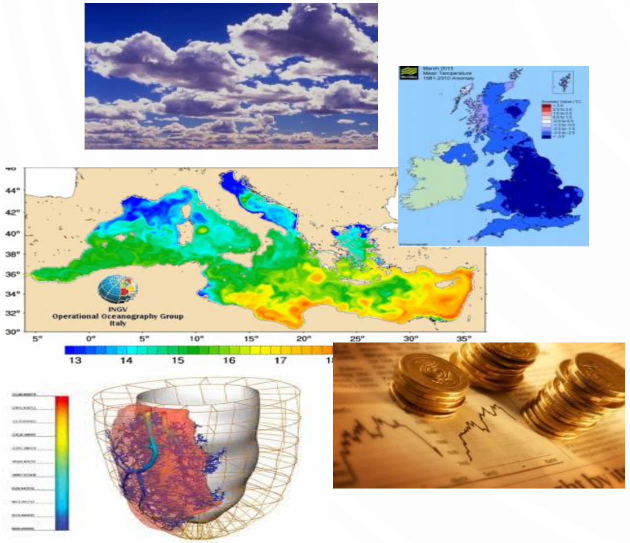
M(P):

$$\begin{cases} L(u(t))=f \\ u(t_0)=u_0 \end{cases}$$

Solution
(forecast)

EXTRA DATA

data (initial condition)



observed data

INVERSE ILL POSED PROBLEM

A NON LINEAR PROBLEM

A BIG DATA PROBLEM

A DATA FILTERING PROBLEM

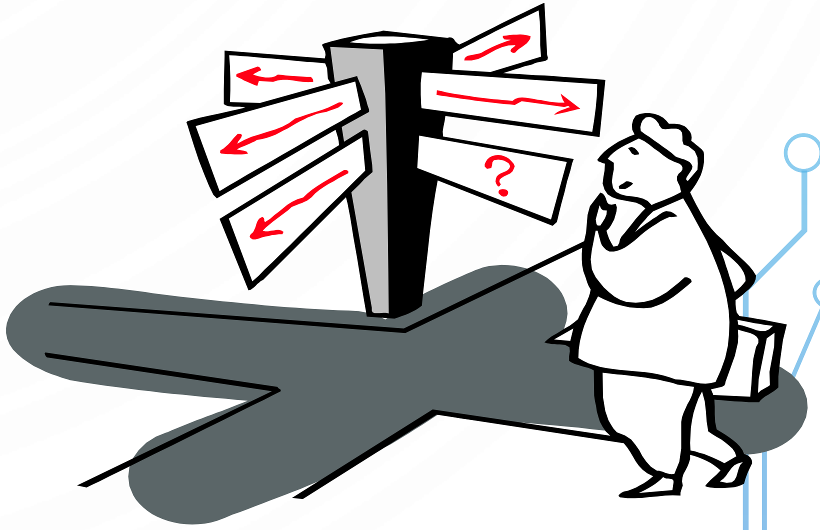
Data Assimilation: try to google it!

AN UNCERTAINTY QUANTIFICATION PROBLEM

A LARGE SIZE COMPUTATIONAL PROBLEM

A COMPUTATIONAL INTENSIVE PROBLEM

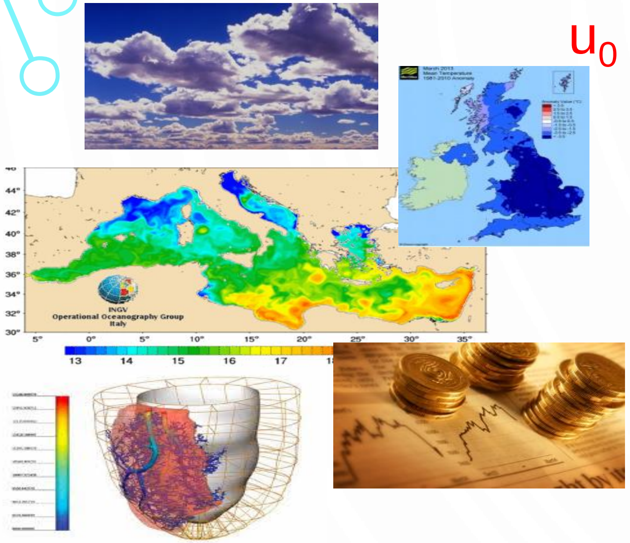
everyone faces it from a point of view…
what is ours?



https://www.youtube.com/watch?v=JUB6__x6-d4

MERGE THE DATA

data (initial condition)



u_0

observed data

y_0

D.A.

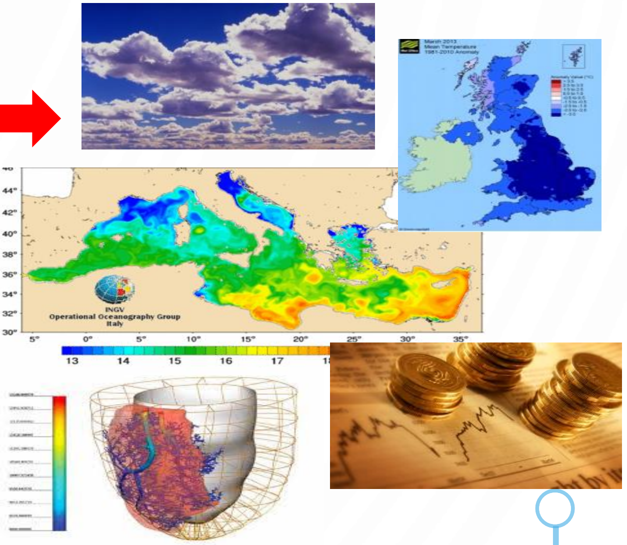
u_0

M(P):

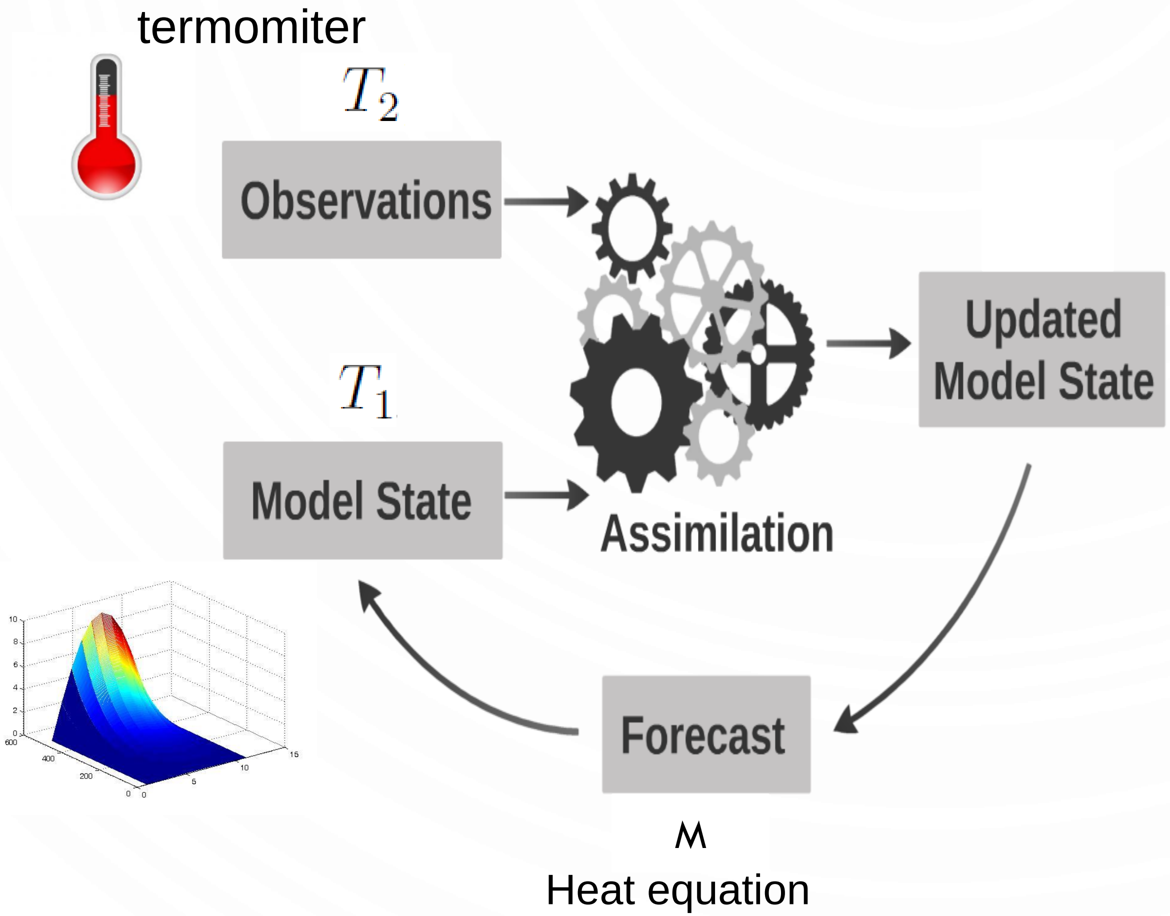
$$\begin{cases} L(u(t)) = f \\ u(t_0) = u_0 \end{cases}$$

$u(t),\ t > t_0$

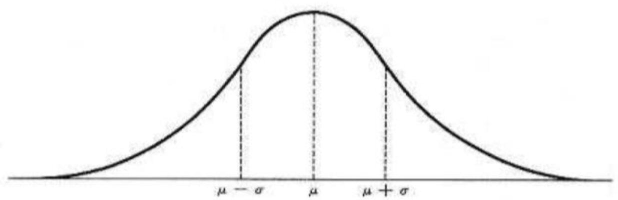
forecast



Data Assimilation: example…



Data Assimilation: example…



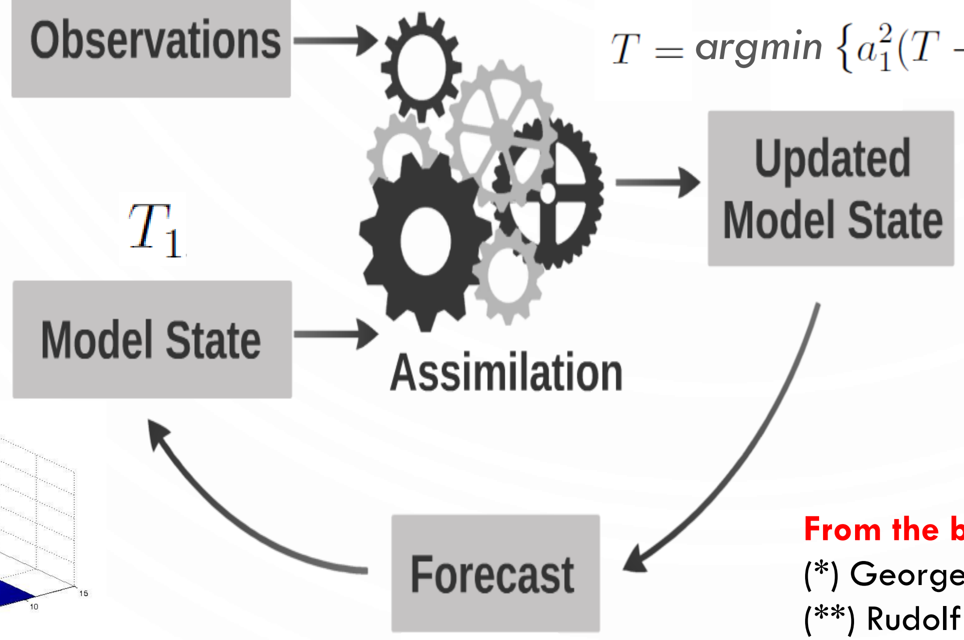
Background and observation
error covariance assumed to be Gaussian (*,**)

$$a_1 = \frac{1}{\sigma_1} \qquad a_2 = \frac{1}{\sigma_2}$$

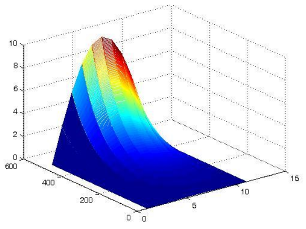
$$T = argmin \left\{ a_1^2 (T - T_1)^2 + a_2^2 (T - T_2)^2 \right\}$$

termomiter

T_2



T_1



M

Heat equation

From the beginning…

(*) George P. Cressman (1959) Cressman analysis

(**) Rudolf Emil Kalman (1960) A new approach to linear filtering and prediction problems - J.Basic Emg. vol.82D, pp.35-45

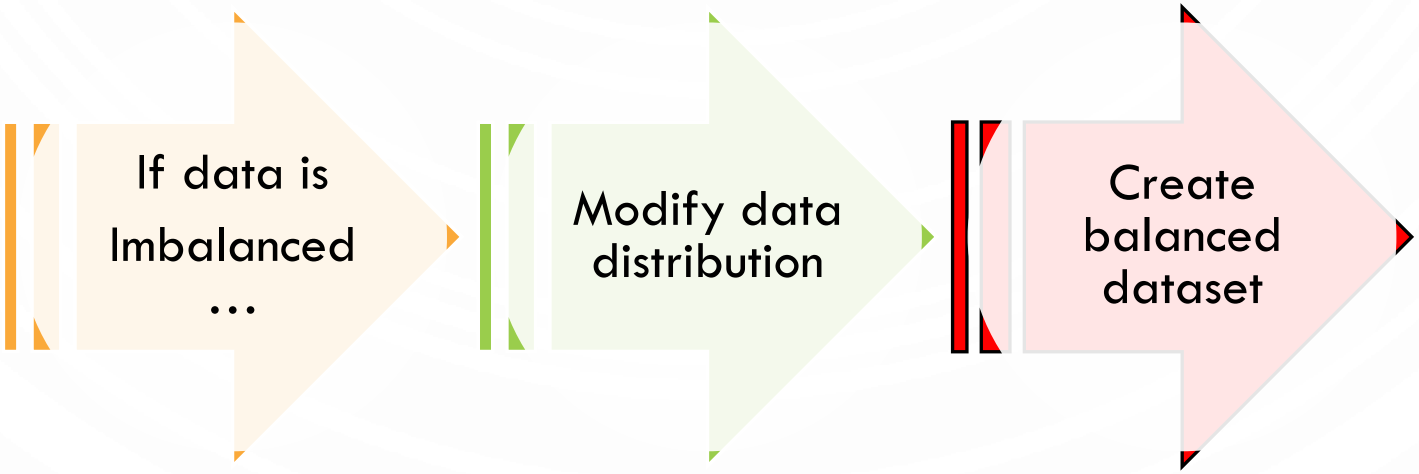
Intrinsic and *extrinsic* imbalance

Intrinsic:

- Imbalance due to the nature of the dataspace

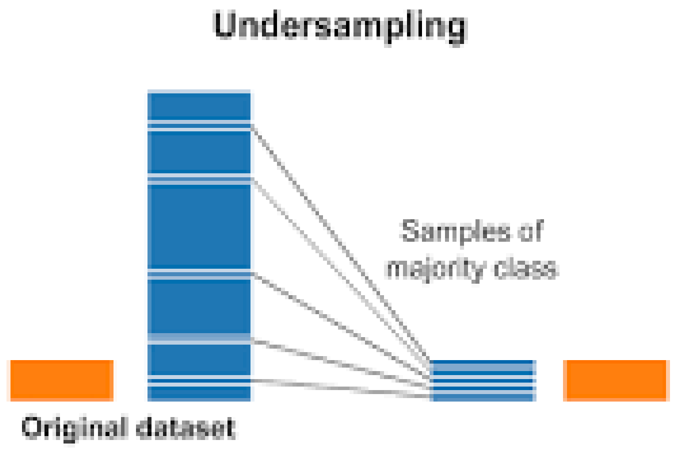
Extrinsic:

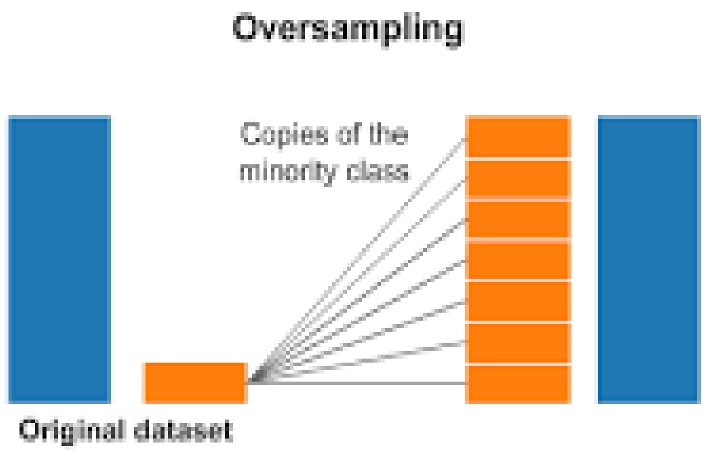
- Imbalance due to time, storage, and other factors



Create balance though sampling

Undersampling and Oversampling





Loss of important information

Possible overfitting

Undersampling and Oversampling

Unsupervised (undersampling):
use random subsets of the majority class to create balance and form multiple classifiers

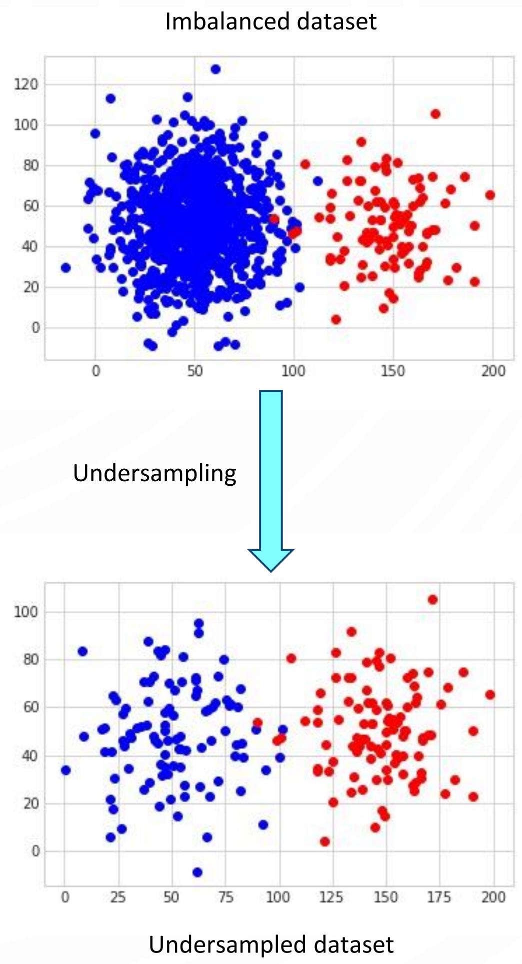
Supervised (undersampling or oversampling):
iteratively (or not) create balance and pull out (or in) redundant (novel) samples in majority (minority) class to form a final classifier

Trying to reduce the error!!!

CORRECTING FOR IMBALANCED DATASETS

Undersampling the majority class

The idea here is to create a new dataset to train our algorithm that is not imbalanced. This is typically achieved by creating a new dataset where we undersample (pick with a lower probability) data points that belong to the majority class.



1. We keep all samples from the minority class. Let N be their number.

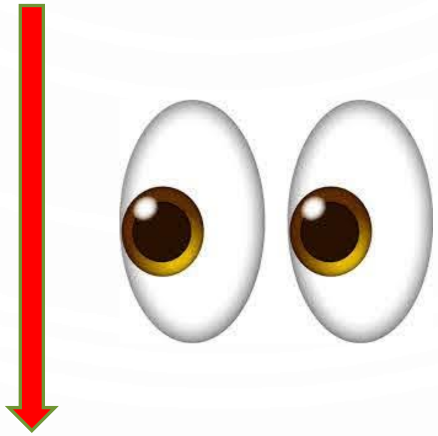
2. We draw ("sample") uniformly at random N data points from the majority class.

3. We use the new dataset, containing 2N data points (N for each class), to fit our model.

Undersampling and Oversampling

Unsupervised (undersampling):
use random subsets of the majority class to create balance and form multiple classifiers

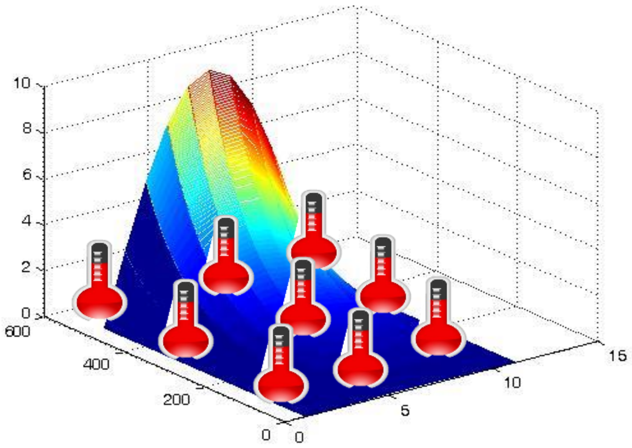
Supervised (undersampling or oversampling):
iteratively (or not) create balance and pull out (or in) redundant (novel) samples in majority (minority) class to form a final classifier

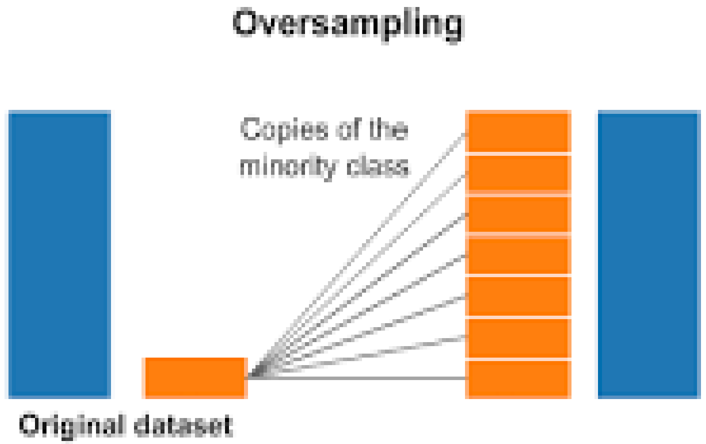


Trying to reduce the error!!!

Oversampling

thermometer

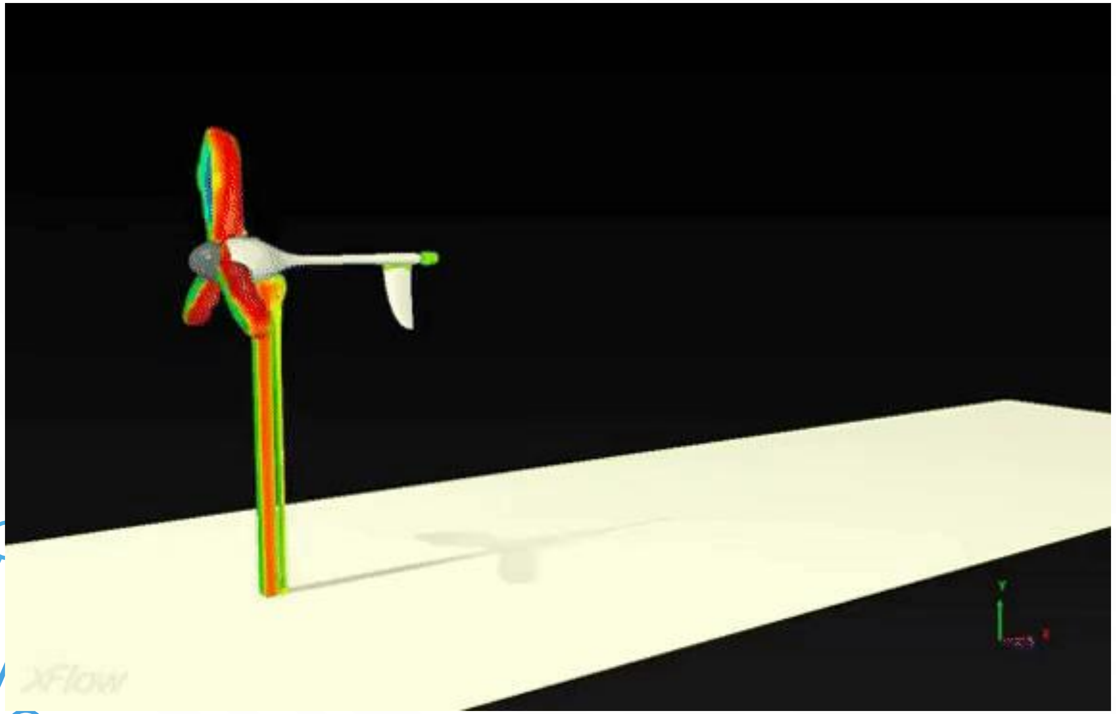




Computational model

observations

When working with Numerical Models…



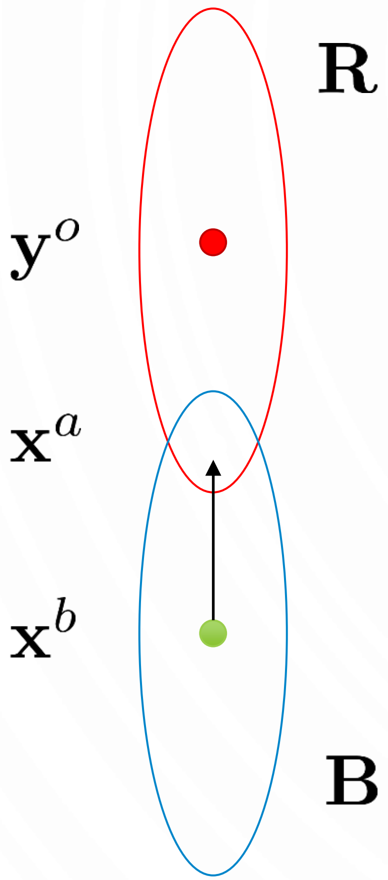
- Finite precision introduces error
- Does not capture randomness of real situations
- Very sensitive to initial conditions

What is Data Assimilation

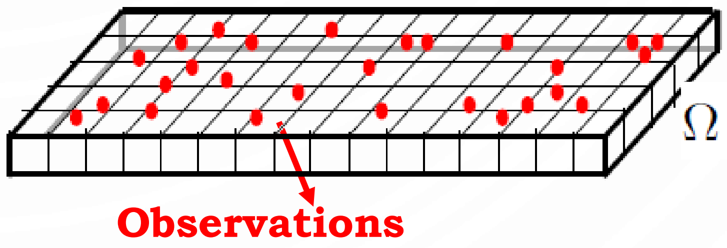
Data assimilation is a technique where observational data is incorporated

with the output of a numerical model or simulation to produce an optimal

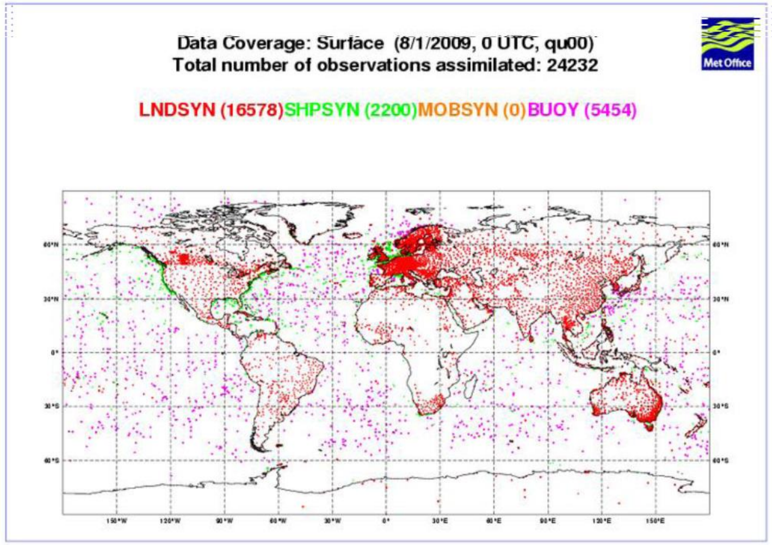
state of an evolving dynamic system



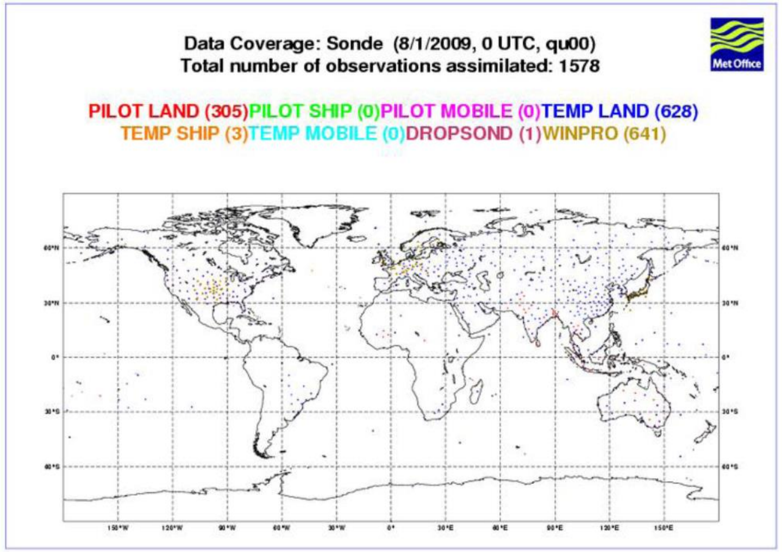
Given a set of observations, $\boldsymbol{y}^o$ with known error $\boldsymbol{R}$, correct the background state or model output $\boldsymbol{x}^b$ with known error $\boldsymbol{B}$, to output an analysis, $\boldsymbol{x}^a$



Observations: why not just use these data?



Surface



Radiosonde

The data are not "dense" enough and the math problem to compute the solution "everywhere" is an

ill posed inverse problem

The Tikhonov-regularized formulation

MODEL EQUATIONS

<u>Full Model</u>

$$\mathbf{x}_{k+1} = \boldsymbol{\mathcal{M}}_{k+1}\mathbf{x}_k$$

$\boldsymbol{\mathcal{M}}_k$ = Model Operator at time k

$$\mathbf{y}_k^o = \boldsymbol{\mathcal{H}}_k\mathbf{x}_k + \boldsymbol{\epsilon}_k^o$$

$\boldsymbol{\mathcal{H}}_k$ = Observation Operator at time k

<u>Tangent Linear Model</u>

$$\mathbf{x}_{k+1} = \mathbf{M}_{k+1}\mathbf{x}_k$$

$\boldsymbol{M}_{k+1}$ = Linearized $\dfrac{\delta\mathbf{x}_{k+1}}{\delta\mathbf{x}_k}$

$$\mathbf{y}_k^o = \mathbf{H}_k\mathbf{x}_k + \boldsymbol{\epsilon}_k^o$$

$\boldsymbol{H}_{k+1}$ = Linearized $\dfrac{\delta\mathbf{y}_k^o}{\delta\mathbf{x}_k}$

The Tikhonov-regularized formulation

FULL FIELD COST FUNCTION (TIKHONOV REGULARISATION)

$$J(\mathbf{x}) = \frac{1}{2}\left(\mathbf{x}-\mathbf{x}^b\right)^T \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}^b\right) + \frac{1}{2}\left(\mathcal{H}\mathbf{x}-\mathbf{y}^o\right)^T \mathbf{R}^{-1}\left(\mathcal{H}\mathbf{x}-\mathbf{y}^o\right)$$

$$\nabla J(\mathbf{x}) = \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}^b\right) - \mathbf{H}^T\mathbf{R}^{-1}\left(\mathbf{y}^o-\mathbf{H}\mathbf{x}\right) = \cancel{0}$$

Use L-BFGS Method to Iteratively Solve

$\boldsymbol{B}$ = Background Error covariance matrix

$\boldsymbol{R}$ = Observation Error covariance matrix

- Difficult to minimise directly
- Multiple local minima

The Tikhonov-regularized formulation – 4D

FULL FIELD COST FUNCTION (TIKHONOV REGULARISATION)

$$diag\left[\mathbf{H}_0, \mathbf{H}_1\mathbf{M}_{0,1}, \ldots, \mathbf{H}_{N-1}\mathbf{M}_{N-2,N-1}\right]$$

$$J(\mathbf{x}) = \frac{1}{2}\left(\mathbf{x}-\mathbf{x}^b\right)^T\mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}^b\right) + \frac{1}{2}\left(\mathcal{G}\mathbf{x}-\mathbf{y}^o\right)^T\mathbf{R}^{-1}\left(\mathcal{G}\mathbf{x}-\mathbf{y}^o\right)$$

From the Tikhonov-regularized formulation

NOT considering the temporal variable

$$min\left\{\|\mathbf{Hu}-\mathbf{v}\|^2_{\mathbf{R}}+\|\mathbf{u}-\mathbf{u}_0\|^2_{\mathbf{B}}\right\}$$

Variational approach

$$J(u)=\|\mathbf{Hu}-\mathbf{v}\|^2_{\mathbf{R}}+\|\mathbf{u}-\mathbf{u}_0\|^2_{\mathbf{B}}$$

$$u^{DA}=min_u\left\{J(u)\right\}$$

3DVariational

$$J(u)=(\mathbf{Hu}-\mathbf{v})^T\mathbf{R}^{-1}(\mathbf{Hu}-\mathbf{v})+(\mathbf{u}-\mathbf{u}_0)^T\mathbf{B}^{-1}(\mathbf{u}-\mathbf{u}_0)$$

Normal equations

$$S=\|\mathbf{Hu}-\mathbf{v}\|^2_{\mathbf{R}}+\|\mathbf{u}-\mathbf{u}_0\|^2_{\mathbf{B}}$$

$$\frac{\partial S}{\partial u}=0$$

Kalman Filter, Optimal Interpolation

$$\mathbf{u}^{DA}=\mathbf{u}_0+\mathbf{K}(\mathbf{Hu}-\mathbf{v})$$

$$\mathbf{K}=\mathbf{RH}^T(\mathbf{H}^T\mathbf{RH}+\mathbf{B})^{-1}$$

considering the temporal variable

$$min\left\{\|\mathbf{Gu}-\mathbf{v}\|^2_{\mathbf{R}}+\|\mathbf{u}-\mathbf{u}_0\|^2_{\mathbf{B}}\right\}$$

Variational approach

$$J(u)=\|\mathbf{Gu}-\mathbf{v}\|^2_{\mathbf{R}}+\|\mathbf{u}-\mathbf{u}_0\|^2_{\mathbf{B}}$$

$$u^{DA}=min_u\left\{J(u)\right\}$$

4DVariational

$$J(u)=(\mathbf{Gu}-\mathbf{v})^T\mathbf{R}^{-1}(\mathbf{Gu}-\mathbf{v})+(\mathbf{u}-\mathbf{u}_0)^T\mathbf{B}^{-1}(\mathbf{u}-\mathbf{u}_0)$$

Normal equations

$$S=\|\mathbf{Gu}-\mathbf{v}\|^2_{\mathbf{R}}+\|\mathbf{u}-\mathbf{u}_0\|^2_{\mathbf{B}}$$

$$\frac{\partial S}{\partial u}=0$$

Ensemble/Extended Kalman Filter

$$\mathbf{u}^{DA}=\mathbf{u}_0+\mathbf{K}(\mathbf{Gu}-\mathbf{v})$$

$$\mathbf{K}=\mathbf{RG}^T(\mathbf{G}^T\mathbf{RG}+\mathbf{B})^{-1}$$

Data Assimilation: a Big Data problem

1. **High resolution** models
2. The domain of validity of **the linear hypothesis** shrinks with increasing resolution and integration length

So **high resolution linearized models** require time-consuming computations.

Data Assimilation: a Big Data problem

<u>DA is a large size computational problem</u>

that should be solved in near **<u>real-time</u>**.

1. **High resolution** models
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Data Assimilation: a Big Data problem

DA is a large size computational problem

that should be solved in near **real-time**.

1. **High resolution** models
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So **high resolution linearized models** require time-consuming computations.

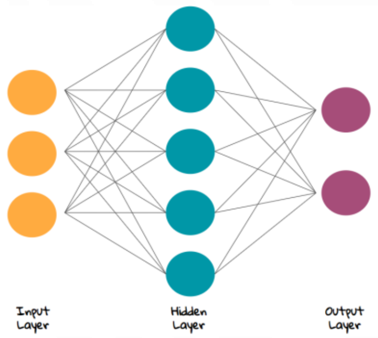
due to the computation **complexity of the DA model**, it is impossible to solve a DA problem by using high resolutions for the model.

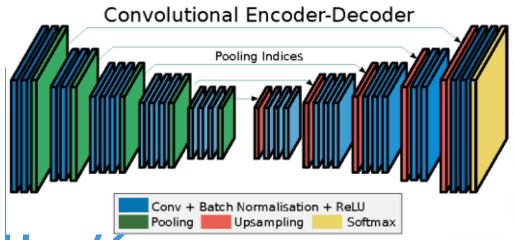
Two main “possibilities”

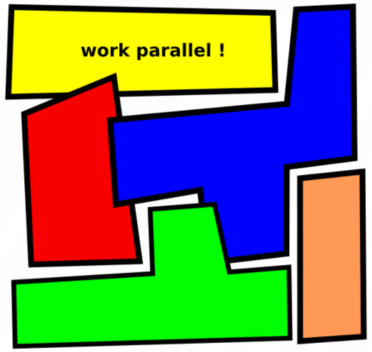
To use some simplifications, (e.g. reduced models, nested models, etc..)

To use some decompositions, to exploit the high performance of emerging computing architectures

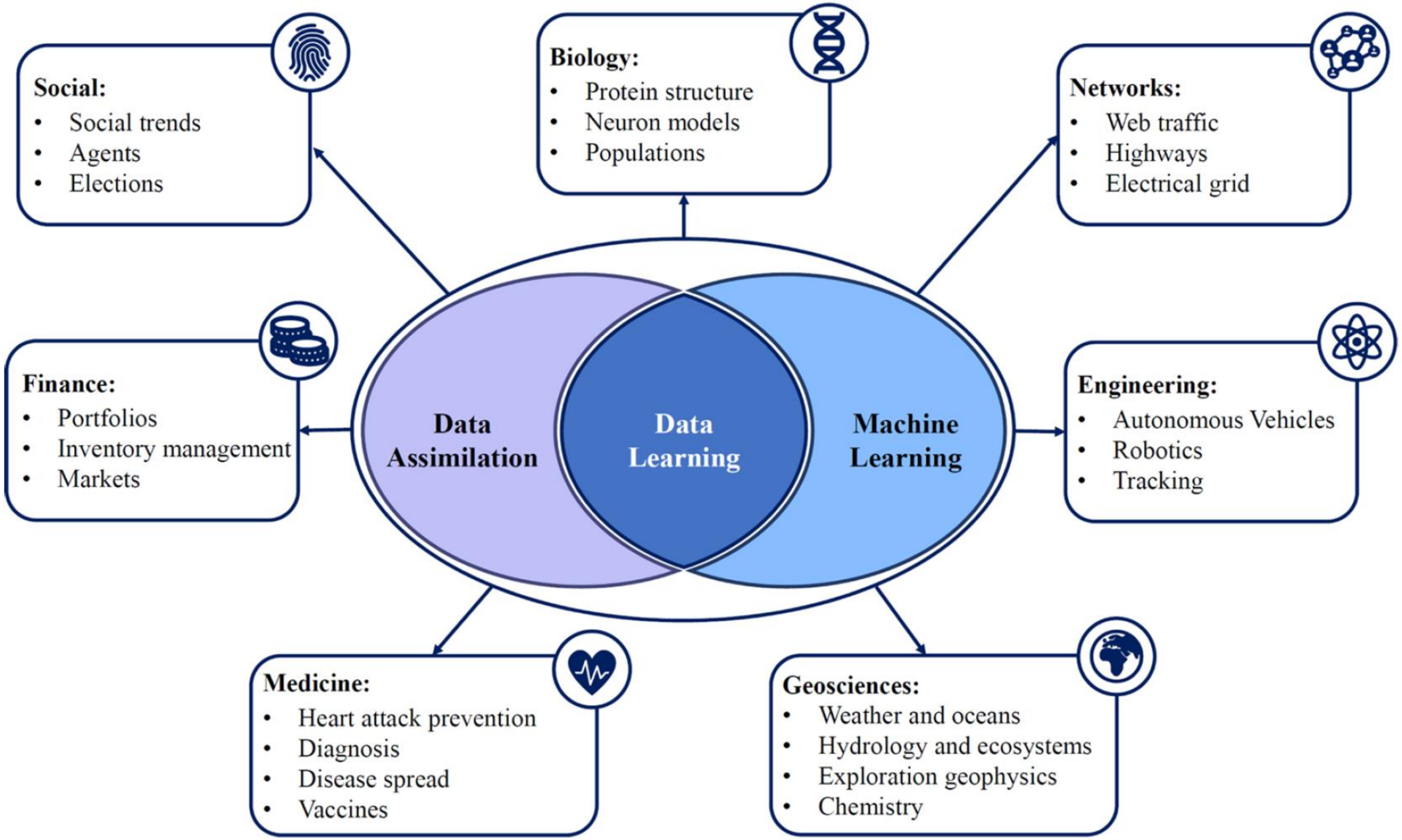
to **develop** scalable algorithms







Data Assimilation + Machine Learning = Data Learning



Data Learning: a modular approach

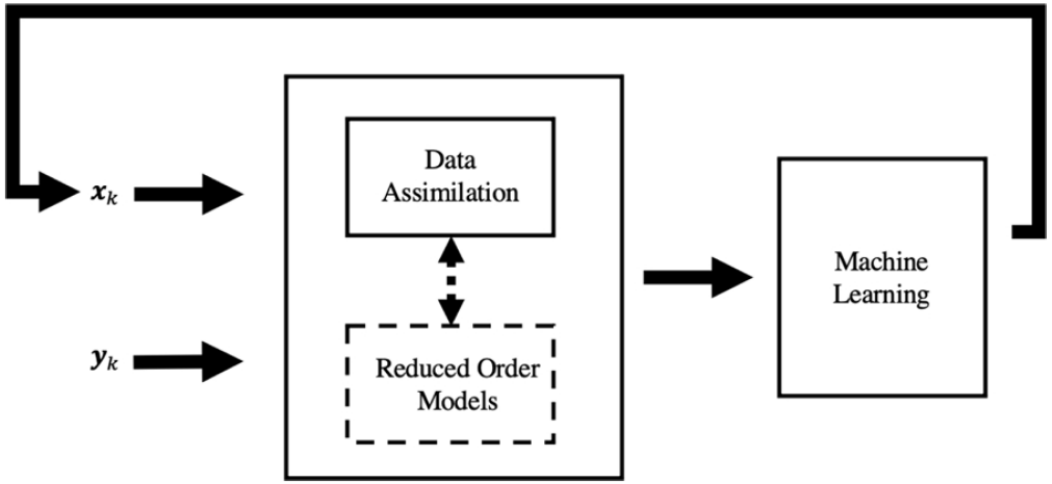
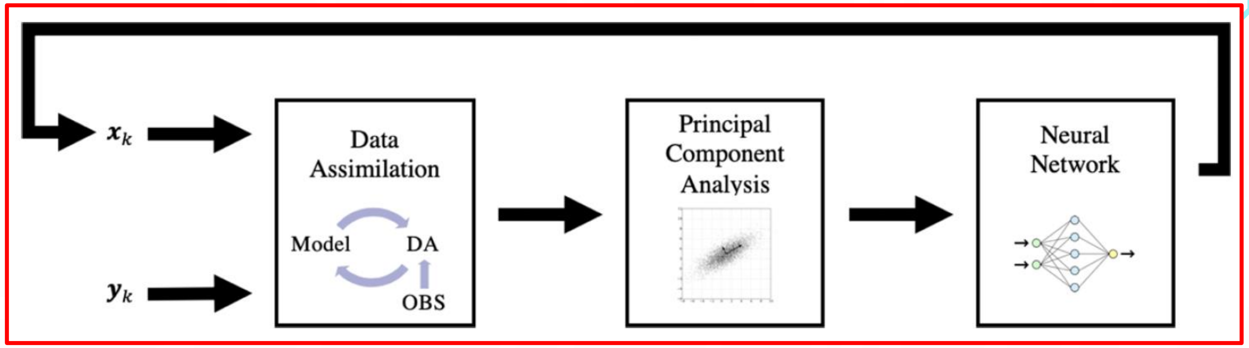
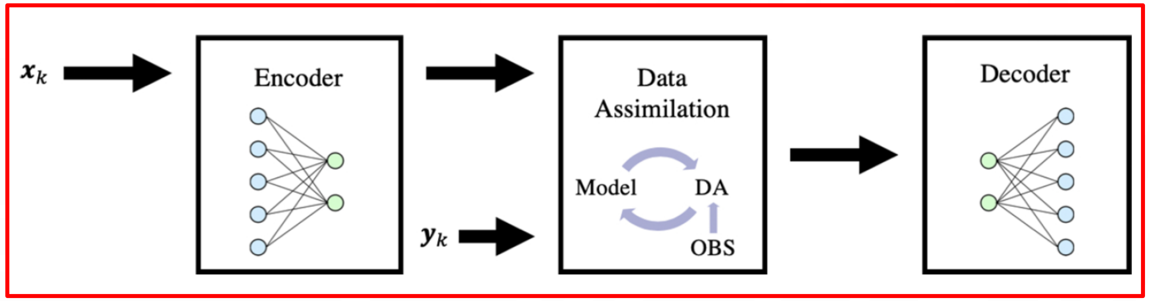
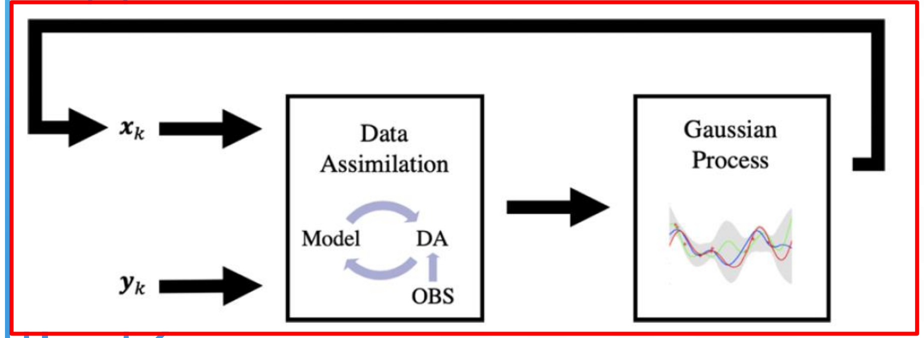
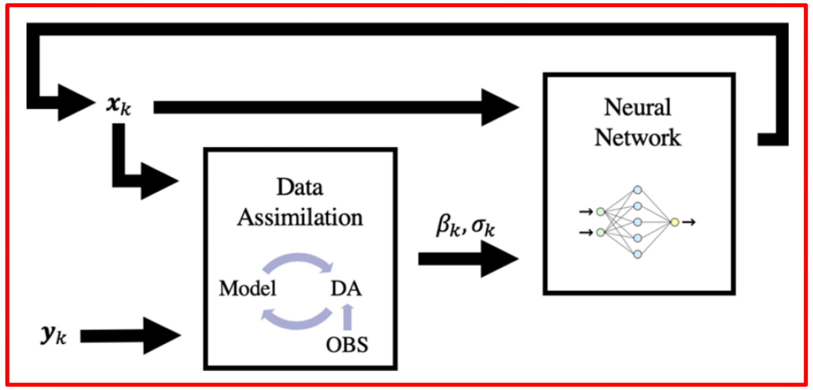


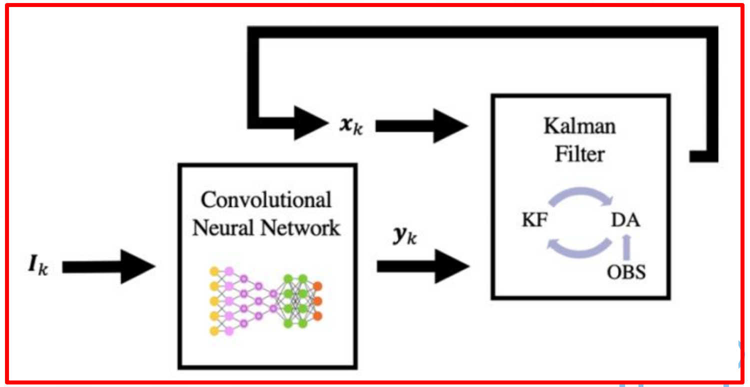
Fig. 1. General Data Learning framework.











Data Assimilation or Latent Assimilation?

$$J(\mathbf{u}) = \alpha\|\mathbf{u}-\mathbf{u}_0\|^2_{\mathbf{B}^{-1}} + \|\mathbf{G}\mathbf{u}-\mathbf{v}\|^2_{\mathbf{R}^{-1}}$$

DA function

3DVar in the control space

$$\mathbf{w} = \mathbf{V}^{+}\delta\mathbf{u}$$
$$\mathbf{B} = \mathbf{V}\mathbf{V}^{T}$$

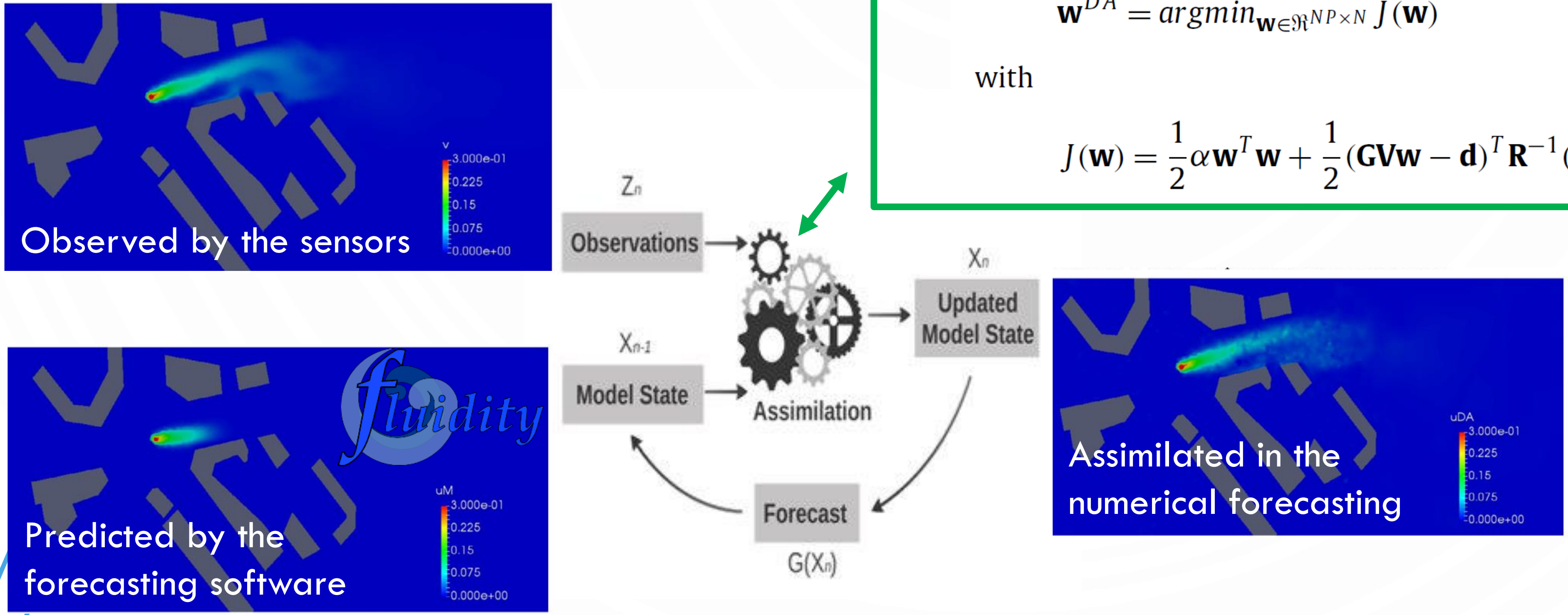
Reduced space, TSVD

$$\mathbf{w}^{DA} = argmin_{\mathbf{w}\in\Re^{NP\times N}} J(\mathbf{w})$$

with

$\sigma=\mu c\delta$

$$J(\mathbf{w}) = \frac{1}{2}\alpha\mathbf{w}^T\mathbf{w} + \frac{1}{2}(\mathbf{G}\mathbf{V}\mathbf{w}-\mathbf{d})^T\mathbf{R}^{-1}(\mathbf{G}\mathbf{V}\mathbf{w}-\mathbf{d})$$

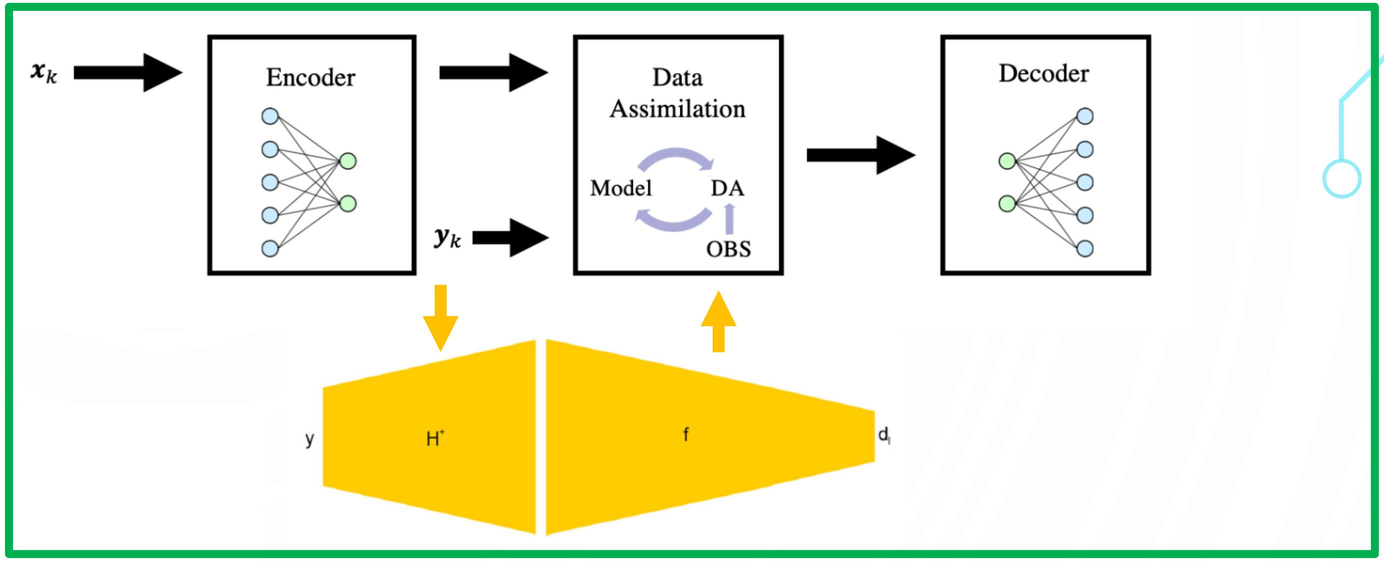


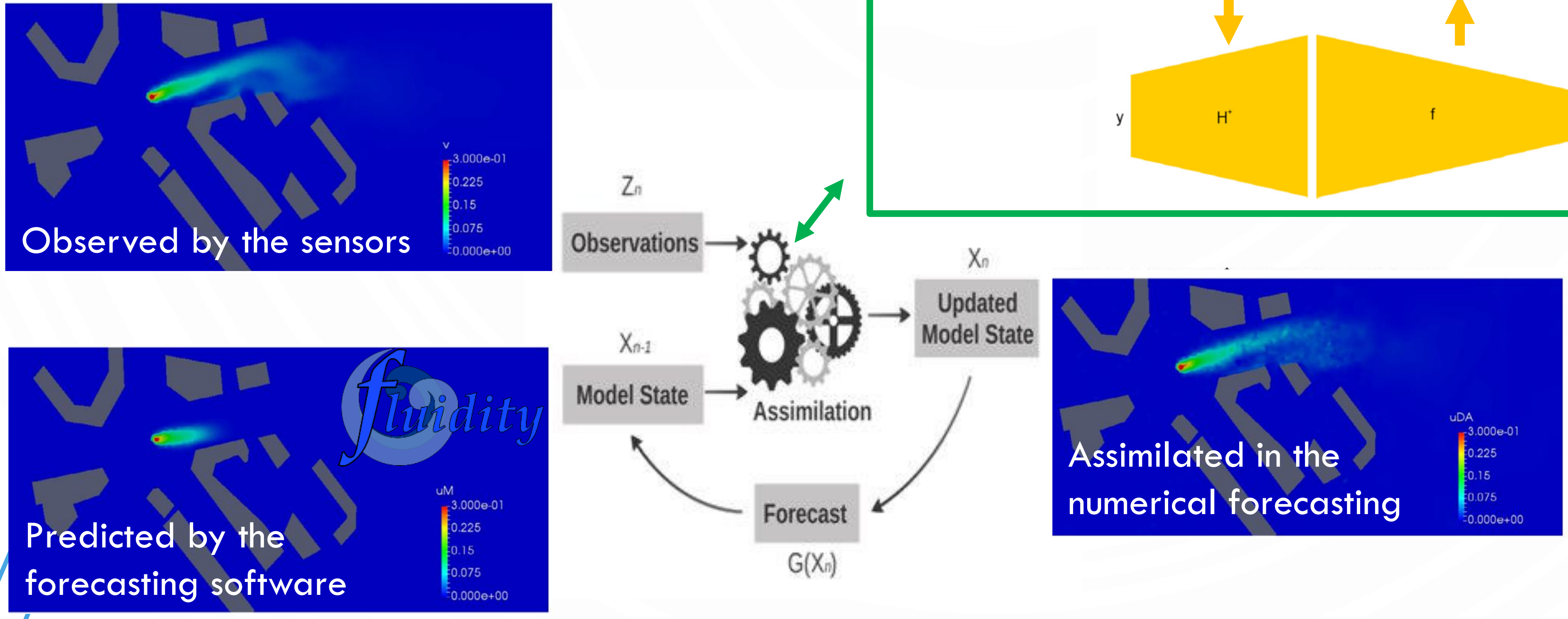
[*] R. Arcucci, L. Mottet, C. Pain and Y. Guo - **Optimal reduced space for Variational Data Assimilation** -Journal of Computational Physics

[**] R. Arcucci, C. Pain, Y. Guo, **Effective variational data assimilation in air-pollution prediction**, Big Data Mining and Analytics

[***] Mack, J., Arcucci, R., Molina-Solana, M., & Guo, Y. K. (2020). **Attention-based Convolutional Autoencoders for 3D-Variational Data Assimilation**. *Computer Methods in Applied Mechanics and Engineering*

Data Assimilation or Latent Assimilation?





EPSRC

INHALE

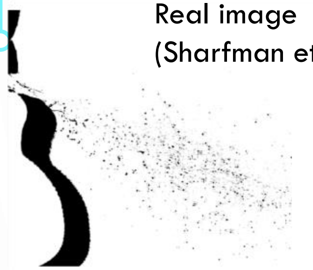
MAGIC
Envisaging a world with greener cities

[*] R. Arcucci, L. Mottet, C. Pain and Y. Guo - **Optimal reduced space for Variational Data Assimilation** -Journal of Computational Physics
[**] R. Arcucci, C. Pain, Y. Guo, **Effective variational data assimilation in air-pollution prediction**, Big Data Mining and Analytics
[***] Mack, J., Arcucci, R., Molina-Solana, M., & Guo, Y. K. (2020). **Attention-based Convolutional Autoencoders for 3D-Variational Data Assimilation**. *Computer Methods in Applied Mechanics and Engineering*

Assimilating Images

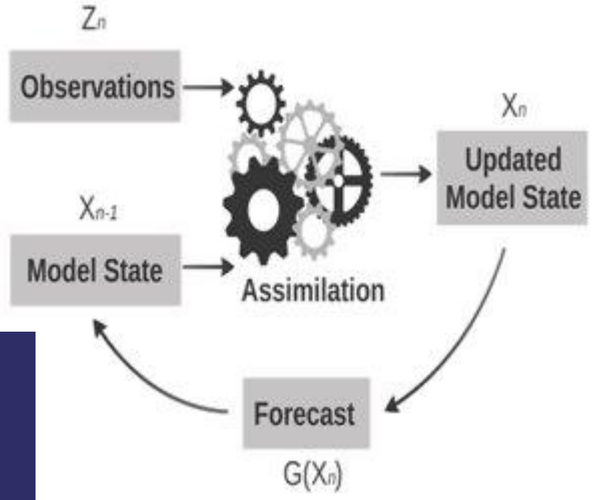
Assimilating Images

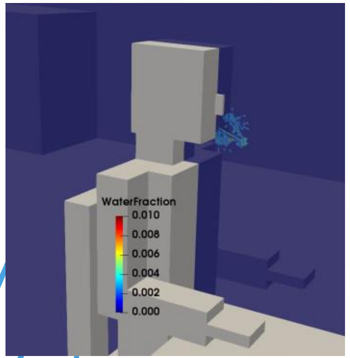
Observed data: experiments

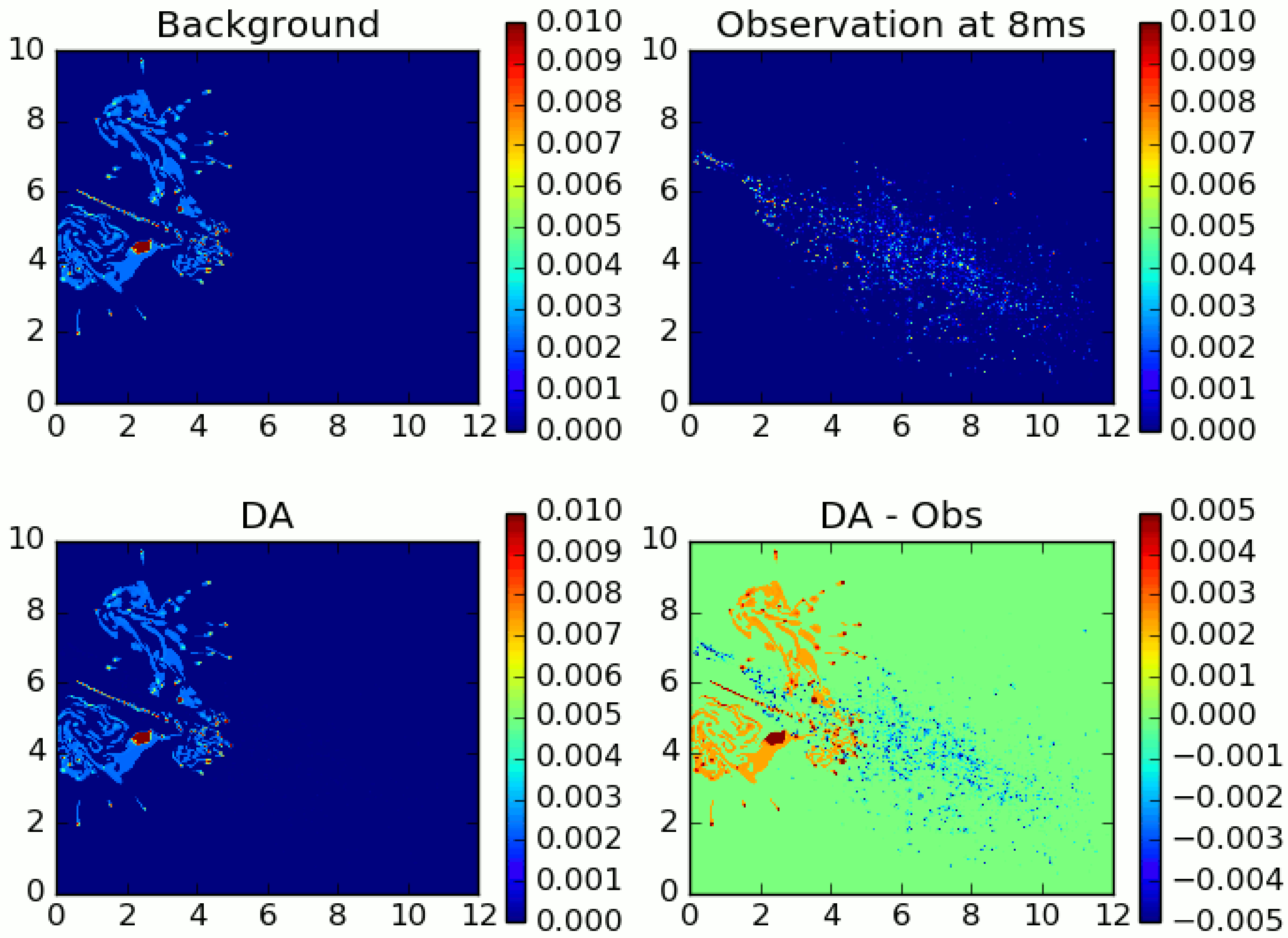


Real image
(Sharfman et al, 2016)

time=8ms







CFD simulation or Surrogate model

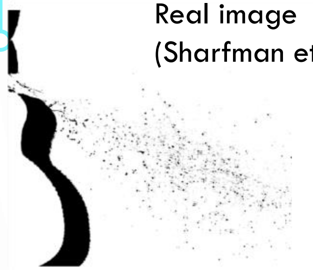
R. Arcucci, L. Mottet, . Quilodran Casas, A. Joshi, A. Obeysekara, Y-K. Guo, C. Pain - Enhancing CFD Simulations of Covid-19 Diffusion by Coughing and Sneezing Using Bayesian Data Assimilation

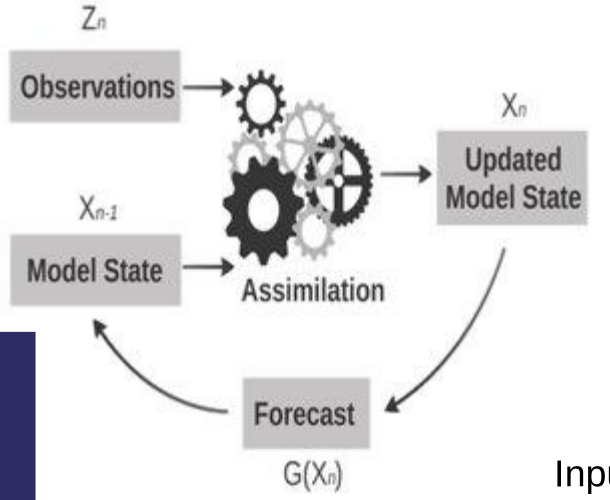
Assimilating Images

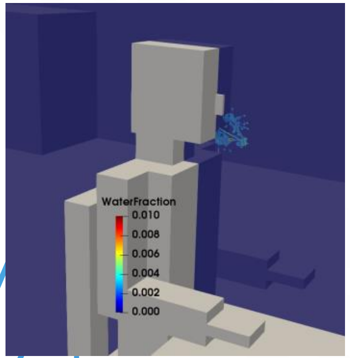
COVID-19: GENERIC CASE - SIMULATION OF DISPERSION IN A CLASS

Observed data: experiments

Real image
(Sharfman et al, 2016)

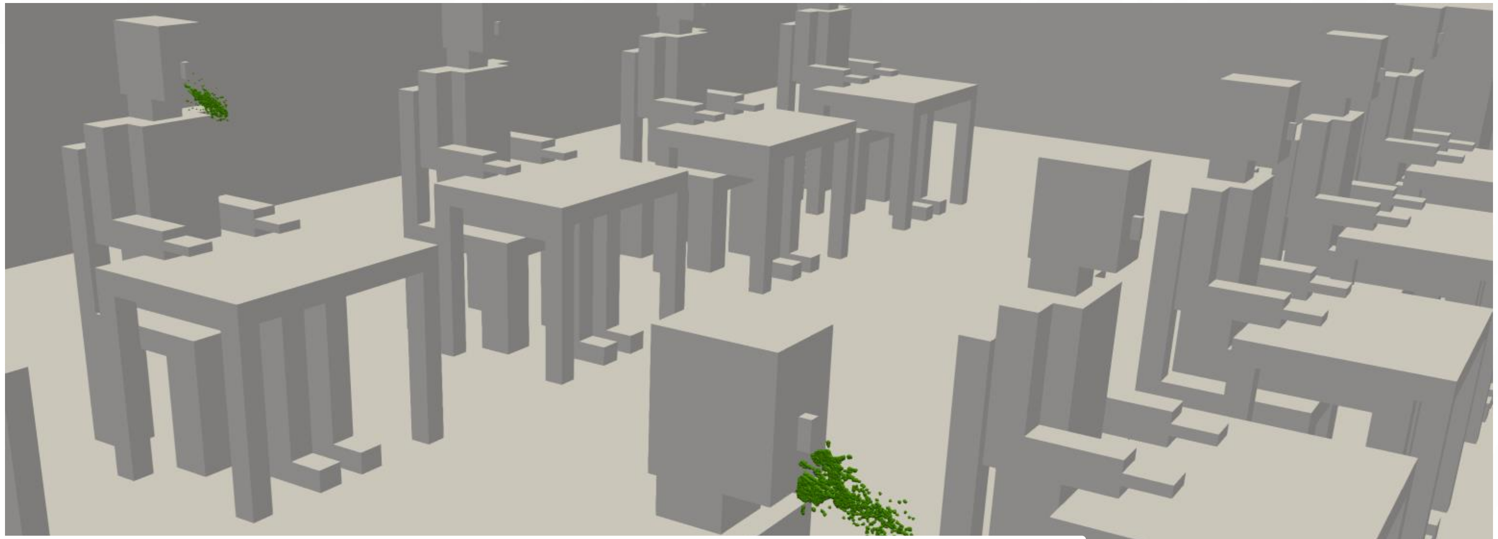






CFD simulation or Surrogate model

Green iso-surface shows dispersion of passive tracer.



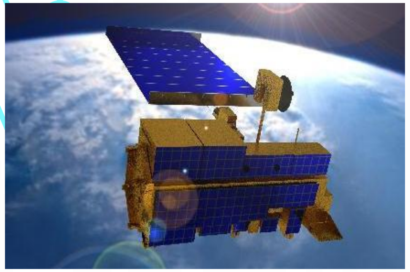
Input data → M(P) → Solution

any perturbation on the data (δ) propagates on the solution (**σ**) by an amplification factor given by **c** = a parameter that depends on the algorithm and **μ** = the Condition number of the problem

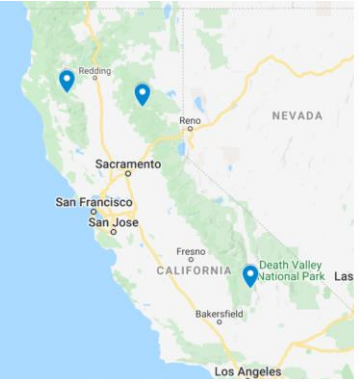
Error on the solution: $\sigma=\mu c \delta$

R. Arcucci, L. Mottet, . Quilodran Casas, A. Joshi, A. Obeysekara, Y-K. Guo, C. Pain - Enhancing CFD Simulations of Covid-19 Diffusion by Coughing and Sneezing Using Bayesian Data Assimilation

Wildfire forecasting

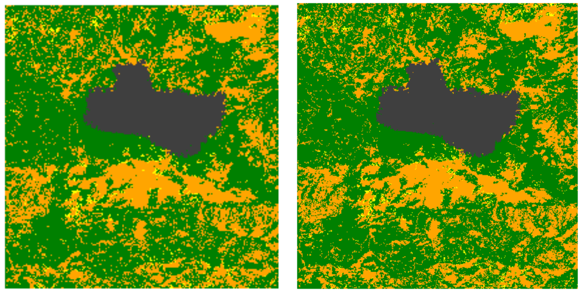


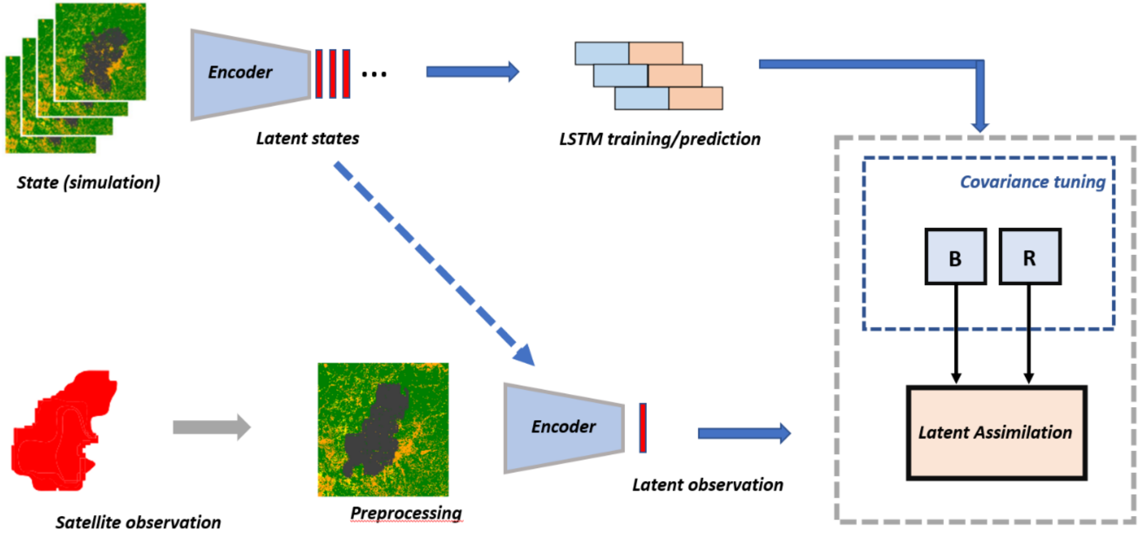
MODIS: every 1-2 days at 1km resolution

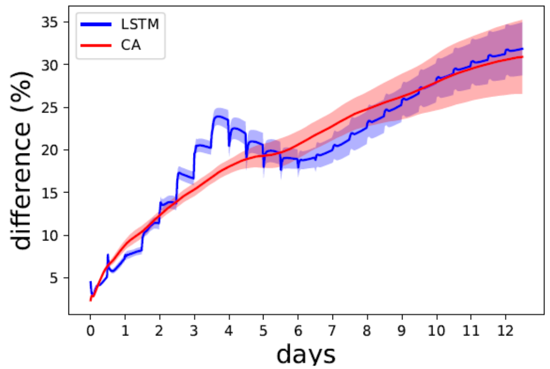


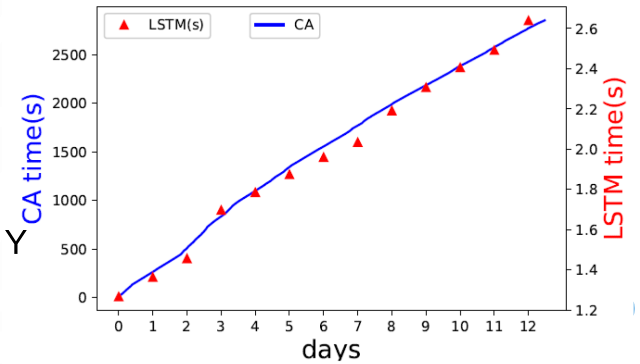
- Learning from simulation data
- Using satellite observations to validate/assimilate

observation prediction









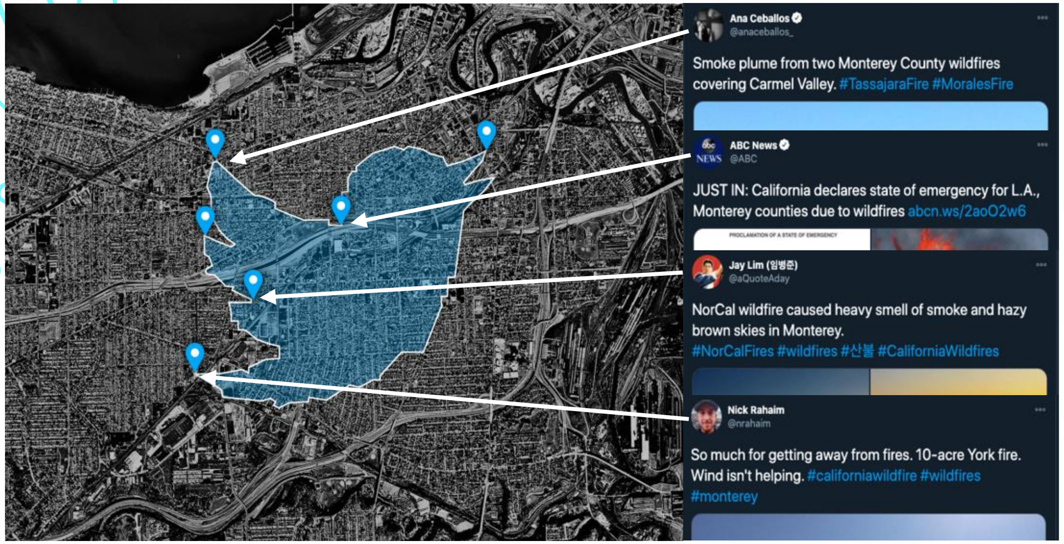
[*] Data-driven surrogate model with latent data assimilation: Application to wildfire forecasting S Cheng, IC Prentice, Y Huang, Y Jin, YK Guo, R Arcucci - Journal of Computational Physics, 111302
[**] Parameter Flexible Wildfire Prediction Using Machine Learning Techniques: Forward and Inverse Modelling S Cheng, Y Jin, SP Harrison, C Quilodrán-Casas, IC Prentice, YK Guo, ..., R.Arcucci - Remote Sensing 14 (13), 3228

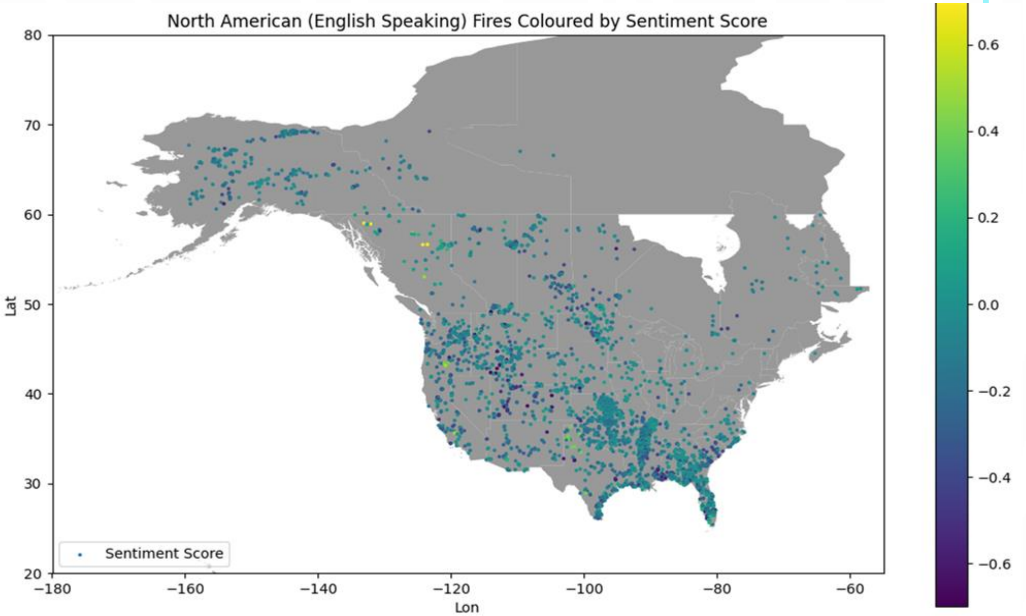
Human Sensors!

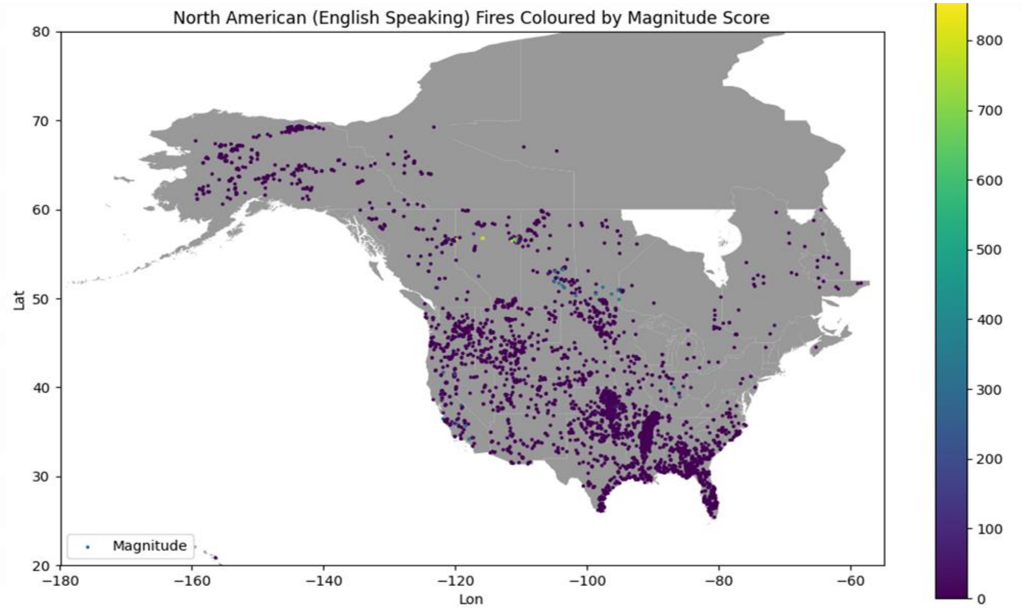
In 2021, the number of mobile devices operating worldwide stood at almost **15 billion**

In 2020, **over 3.6 billion people** were using social media worldwide, a number projected to increase to almost 4.41 billion in 2025.

Social data and satellites: Wildfires System

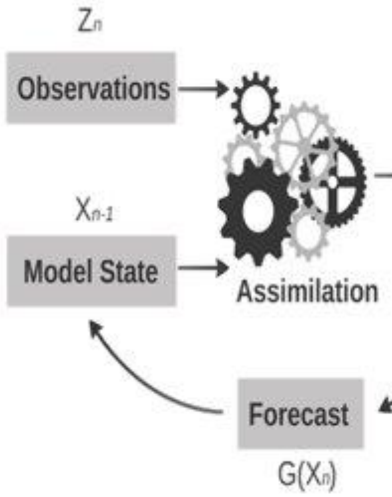


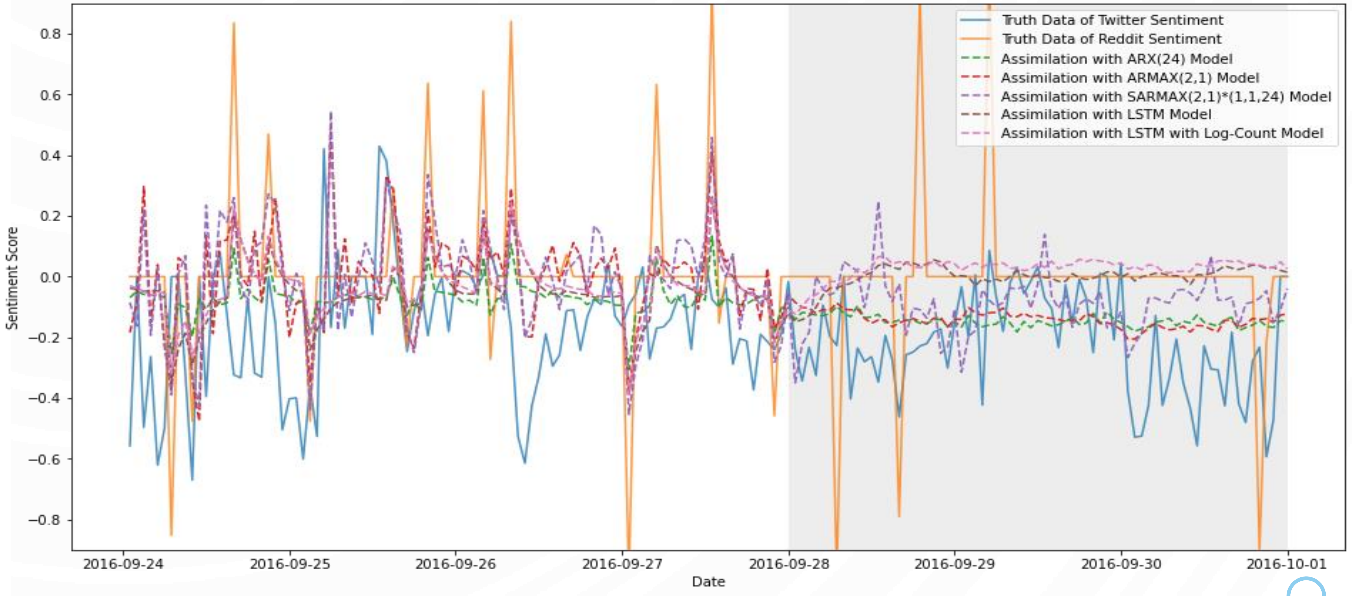




- How do people perceive wildfires? Can this be measured or modelled?
- Idea: can we collect many subjective opinions on certain natural events, and are these opinions reflective of the size and severity of the event?
- Social media and Twitter - human sensors; Sentiment analysis - Converting emotional leaning in a passage of text into a numerical value, evaluating the positivity (or negativity) of the emotions expressed.

Social data and satellites: Wildfires System





[*] Social Data Assimilation of Human Sensor Networks for Wildfires
J Lever, R Arcucci, J Cai - Proceedings of the 15th International Conference PETRA

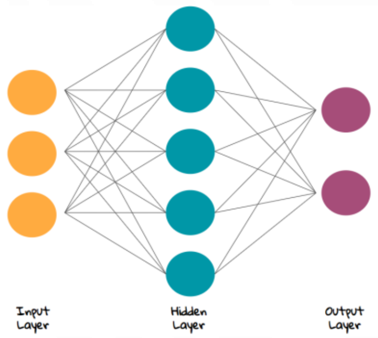
[**] Sentimental wildfire: a social-physics machine learning model for wildfire nowcasting
J Lever, R Arcucci - Journal of Computational Social Science, 1-39

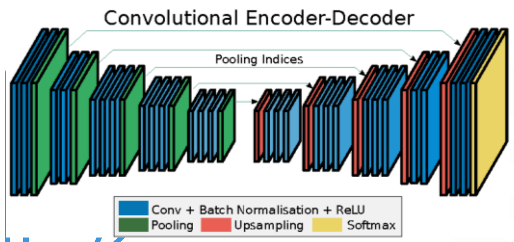
Two main “possibilities”

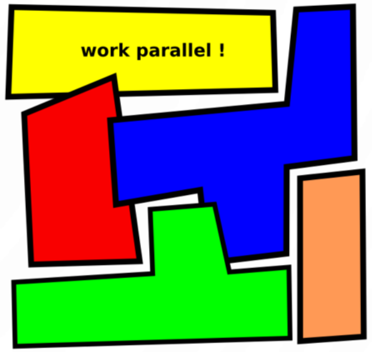
To use some simplifications, (e.g. reduced models, nested models, etc..)

To use some decompositions, to exploit the high performance of emerging computing architectures

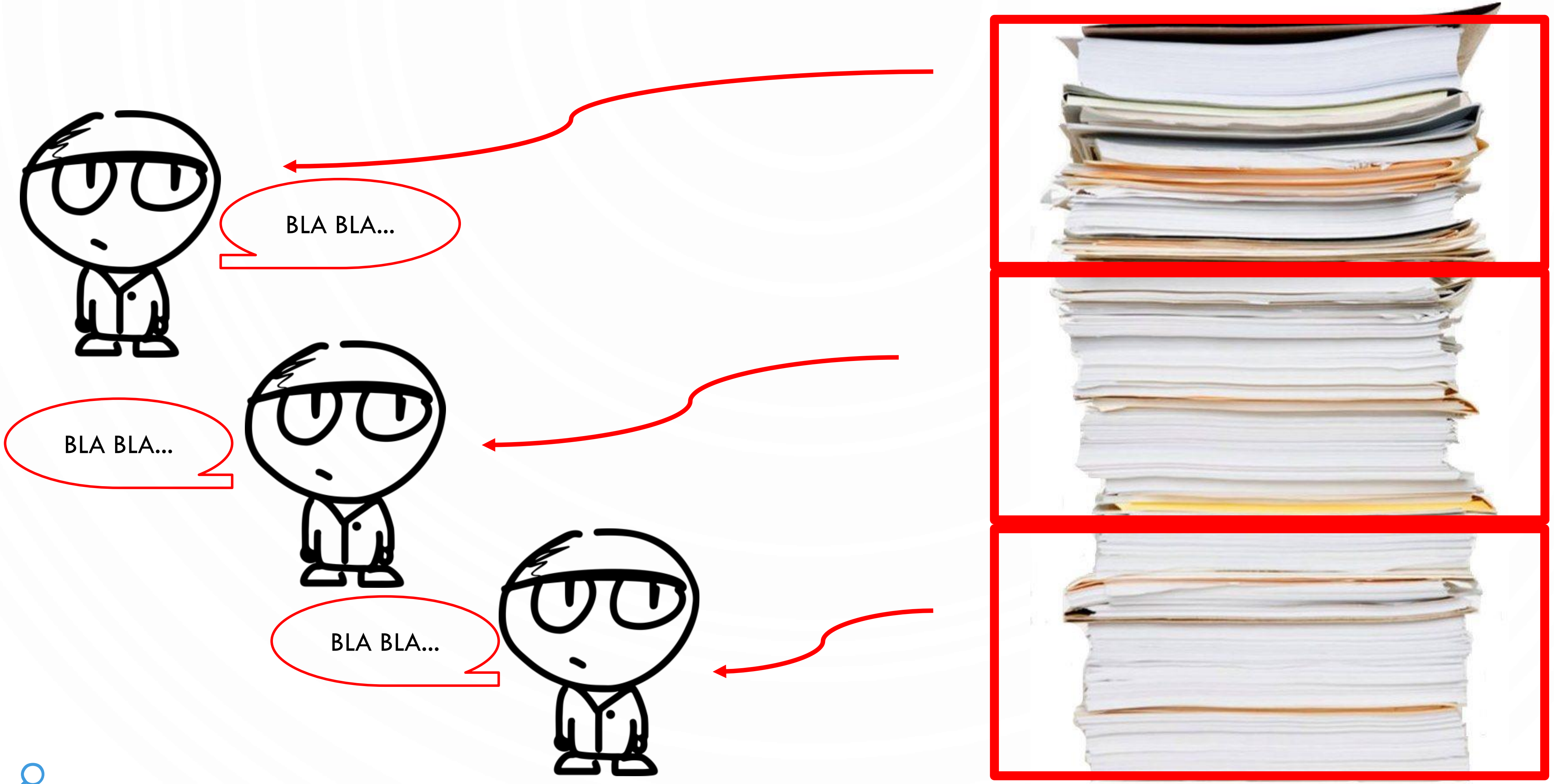
to **develop** scalable algorithms







… to **develop** scalable algorithms

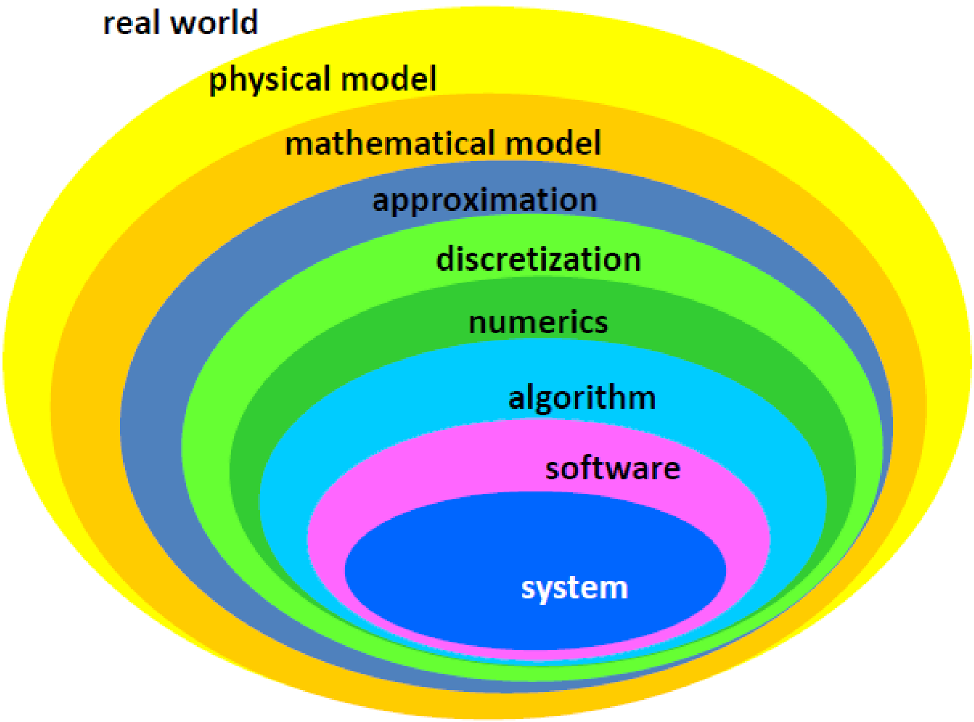


Parallel computing

Domain Decomposition

Domain Decomposition for Data Assimilation

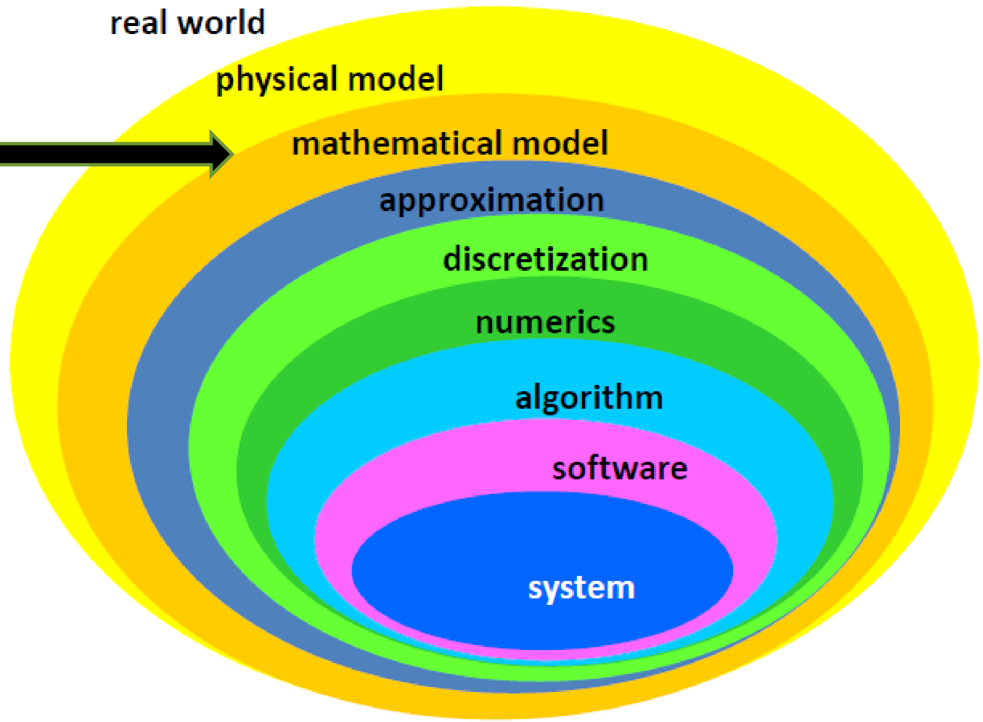
Mathematical Stack



Domain Decomposition for Data Assimilation

«Adapting old programs to fit new machines usually means adapting new machines to behave like old ones.»
Alan Perlis

Parallelization should be introduced at the beginning…



Domain Decomposition for Data Assimilation

Let $\Omega \subset \Re^S$ be decomposed into a sequence of p overlapping sub-domains $\Omega_i \subset \Re^{r_i}$, $r_i \leq N$, $i = 1, \ldots, p$ such that

$$\Omega = \bigcup_{i=1}^{p} \Omega_i$$

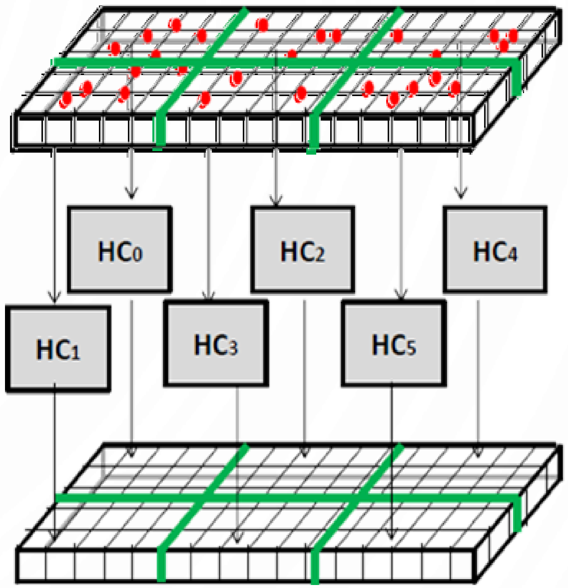
where

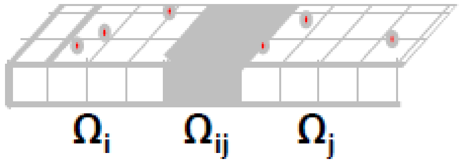
$$\Omega_i \cap \Omega_j = \Omega_{ij} \neq \emptyset$$

if the sub-domains are adjacent.

$$\mathbf{u}_i^{DA} = argmin_{u_i} \left\{ J/\Omega_i + O/\Omega_{ij} \right\}$$

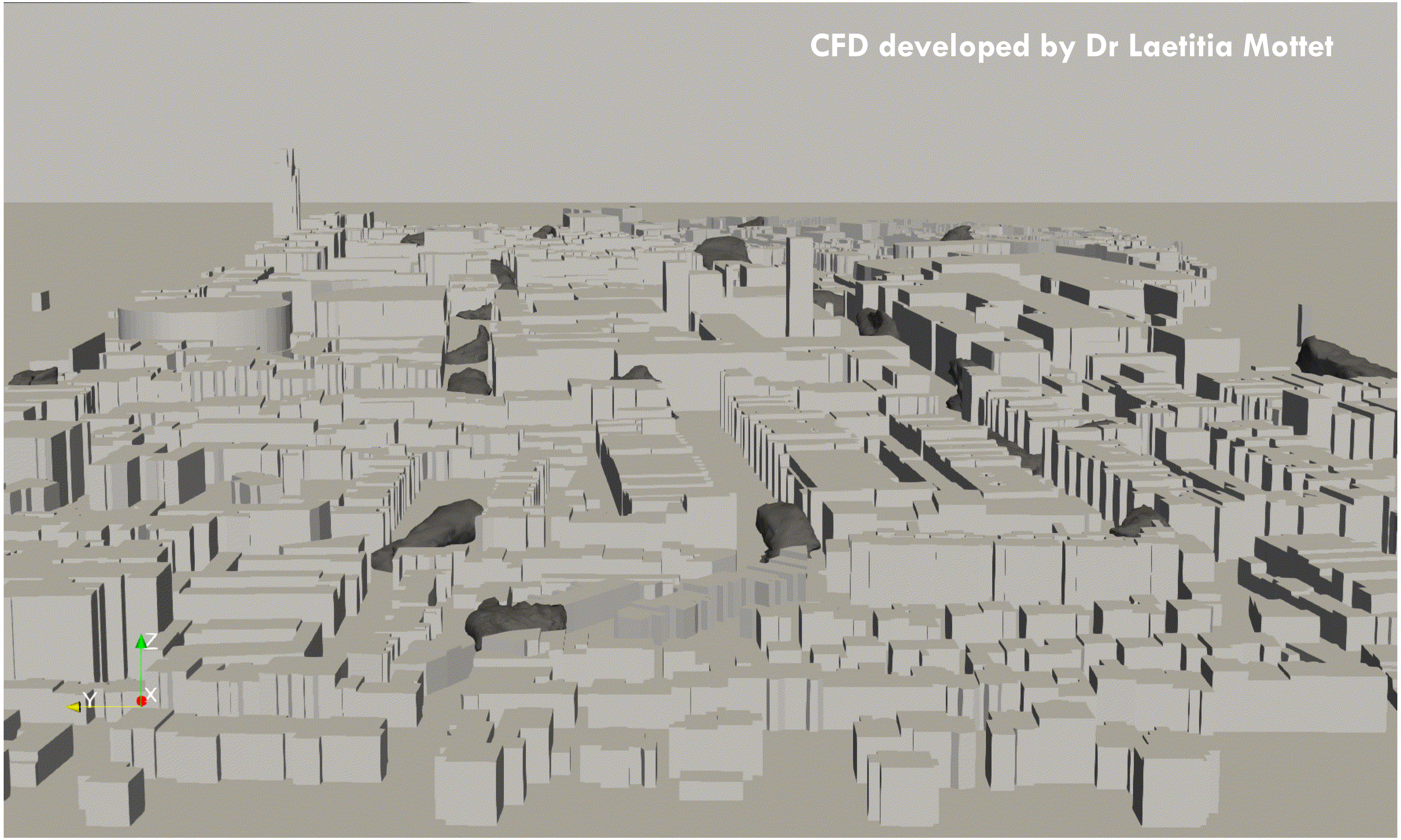
where O/Ω_{ij} is called overlapping operator.





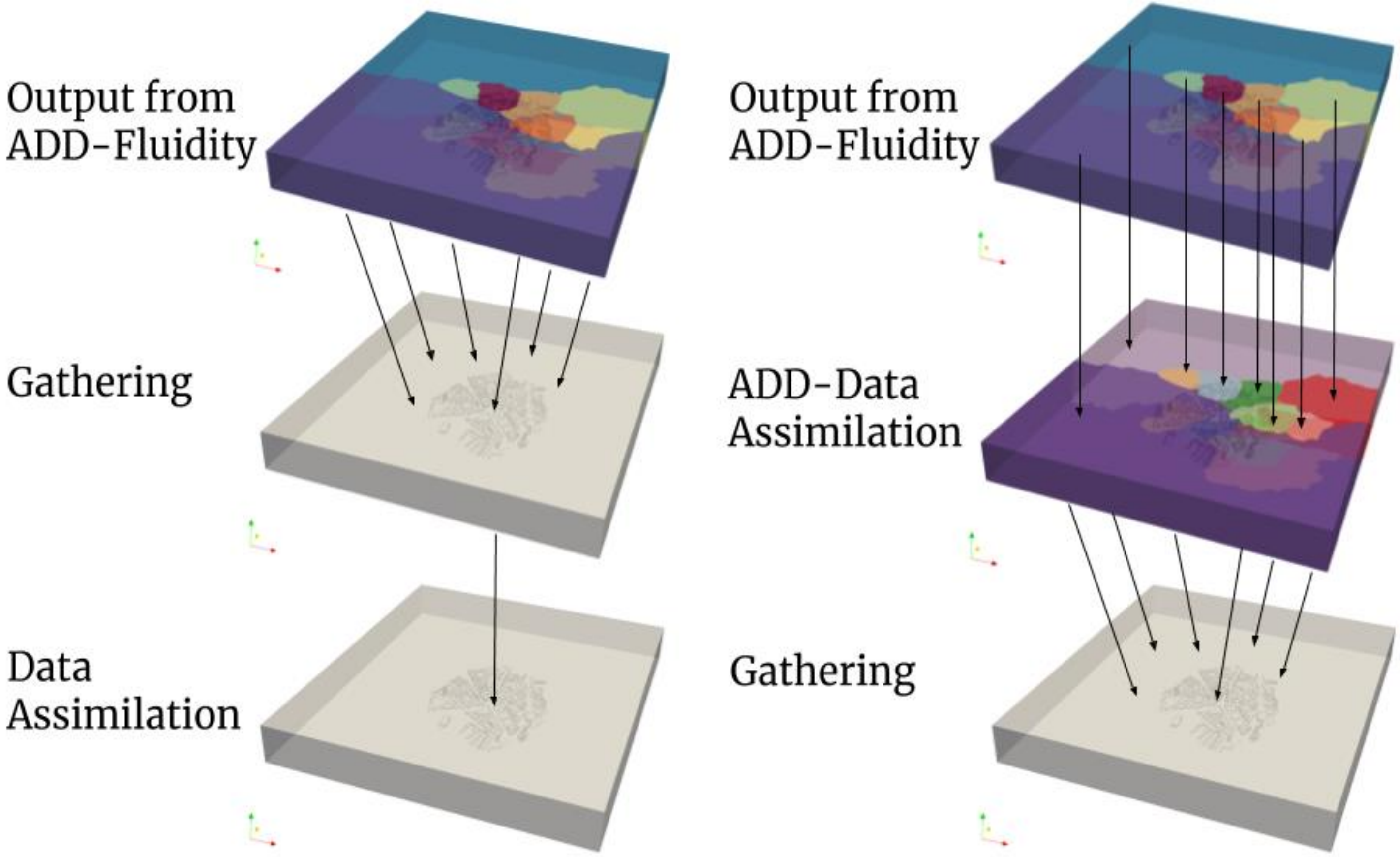
$$J(\mathbf{u}) = \left\{ \|\mathbf{G}\mathbf{u} - \mathbf{v}\|_{\mathbf{R}}^2 + \|\mathbf{u} - \mathbf{u}_0\|_{\mathbf{B}}^2 \right\}$$

A Scalable Numerical Algorithm for solving Tikhonov Regularization Problems – R. Arcucci, L. D'Amore, S. Celestino, G. Laccetti and A. Murli - LNCS 9574 - Ch. 5, 978-3-319-32151


CFD developed by Dr Laetitia Mottet
Z
Y
X

Domain Decomposition for Data Assimilation

How to face a computationally expensive problem (like Data Assimilation) on a domain such as a BIG city



Domain Decomposition for Data Assimilation

How to face a computationally expensive problem (like Data Assimilation) on a domain such as a BIG city

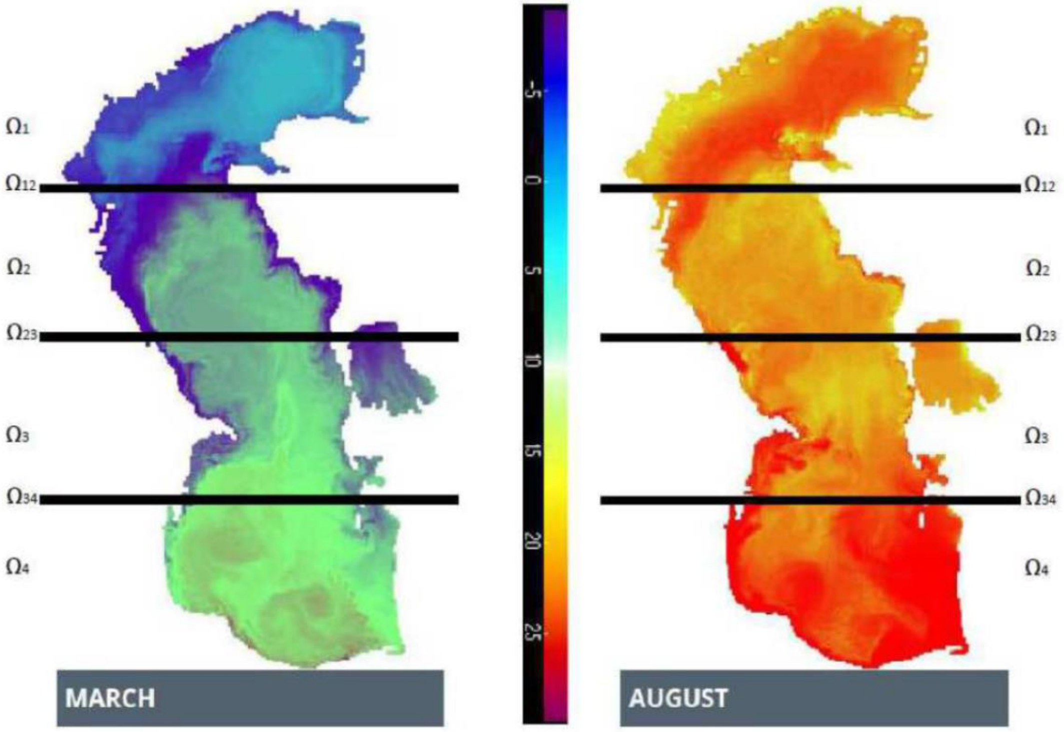
Predicted by the forecasting software

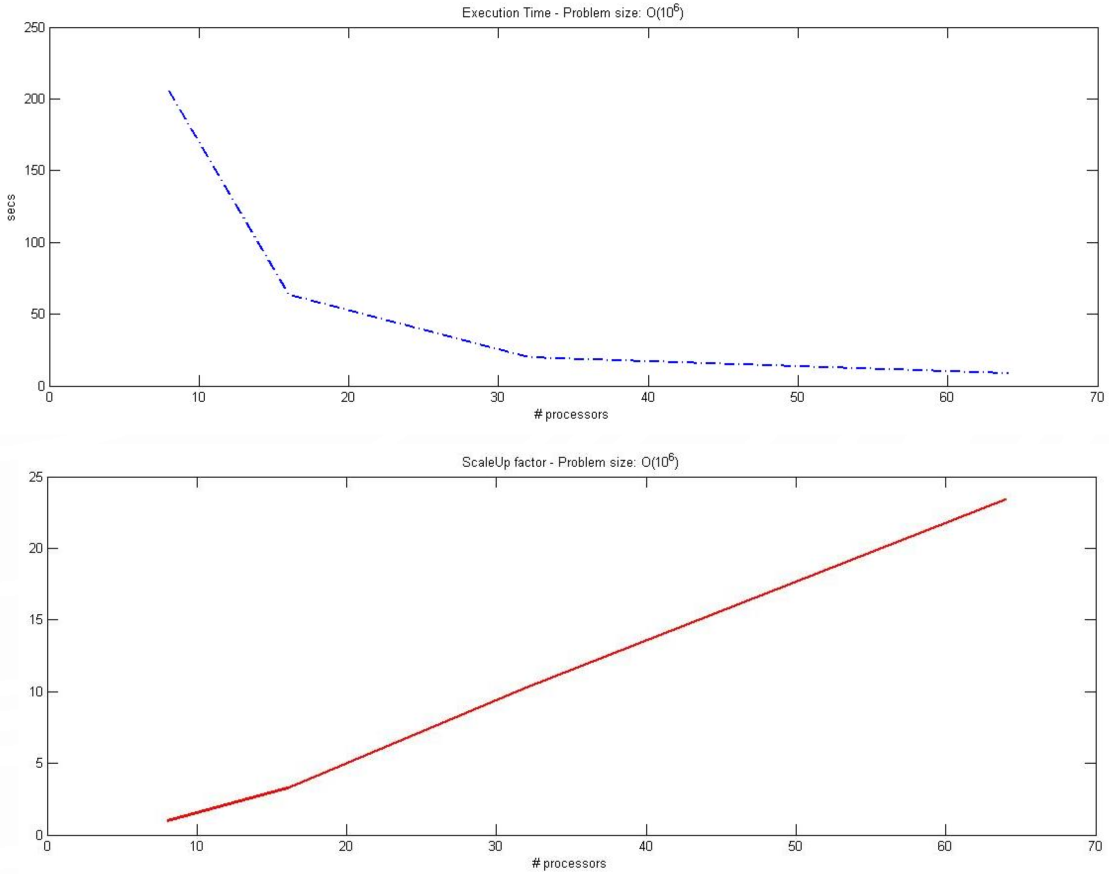
Observed by the sensor

Iso-surface, in white, of the pollutant concentration computed in parallel with 10 processors

Assimilated in the numerical forecasting

Domain Decomposition for Data Assimilation



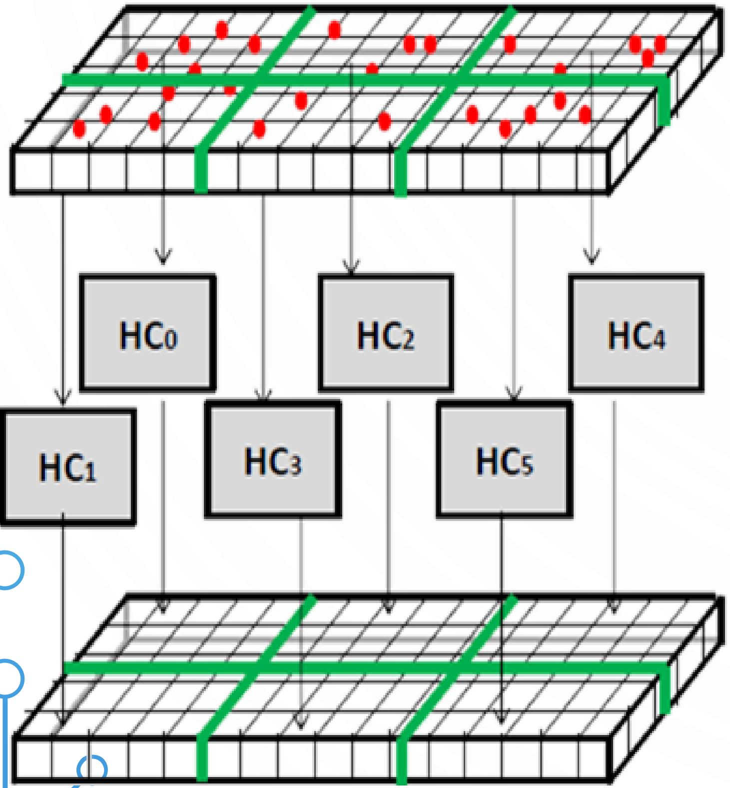


R. Arcucci, L.Carracciuolo and R.Toumi - **Toward a preconditioned scalable 3DVAR for assimilating Sea Surface Temperature collected into the Caspian Sea** - Journal of Numerical Analysis, Industrial and Applied Mathematics (JNAIAM) vol. 11-12, no. 1, 2018, pp. 9-28 ISSN 1790–8140

Domain Decomposition for Data Assimilation … big domains

Sunway TaihuLight，神威·太湖之光

total of 10,649,600 CPU cores across the entire system



Data Assimilation:

Examples and code (https://github.com/DL-WG/DA-tutorial-/)

… we are happy to share

Weekly meetings with invited speakers from other universities or companies:

We meet every Tuesday at 4pm (UK time) on Zoom
Our mailing list:
https://mailman.ic.ac.uk/mailman/listinfo/datalearning

All the talks are recorded and uploaded on our YouTube Channel – Data Learning

International Conference:

Every year, the DataLearning group organises a workshop on **Machine Learning and Data Assimilation for Dynamical Systems (MLDADS)**, as part of the International Conference on Computational Science (ICCS).

Prague – ICCS 2023 **London - ICCS 2022** **Poland - ICCS 2021** **Amsterdam - ICCS 2020** **Faro, Portugal - ICCS 2019**

Sharing contents with our community worldwide:

To get access to our **codes**: **Our GitHub** https://github.com/DL-WG

There is nothing measured that doesn't exist.

Thank you!

Some other papers and applications:
https://sites.google.com/view/rossella-arcucci/datalearning