Workshop LEFE-CYBER / ILICO / ODATIS

Introduction à l'intelligence artificielle dans l'assimilation des données géophysiques

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Outline

- Geophysical state estimation: models vs observations
- IA in geophysical state estimation and DA:
  - Higher resolution interpolation: general framework and applications
  - Generative models and data assimilation for modeling dynamical systems
  - End-to-end (online) Learning in Hybrid Modeling Systems

Geophysical state estimation: models vs observations

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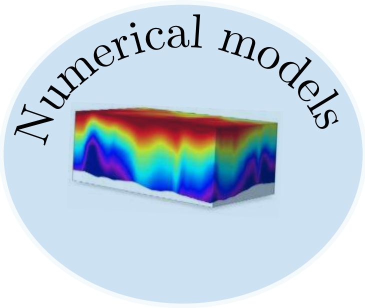

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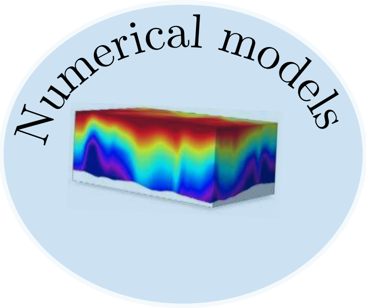

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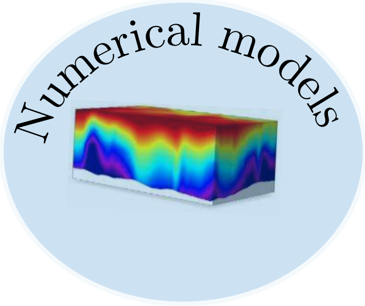

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- Long term simulations
- Understanding of physical processes

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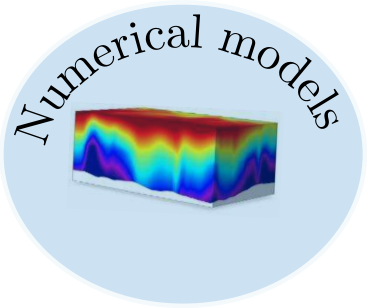

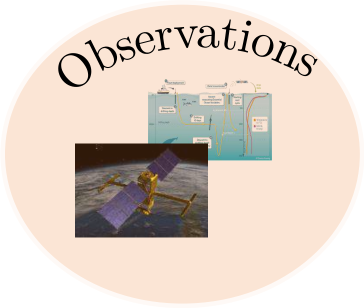

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- Model validation

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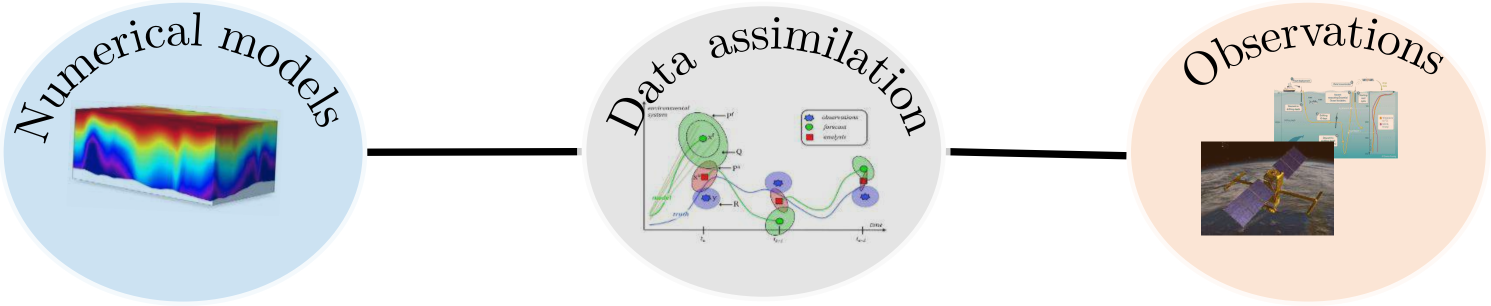

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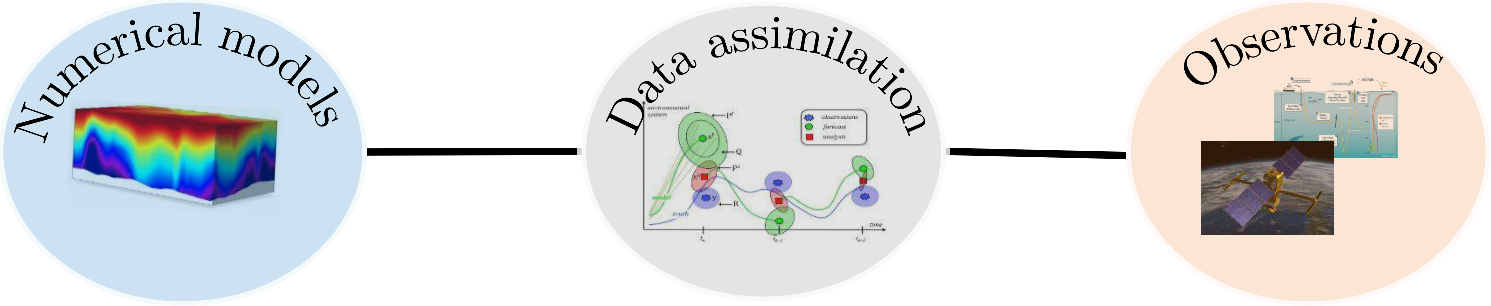

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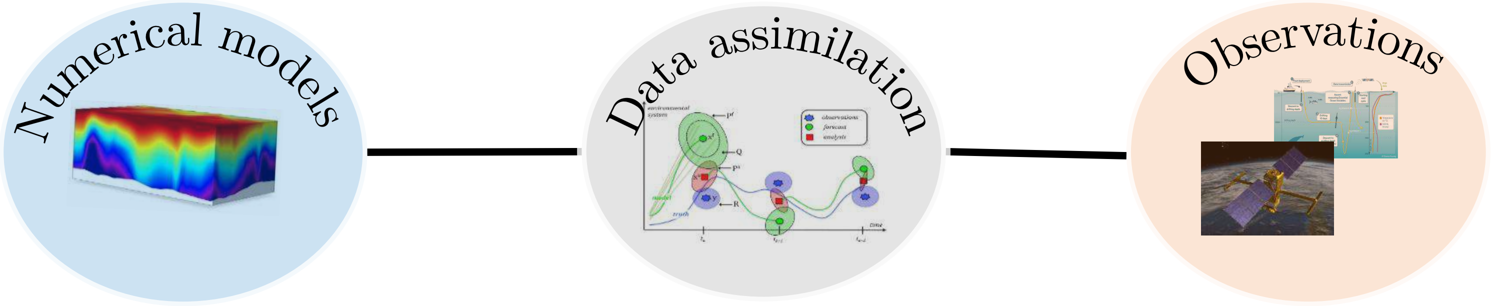
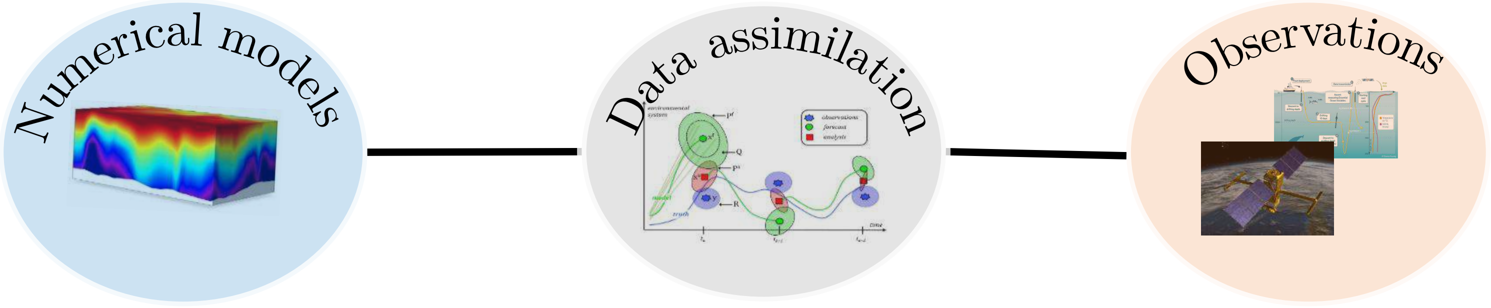
Geophysical state estimation: models vs observations



- Initialization of the models

- Data reconstruction and interpolation

Geophysical state estimation: models vs observations



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- Model bias correction
- Choice of some parameterizations
- How to increase the predictability
- How to model a subset of variables

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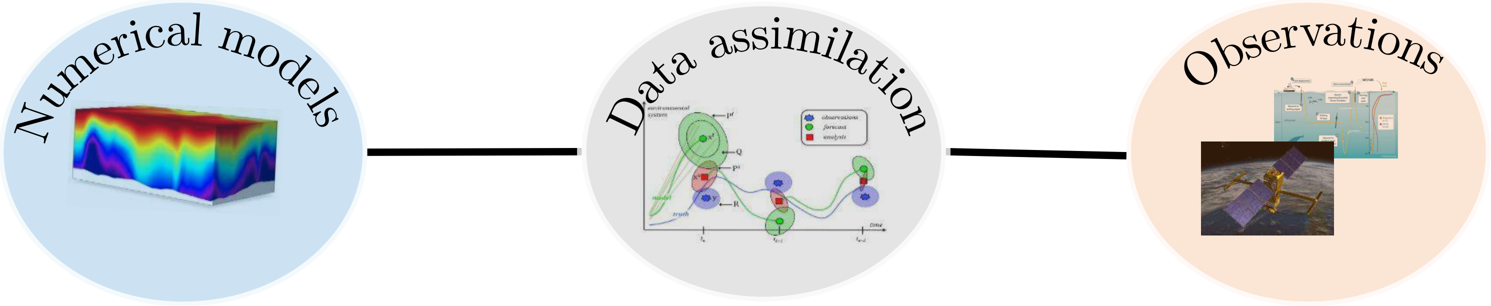

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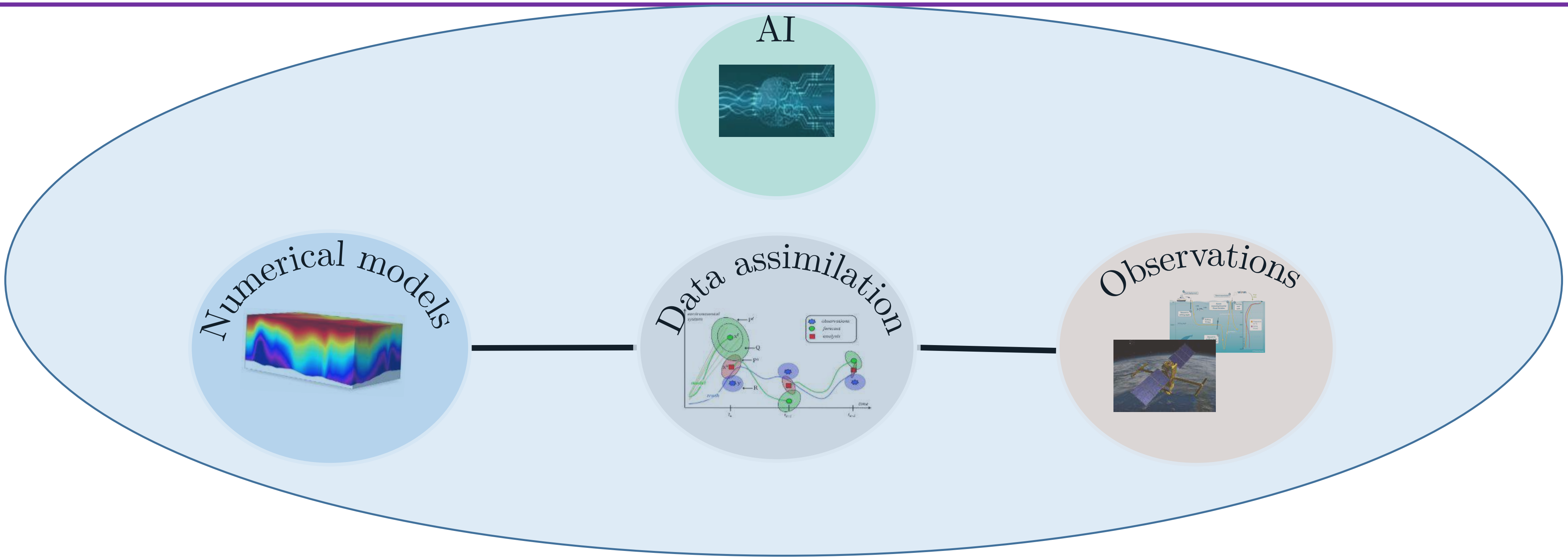
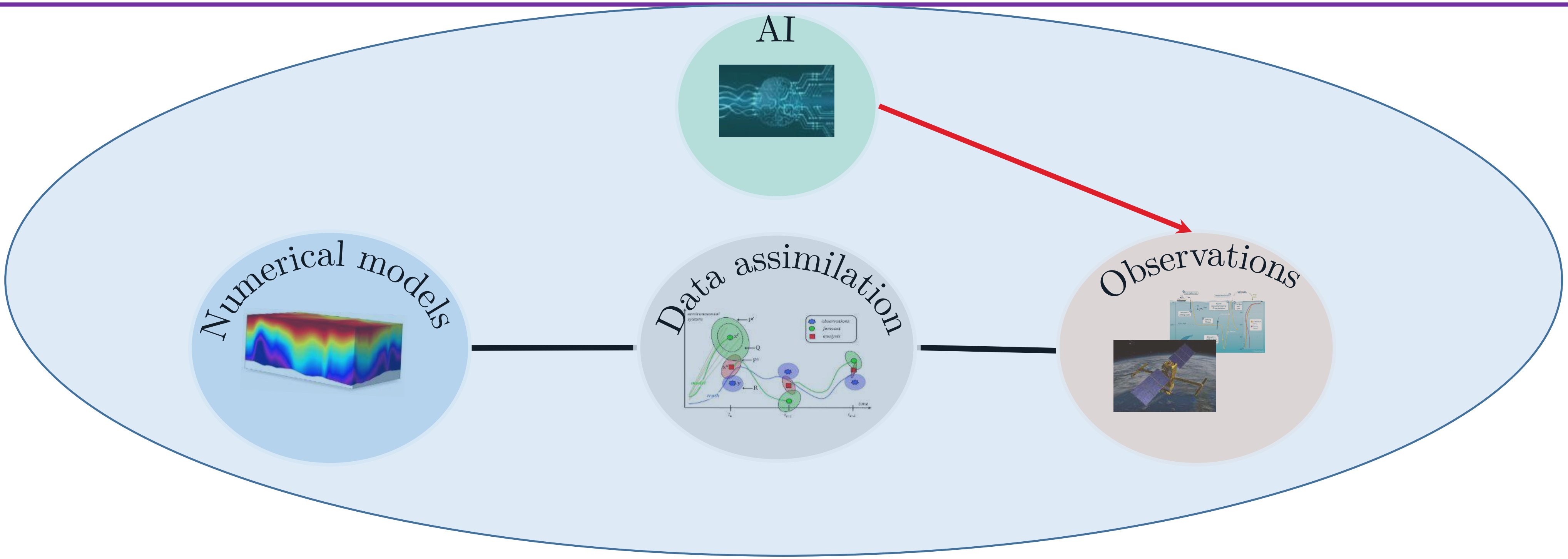
- How to explore these big amounts data
- How to design new sensing missions

IA in geophysical state estimation and DA



Improving geophysical state estimation using machine learning and AI

IA in geophysical state estimation and DA



- Higher resolution interpolation
- Data driven synergy, emulators

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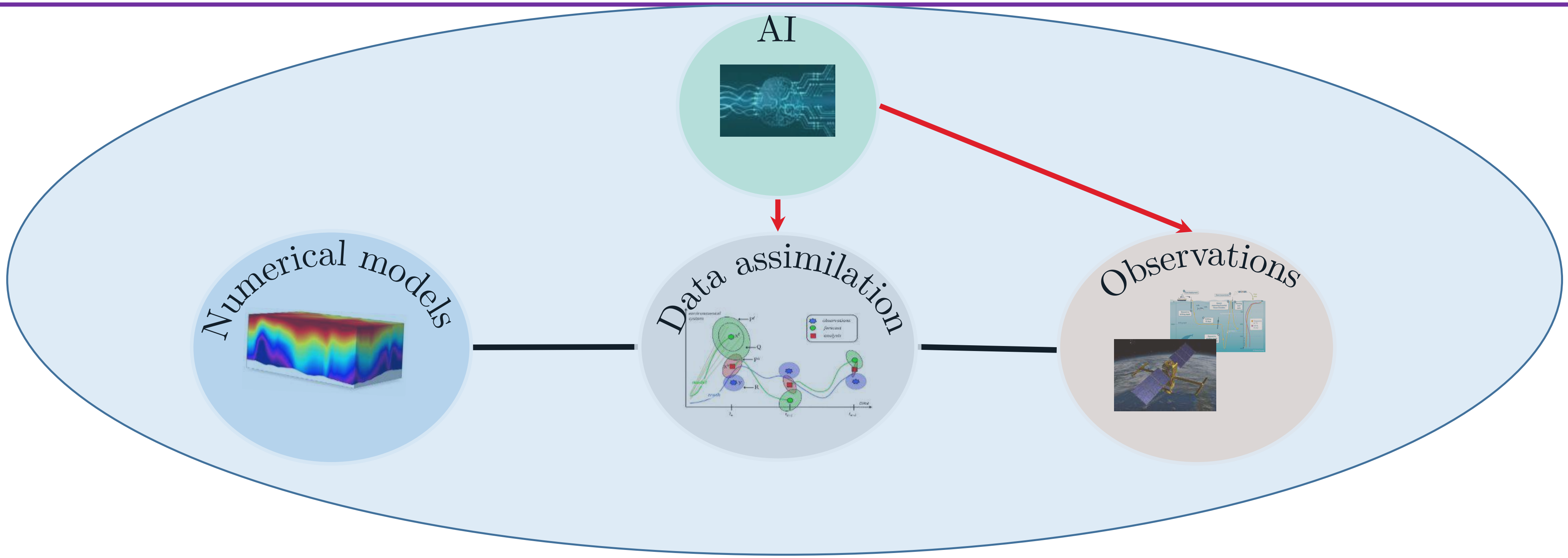
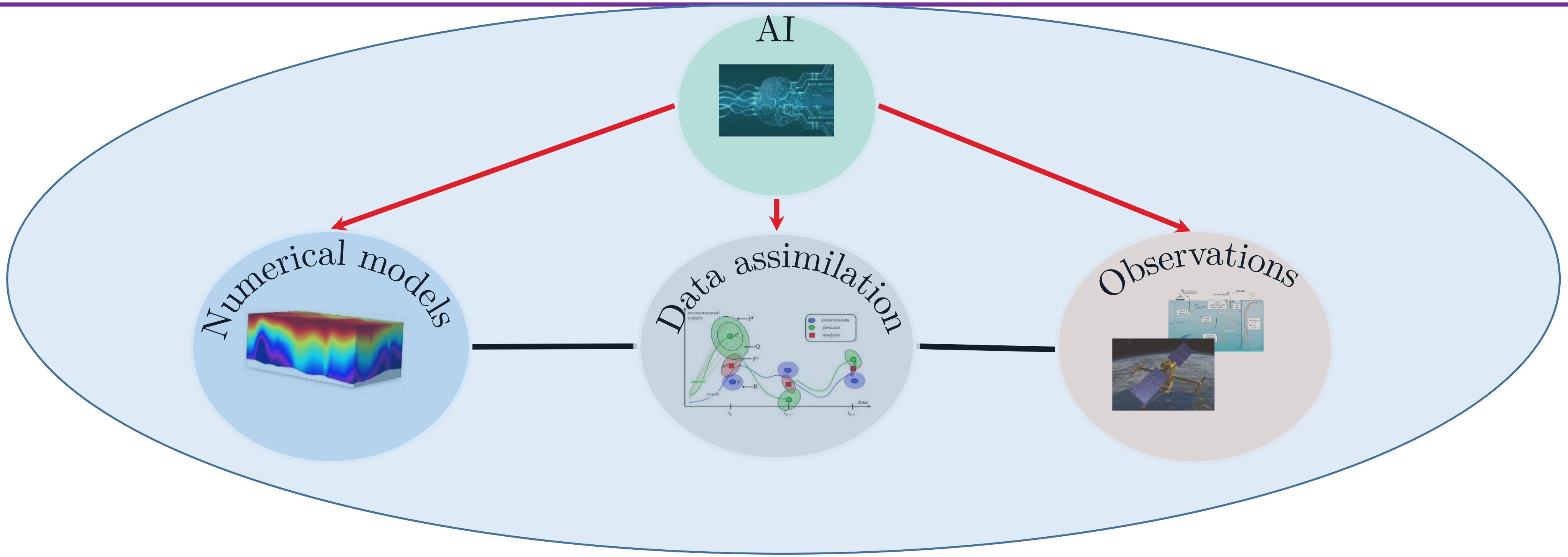


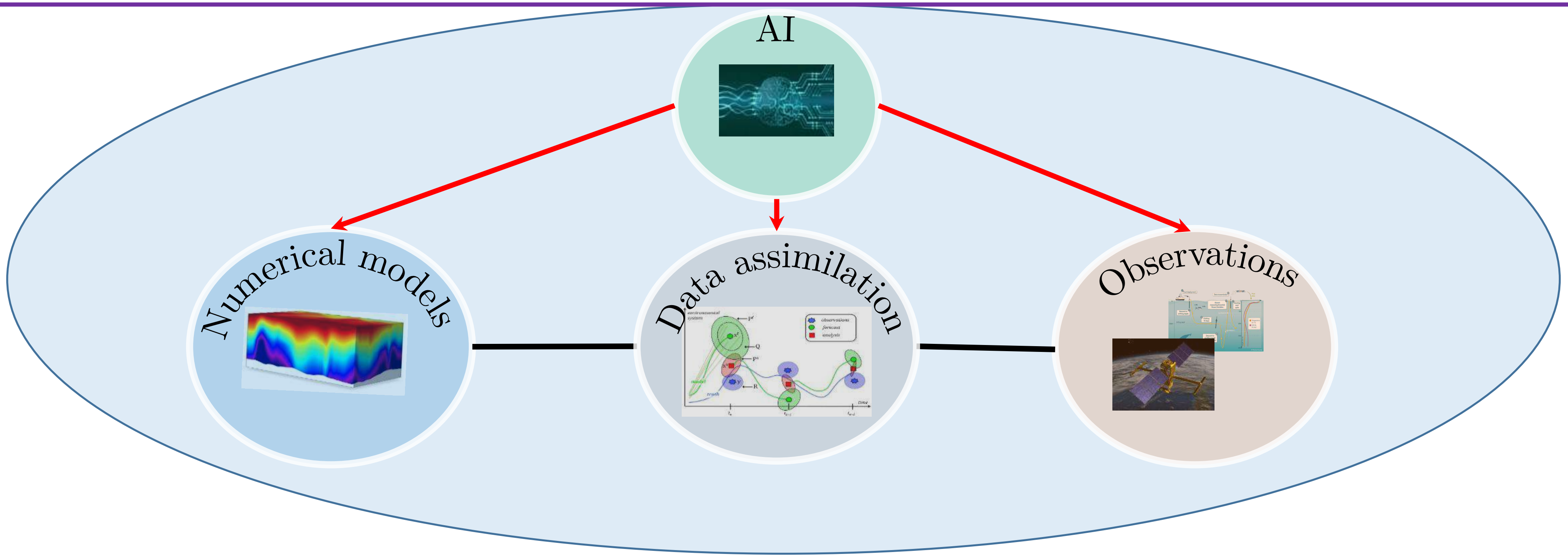
- Point of view from both AI generative models/standard DA schemes for surrogate modeling
  Machine learning, data assimilation and uncertainty quantification

IA in geophysical state estimation and DA



- Surrogate modeling
- Accelerating model resolution
- Model tuning and parameterization, hybrid models

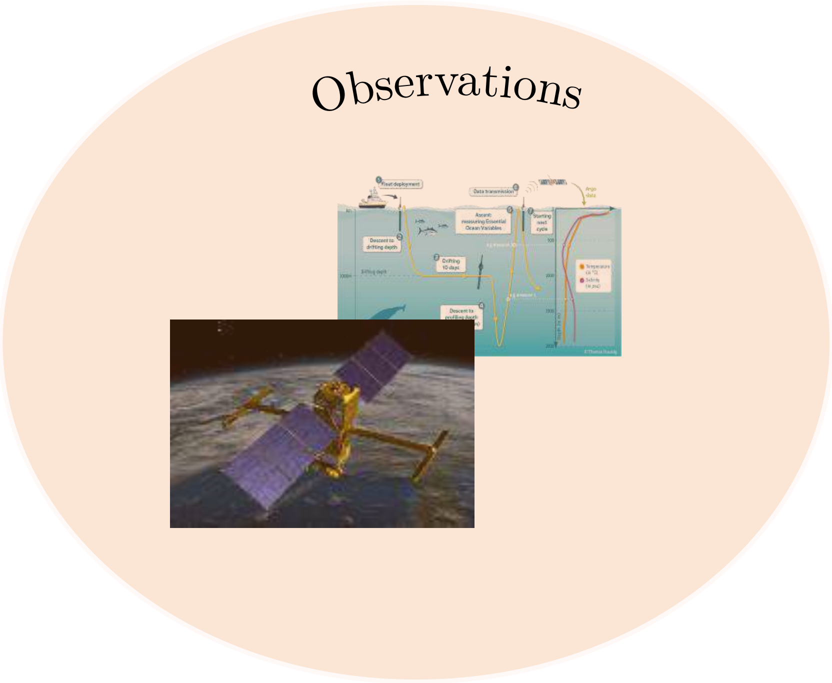
IA in geophysical state estimation and DA



- ➡ **Formulation of higher resolution interpolation with examples**
- ➡ **Generative models and data assimilation for modeling dynamical systems**
- ➡ **End-to-end Learning of sub-models in Hybrid Modeling Systems**

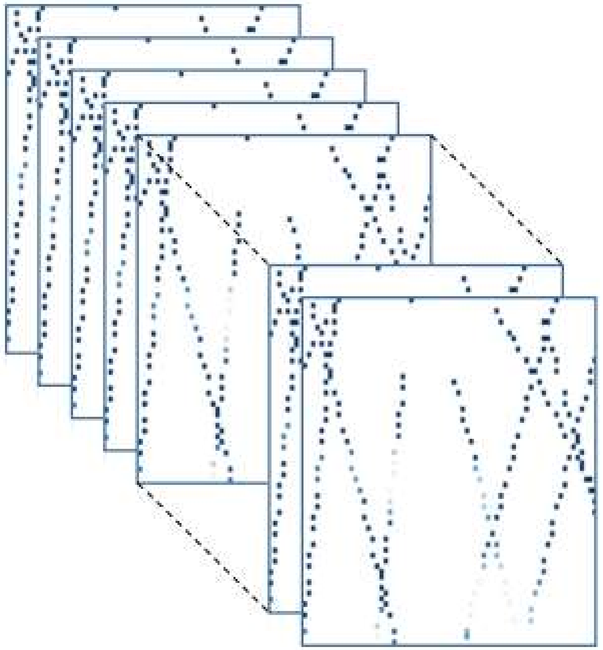
AI for observations

Higher resolution interpolation: general framework and applications



Higher resolution interpolation

Problem statement



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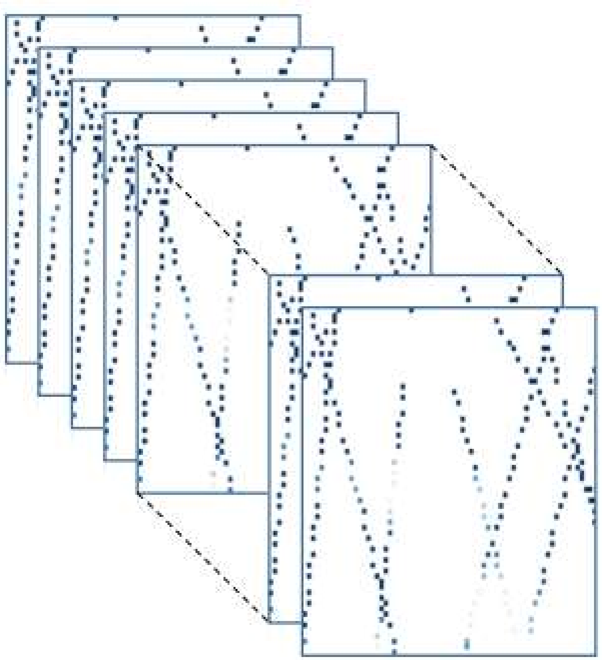

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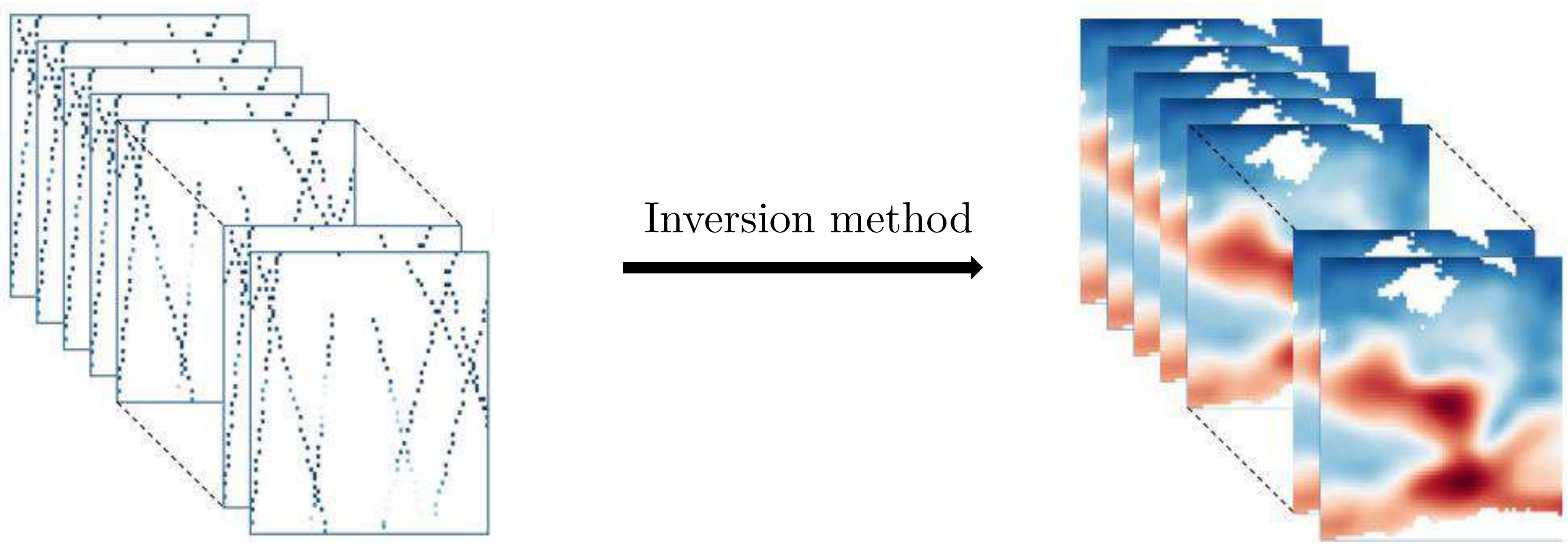

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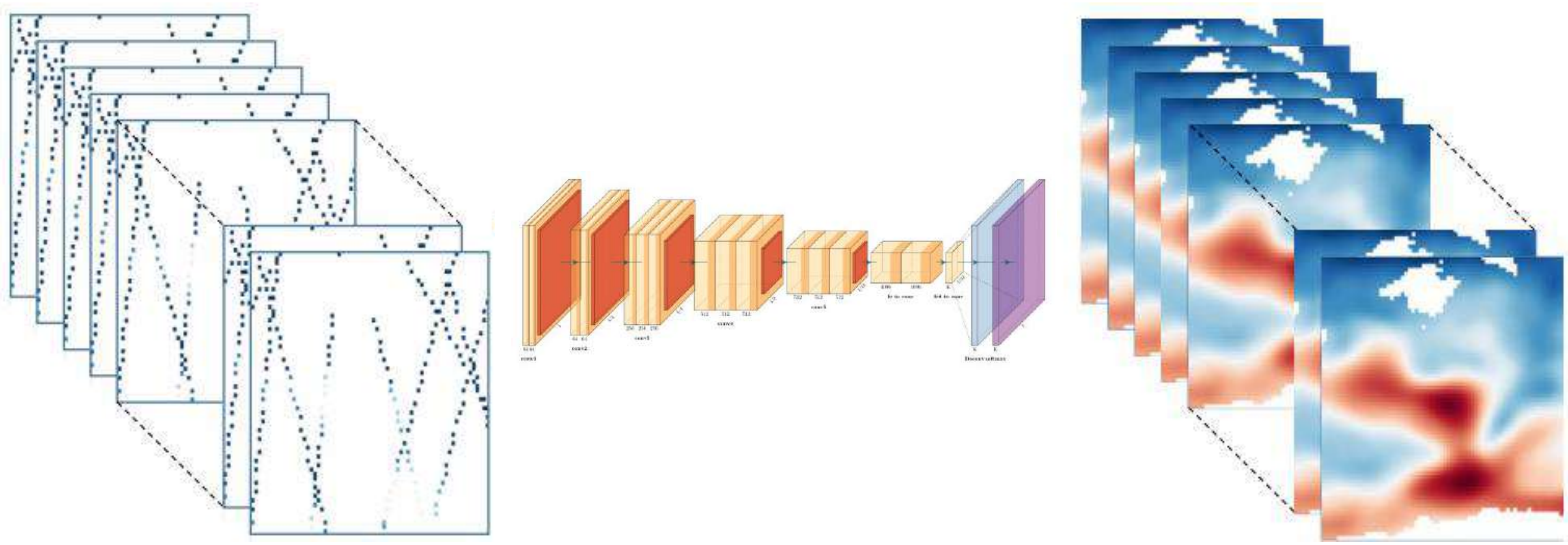

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- Takes advantage of recent developments in AI architectures

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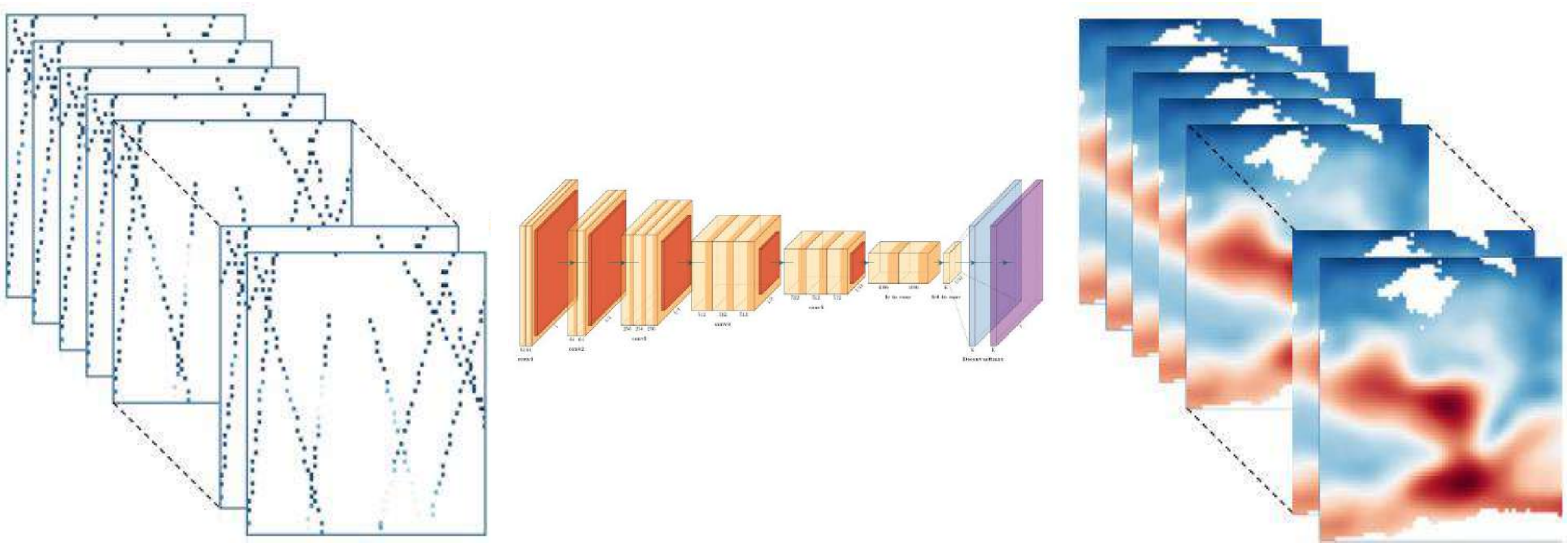

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- Uncertainty quantification ?
- Forecasting applications ?

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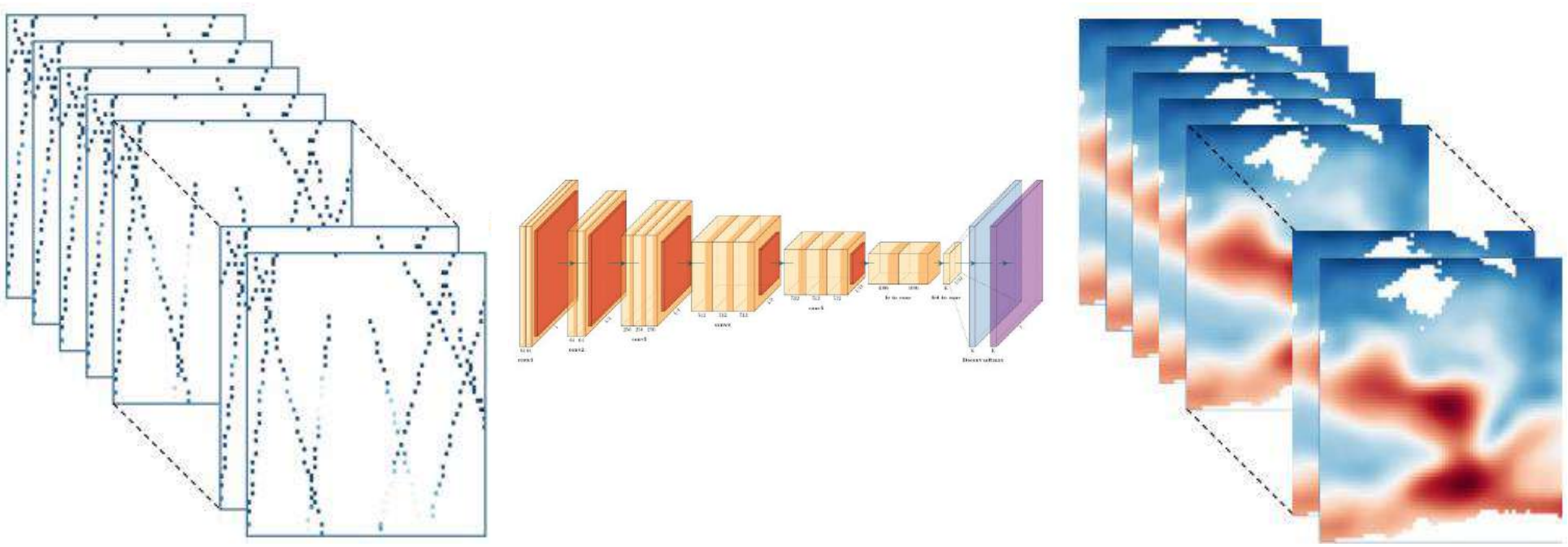

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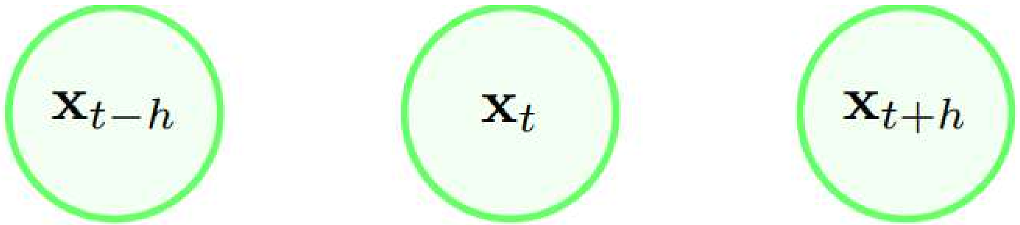

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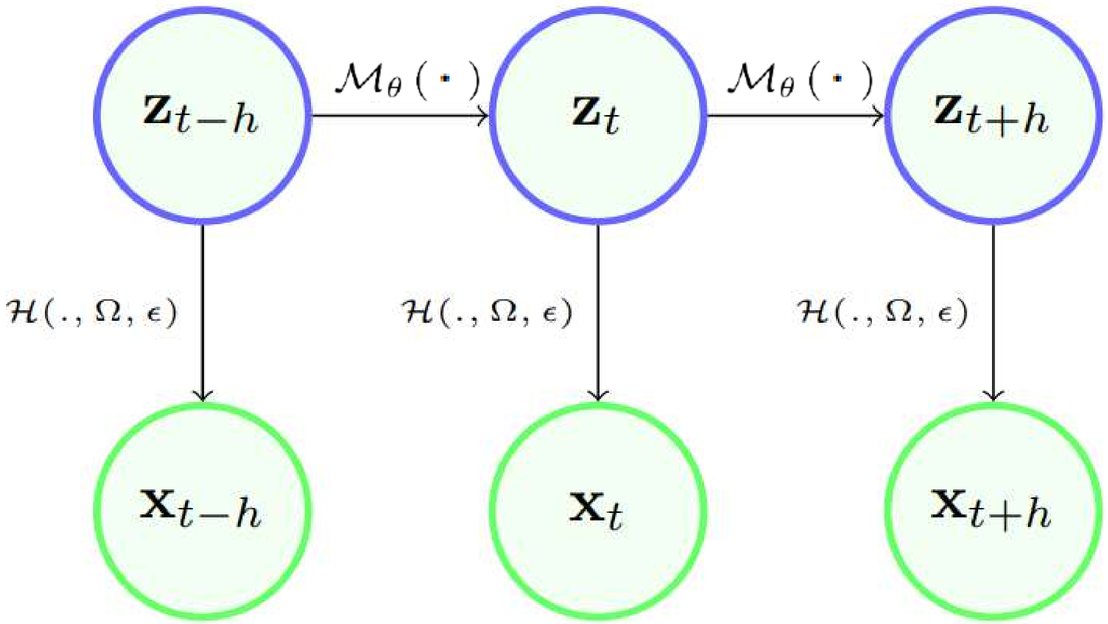
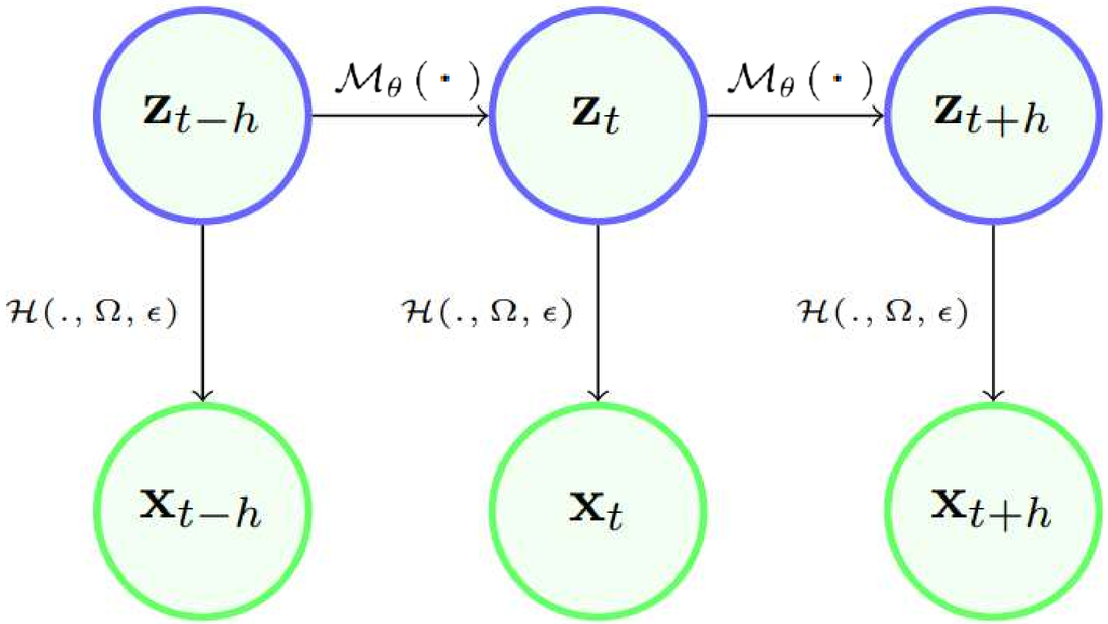


Higher resolution interpolation

Turn spatiotemporal interpolation into a Bayesian filtering problem:

- State variabl
- Observations

$$\begin{cases} \mathbf{z}_{t+1} = \mathcal{M}_\theta(\mathbf{z}_t) + \varepsilon_t \\ \mathbf{x}_t = \mathcal{H}_\theta(\mathbf{z}_t) + \mu_t \end{cases}$$



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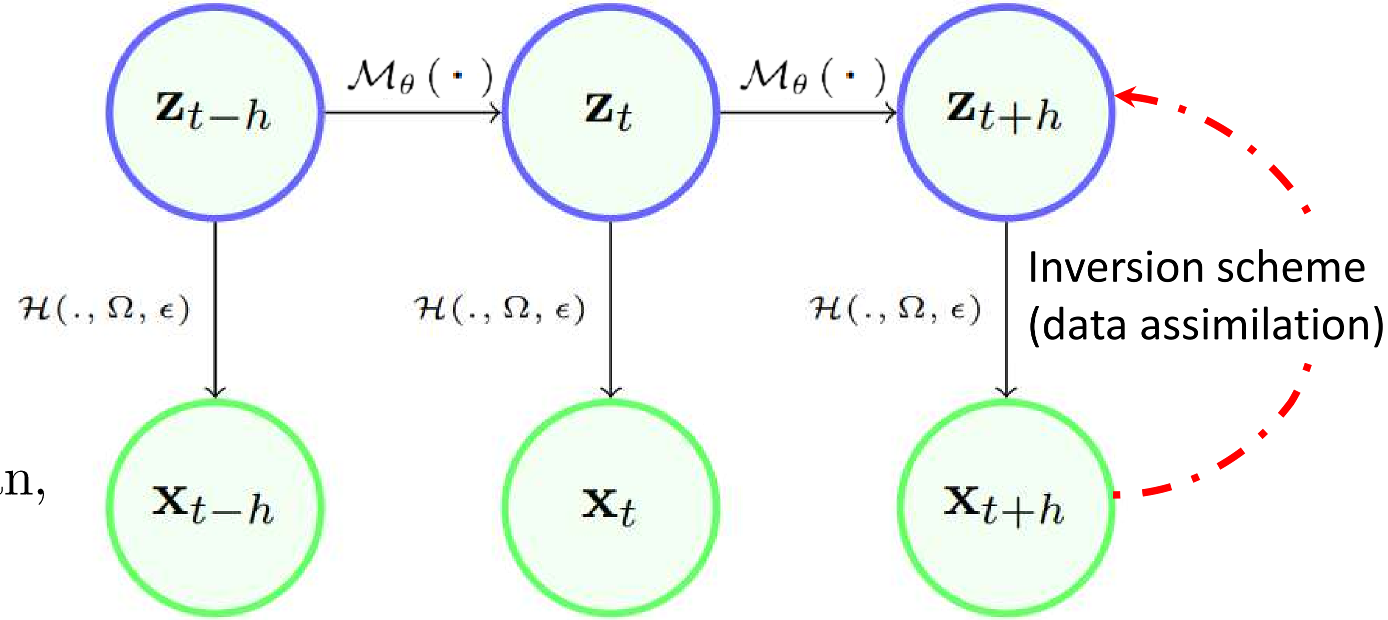

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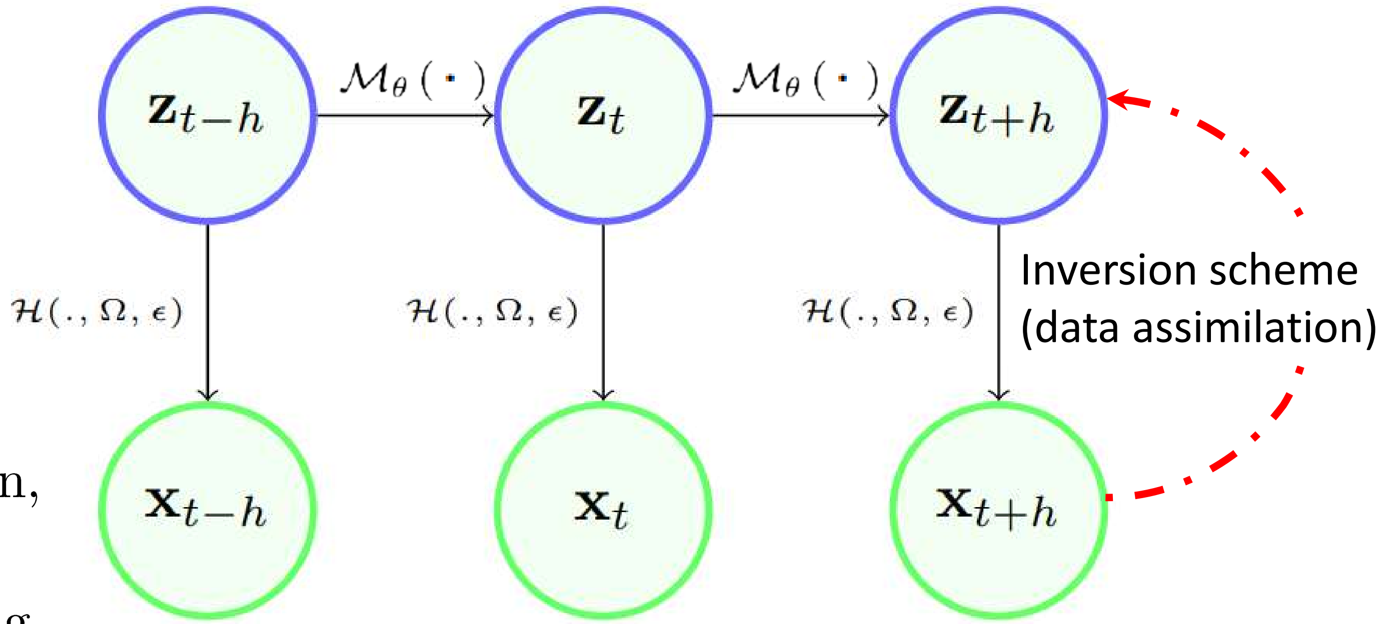

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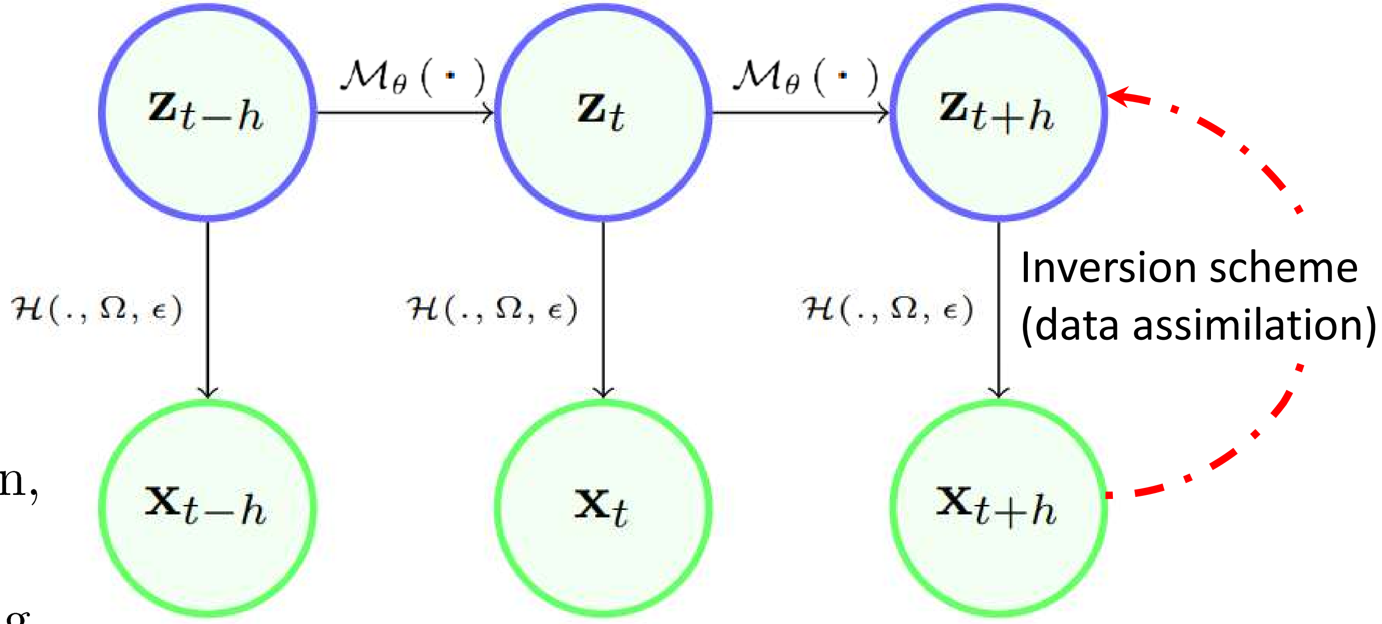

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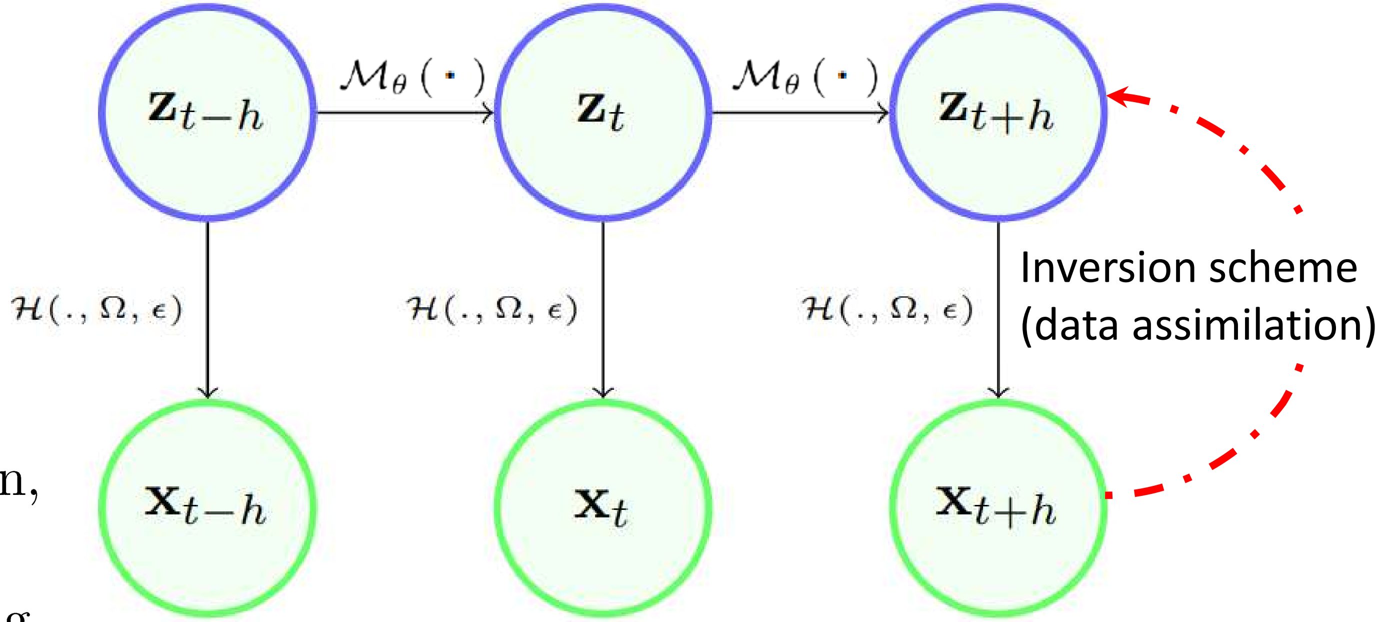

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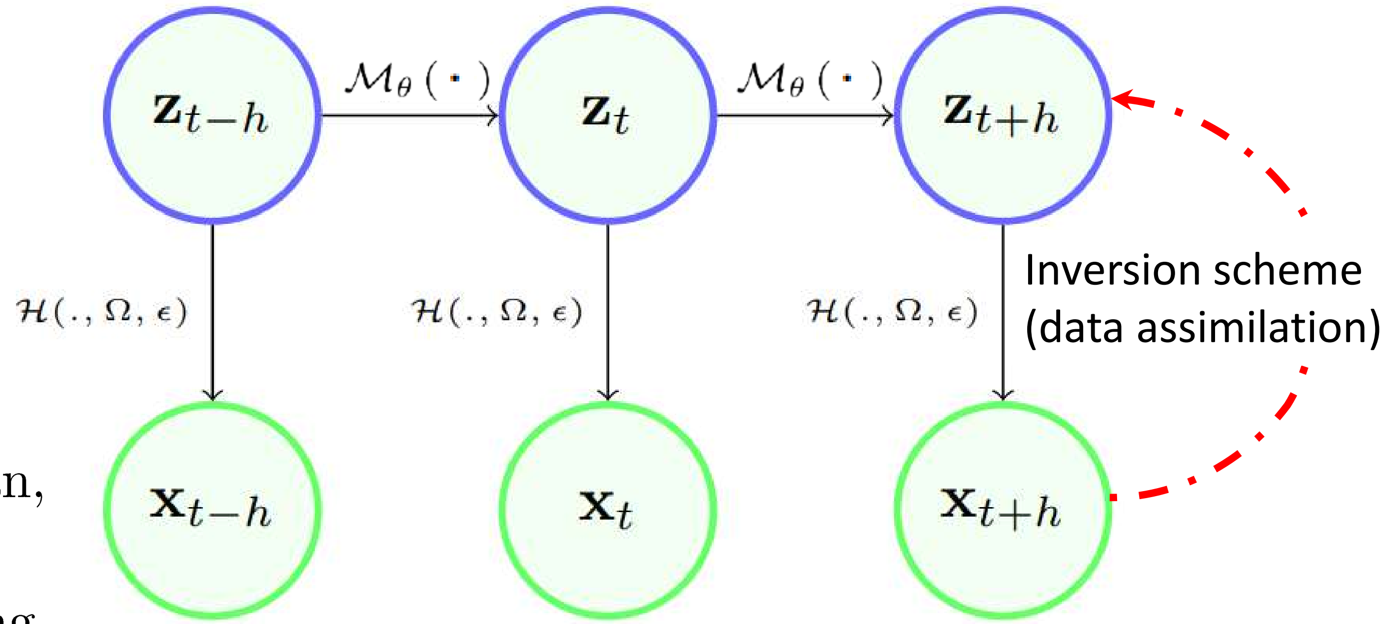

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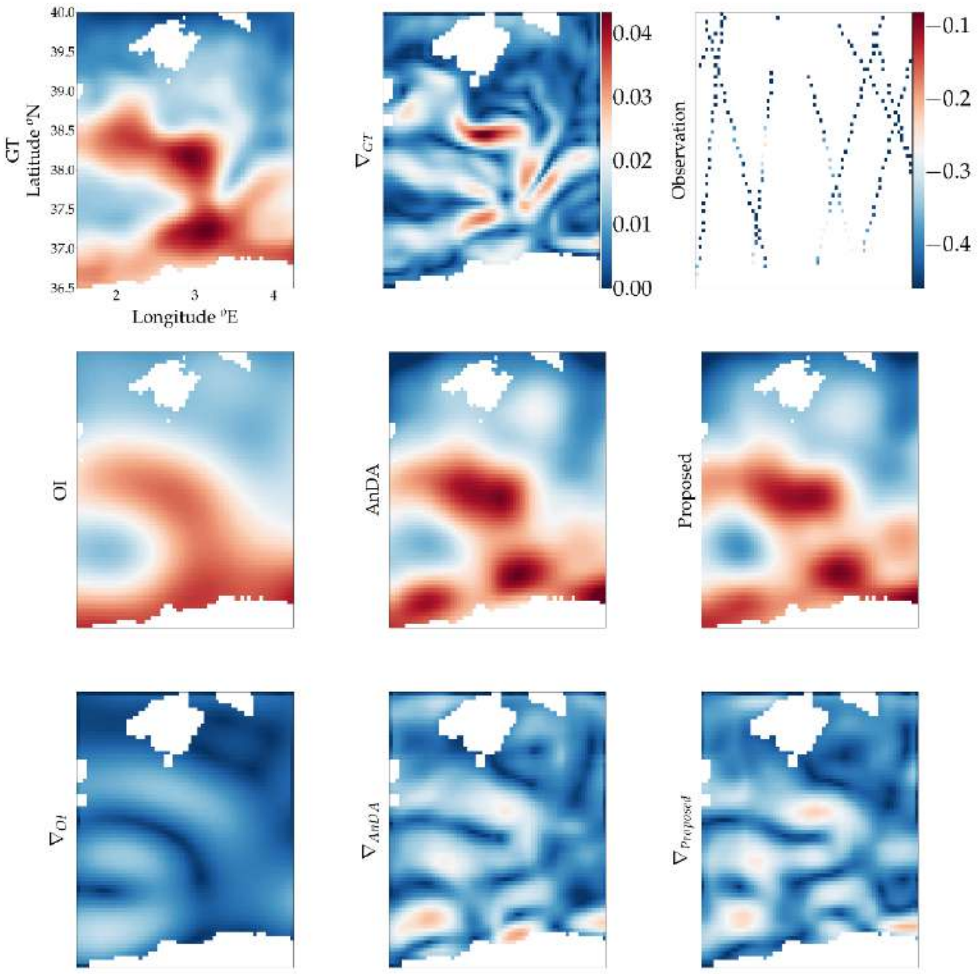
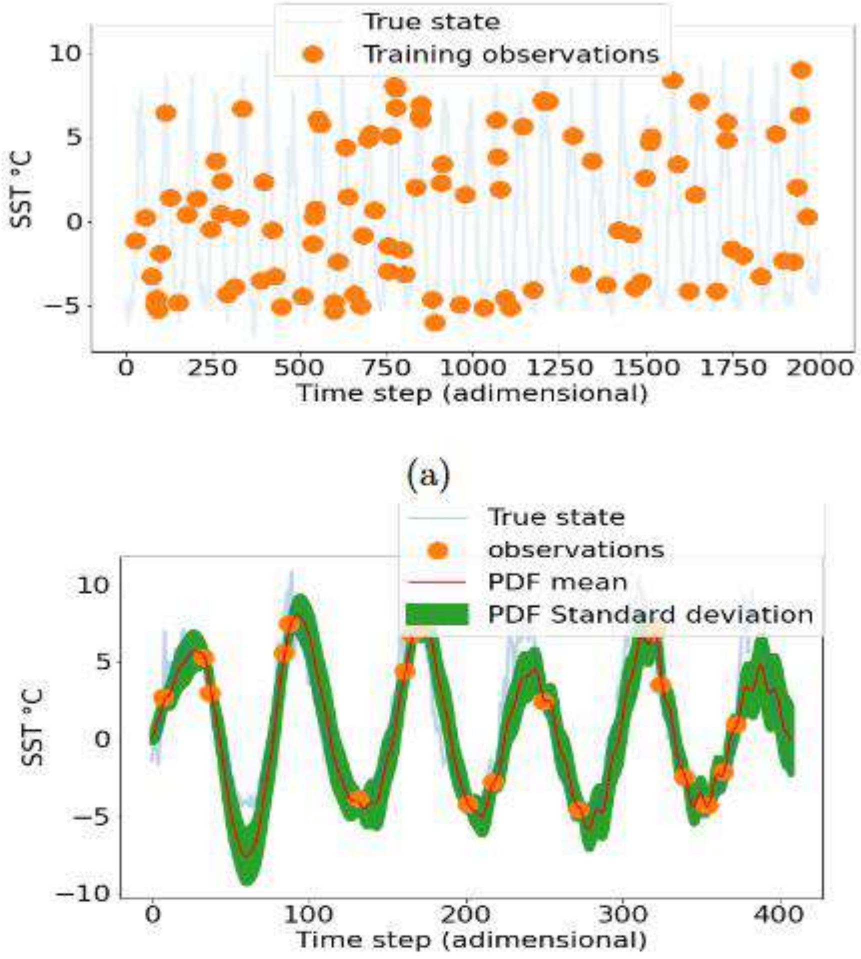
- Probabilistic formulation

Higher resolution interpolation, examples

Interpolation results of SLA data in med sea



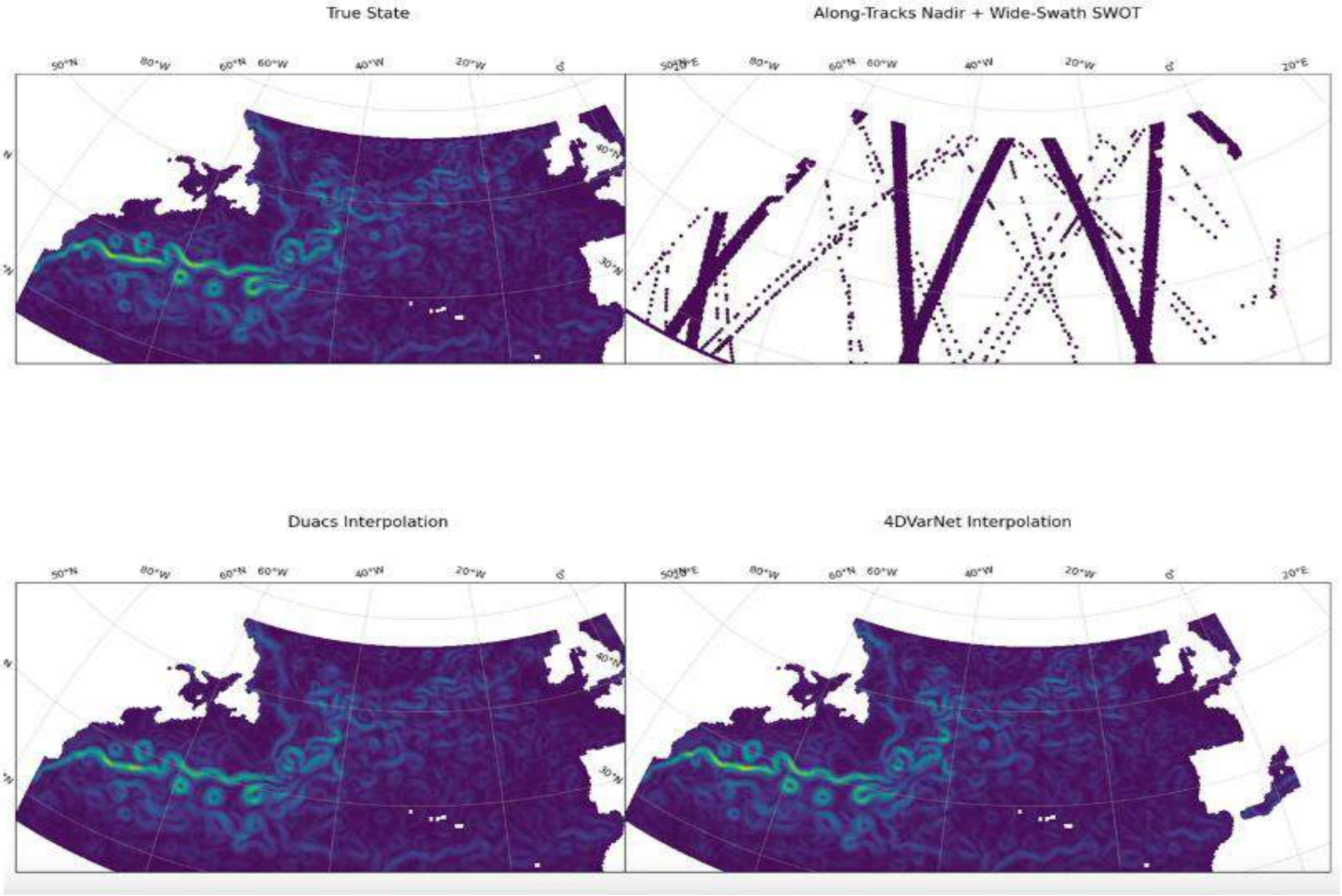
SST anomaly



(a)

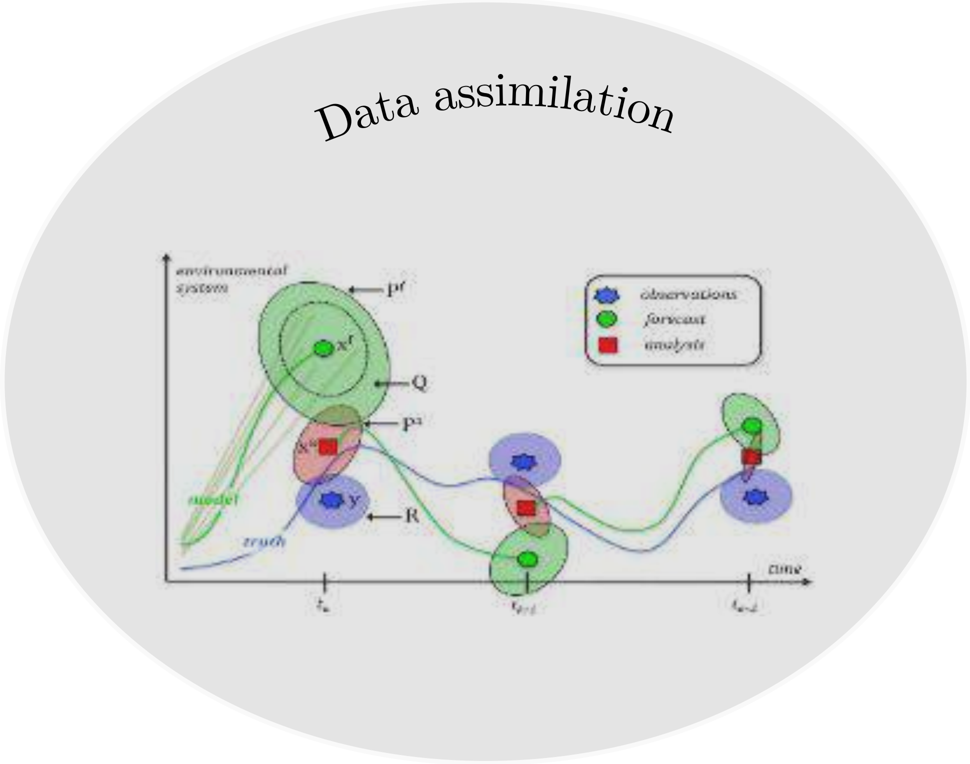
(b)

High


True State
Along-Tracks Nadir + Wide-Swath SWOT
Duacs Interpolation
4DVarNet Interpolation
50°N
80°W
60°N
60°W
40°W
20°W
0°
20°E
40°N
30°N

AI for Data Assimilation

Generative models and data assimilation for modeling dynamical systems



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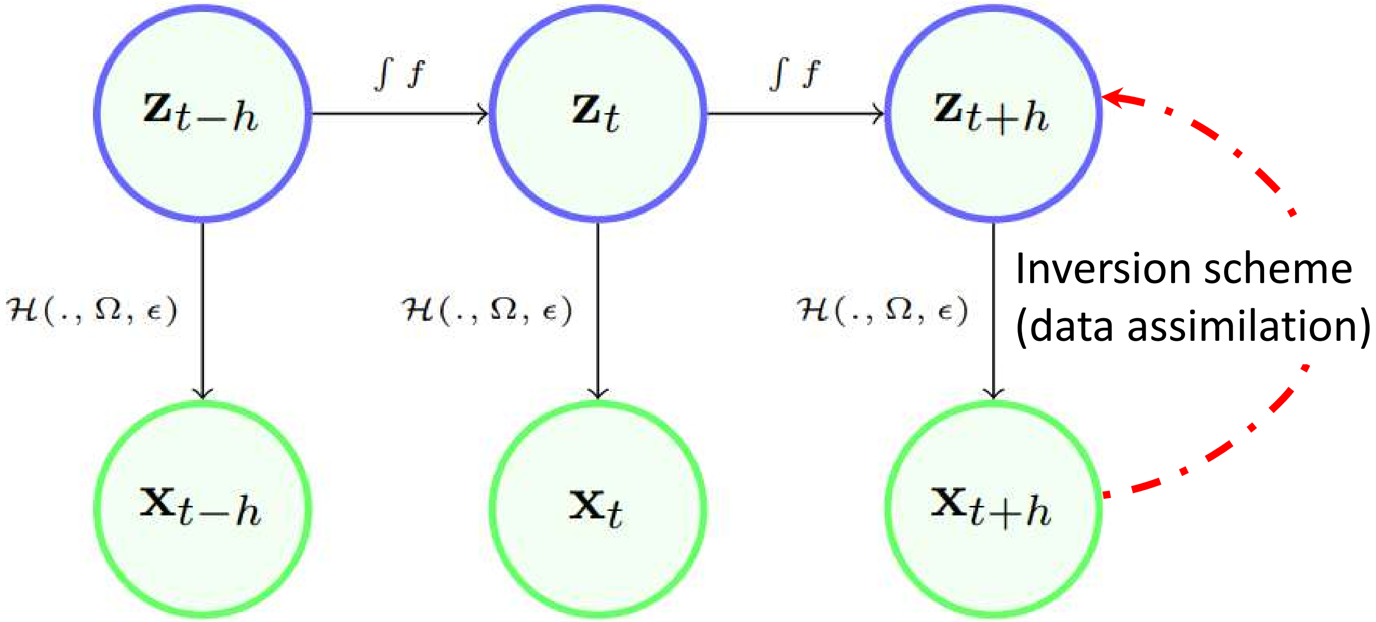

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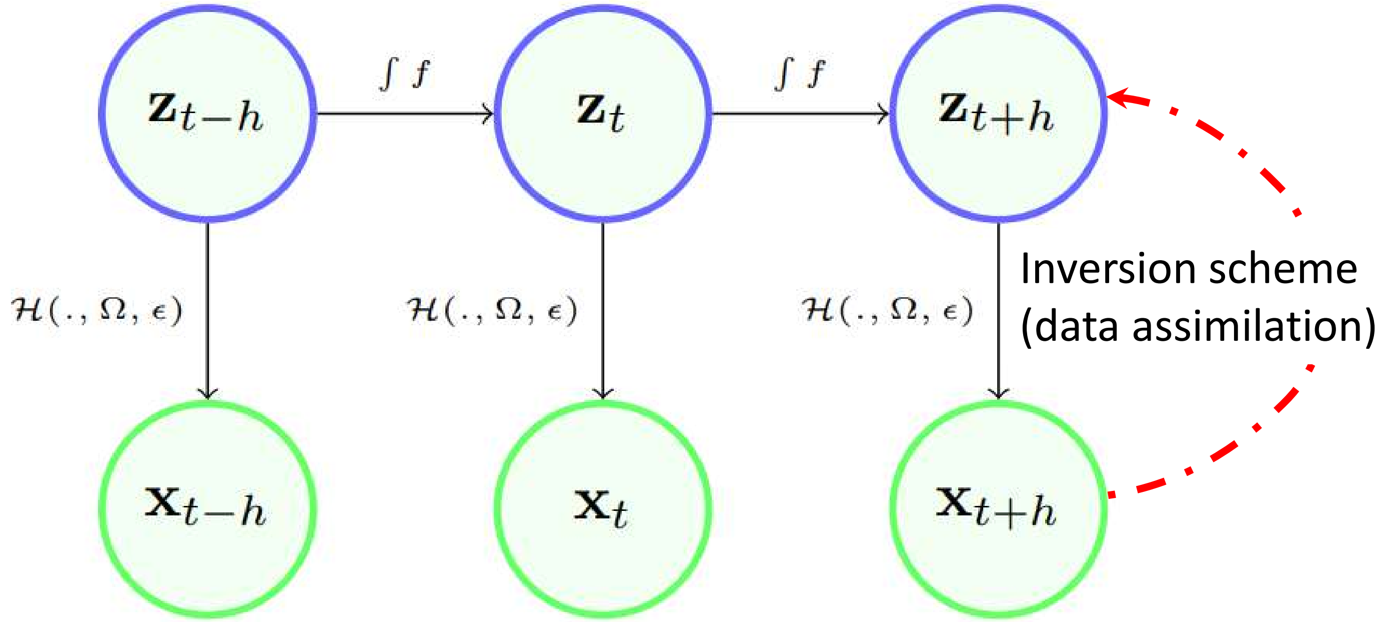

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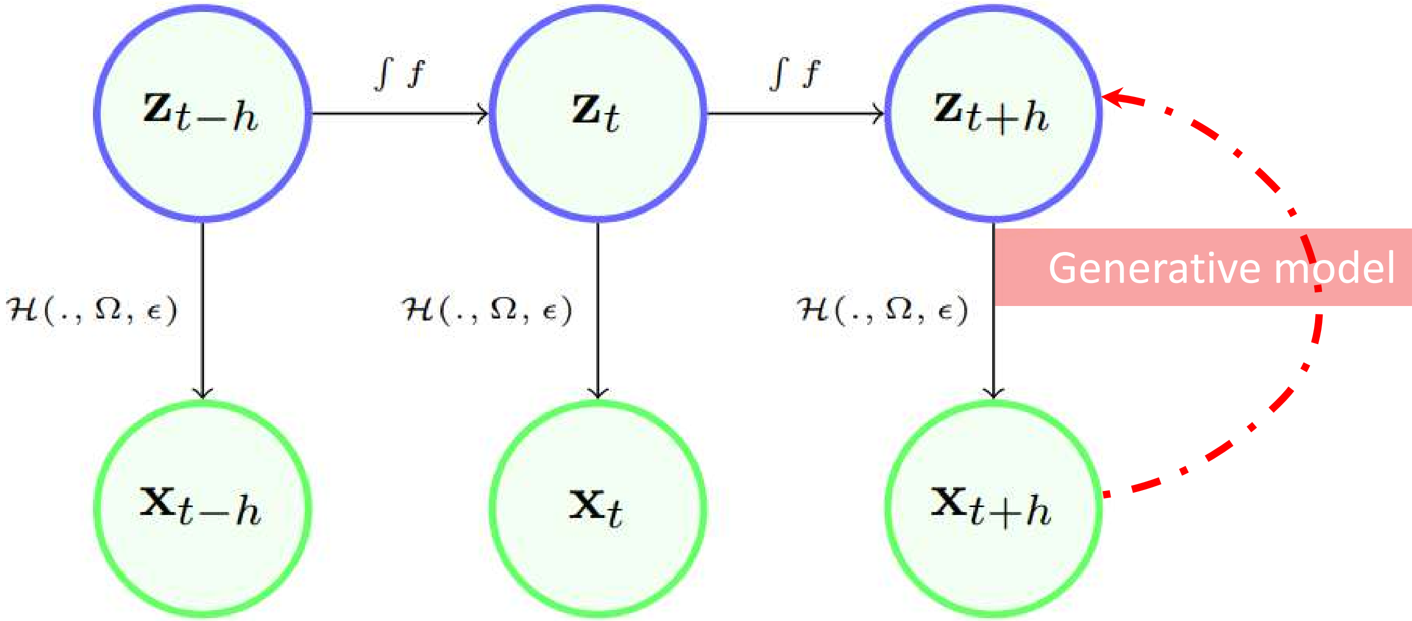

- We showed previously how to use DA to solve interpolation/forecasting problems

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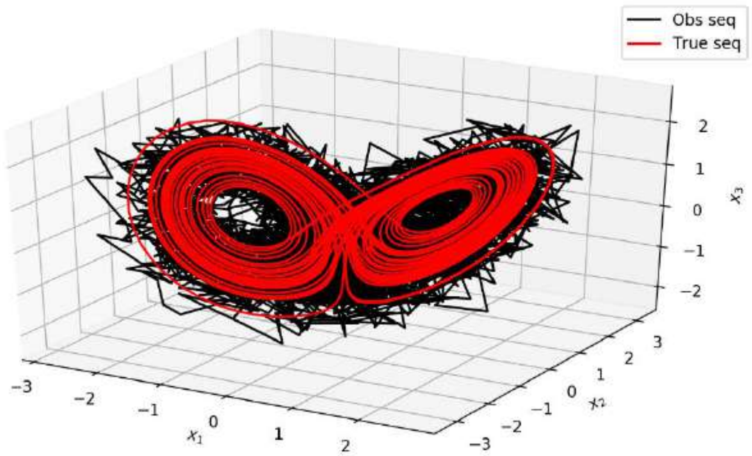
- For instance, we can maximize the evidence lower bound of the SSM:

$$\underbrace{\log p_\theta(\mathbf{x}_{t_0:t_N})}_{\text{Model evidence}} = \underbrace{-\mathbb{E}_{q_\phi}\left[\log q_\phi(\cdot \mid \mathbf{x}_{t_0:t_N})\right] + \mathbb{E}_{q_\phi}\left[\log p_\theta(\cdot, \mathbf{x}_{t_0:t_N})\right]}_{\text{Marginal log Likelihood (ELBO)}} + \underbrace{D_{KL}\left(q_\phi(\cdot \mid \mathbf{x}_{t_0:t_N}) \| p_\theta(\cdot \mid \mathbf{x}_{t_0:t_N})\right)}_{\text{Intratable, } > 0}$$

Generative models and data assimilation

Application example, Learning dynamical systems from noisy/partial observations

Lorenz 63 system



Training both the:

- Dynamical model
- The noise variances
- The Filter

Generative models and data assimilation

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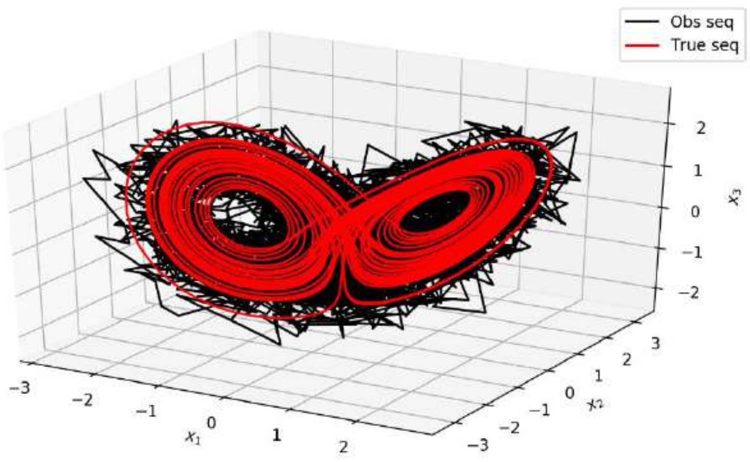

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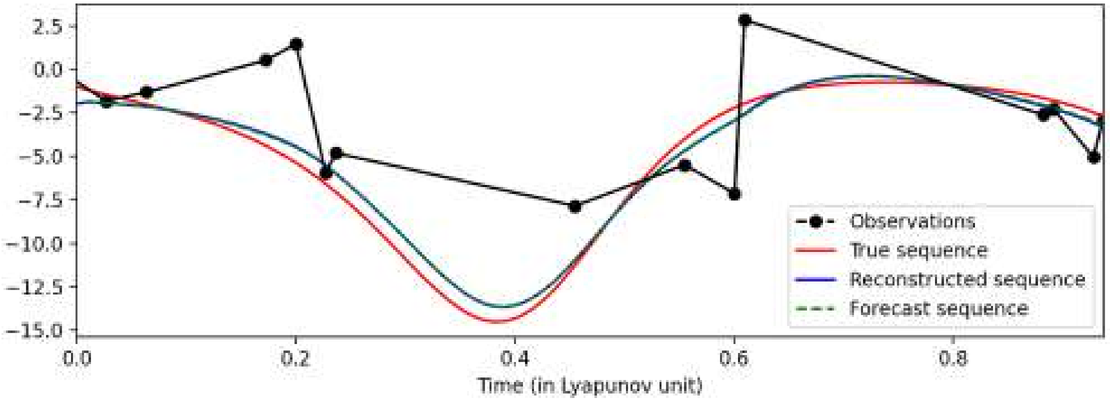
An example of the first dimension of the L63 system reconstructed by the inference module of our model. The observations are noisy (r = 33%) and irregularly sampled



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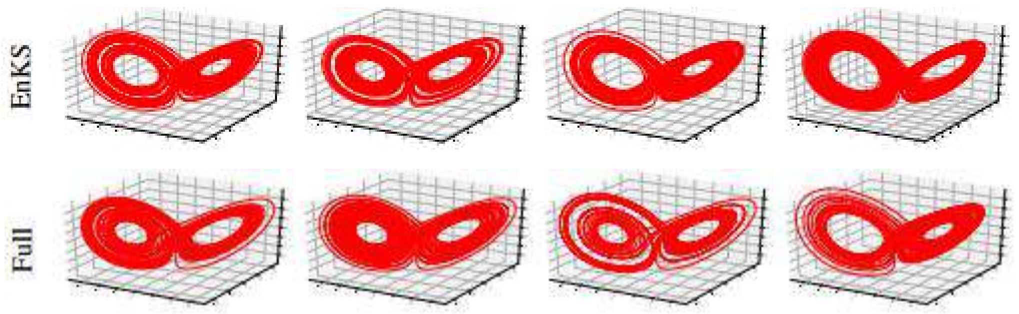

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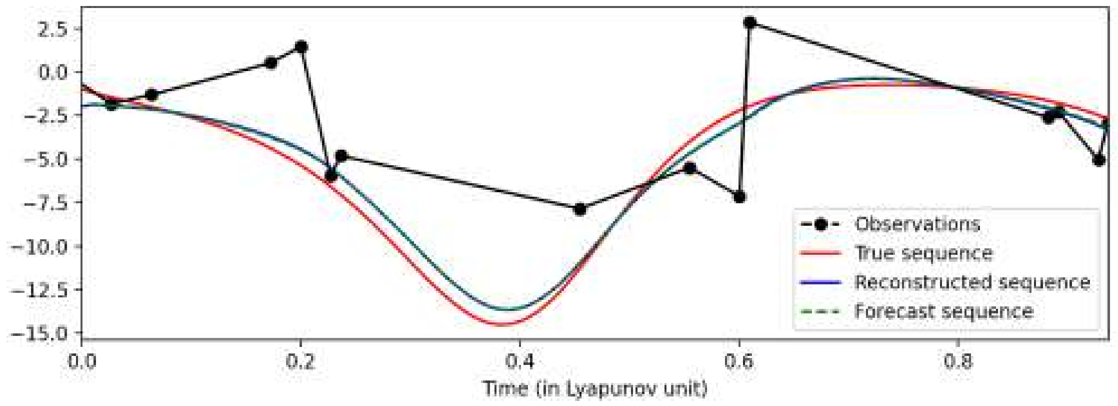

Generative models and data assimilation

Ongoing works on further links between DA and generative models

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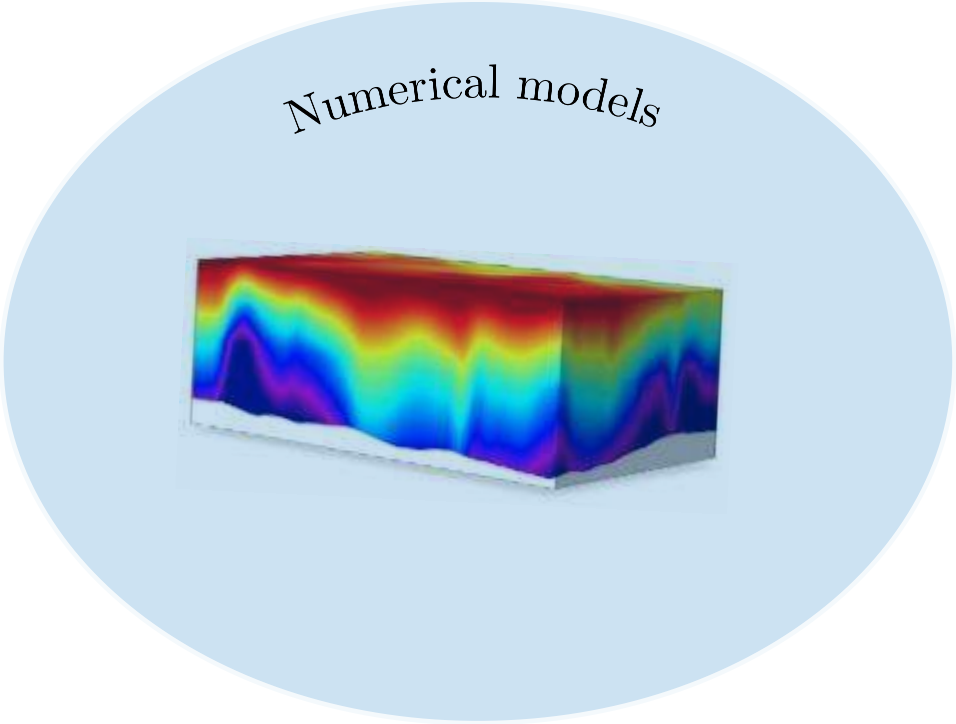
- Given the parameters of the SSM, than maximizing the ELBO gives us a filter
- If the filter converges, we even have an estimate of the model evidence (can be used for model selection)
- Benchmark this framework against standard DA for applications such as filtering, smoothing, and parameters/evidence estimation

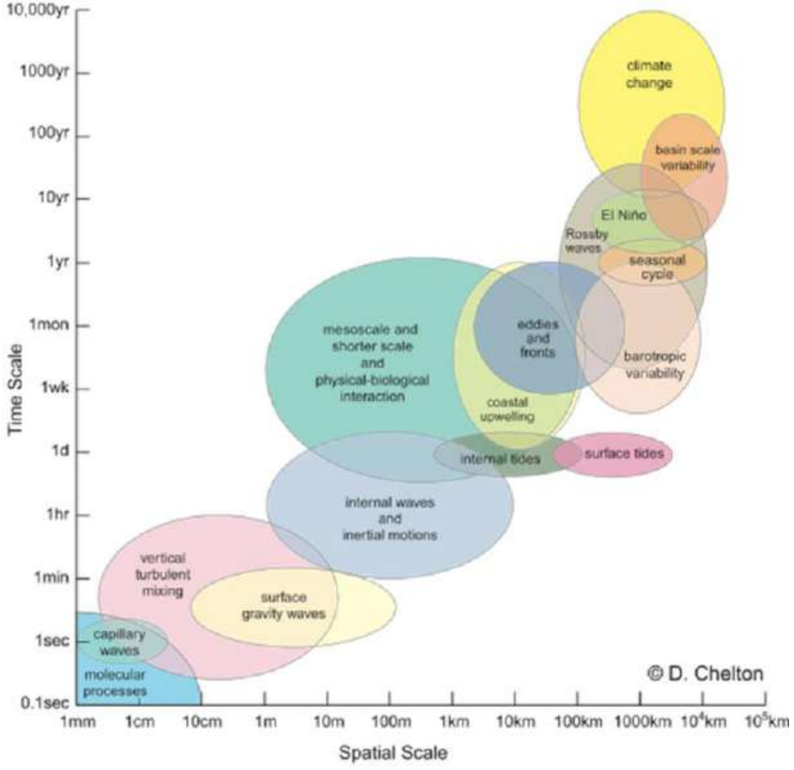
AI for Numerical Models

End-to-end Learning of sub-models in Hybrid Modeling Systems



Online learning of hybrid models
Tuning geophysical models

Reality



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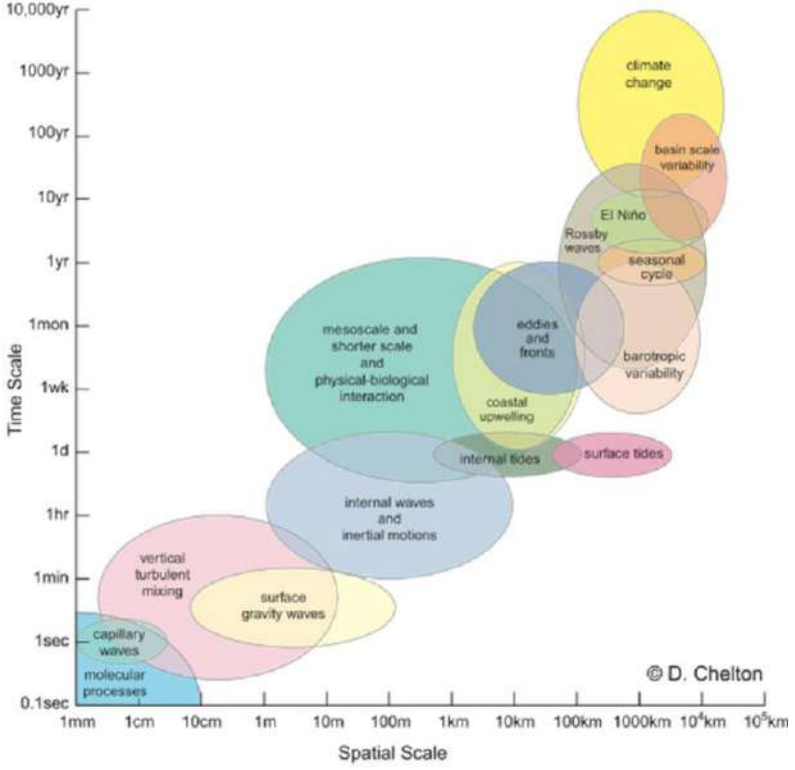

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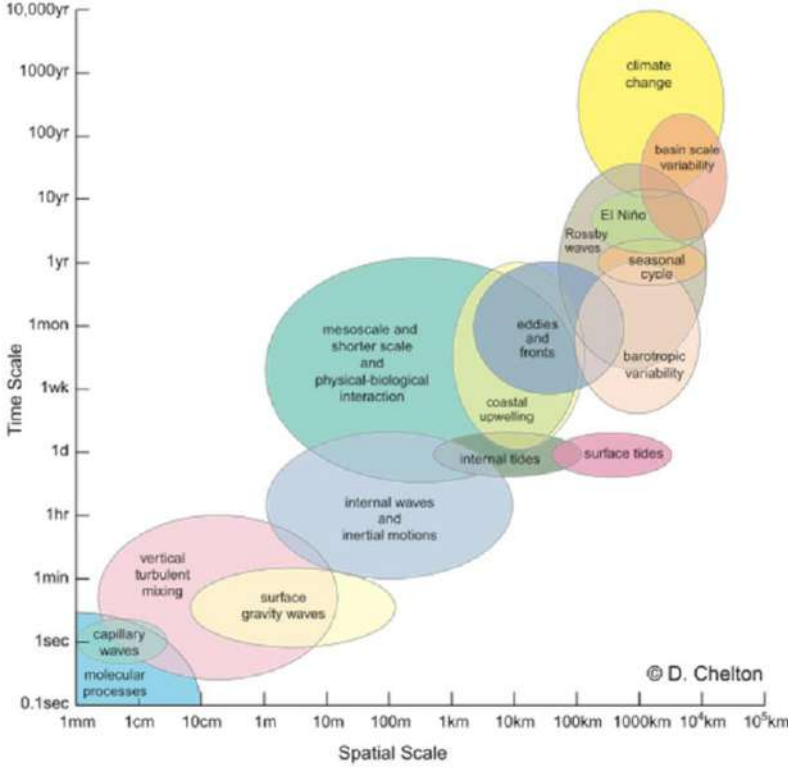
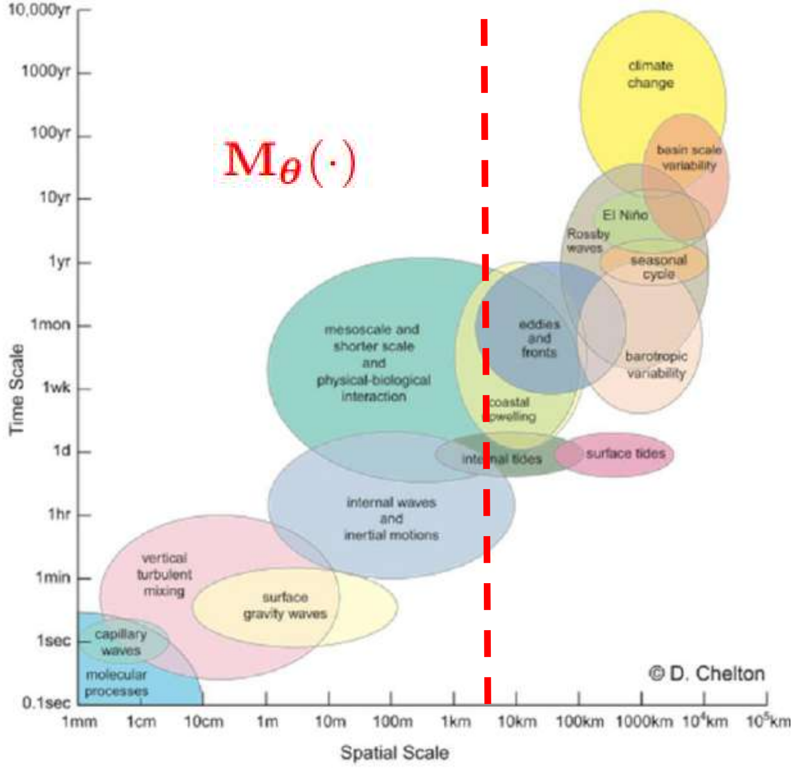


Computer



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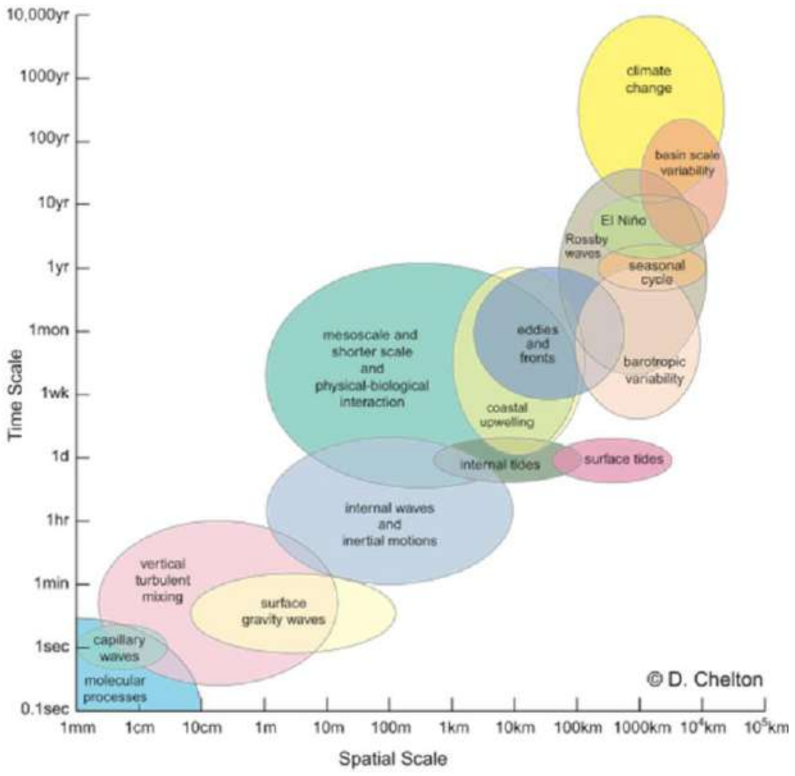
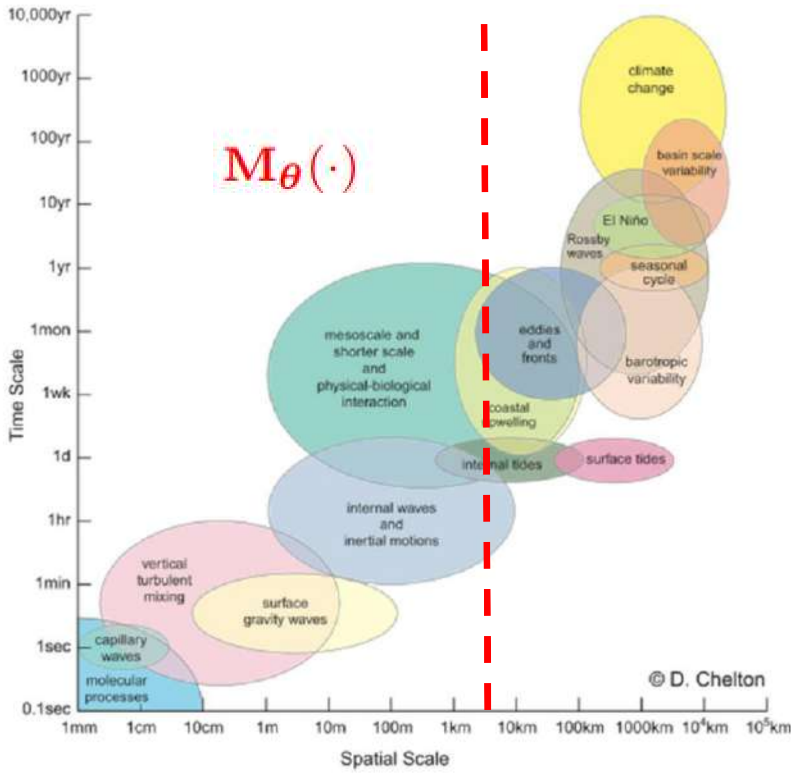


Computer



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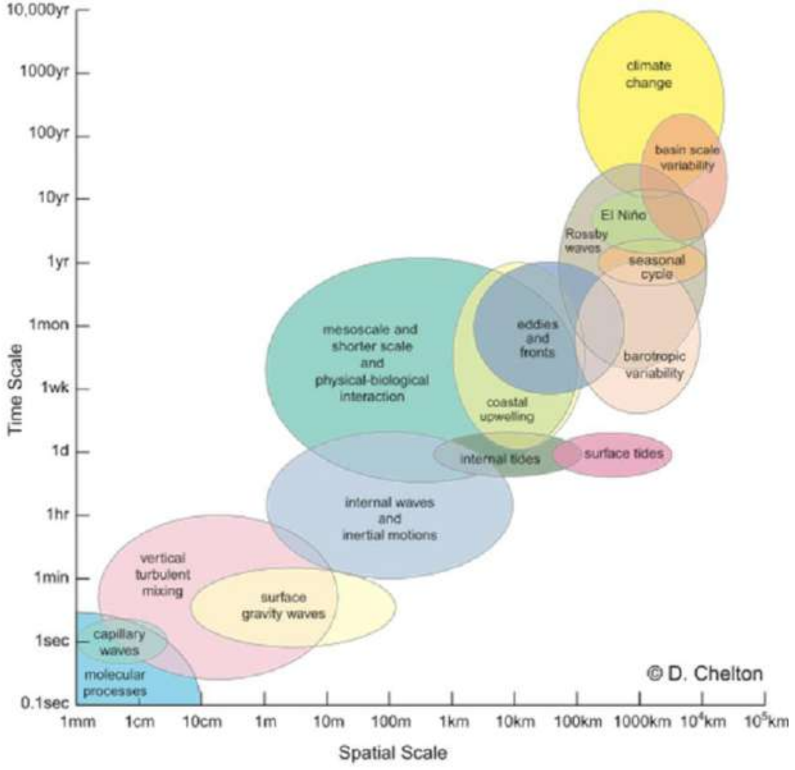
Online learning of hybrid models
Tuning geophysical models

Reality



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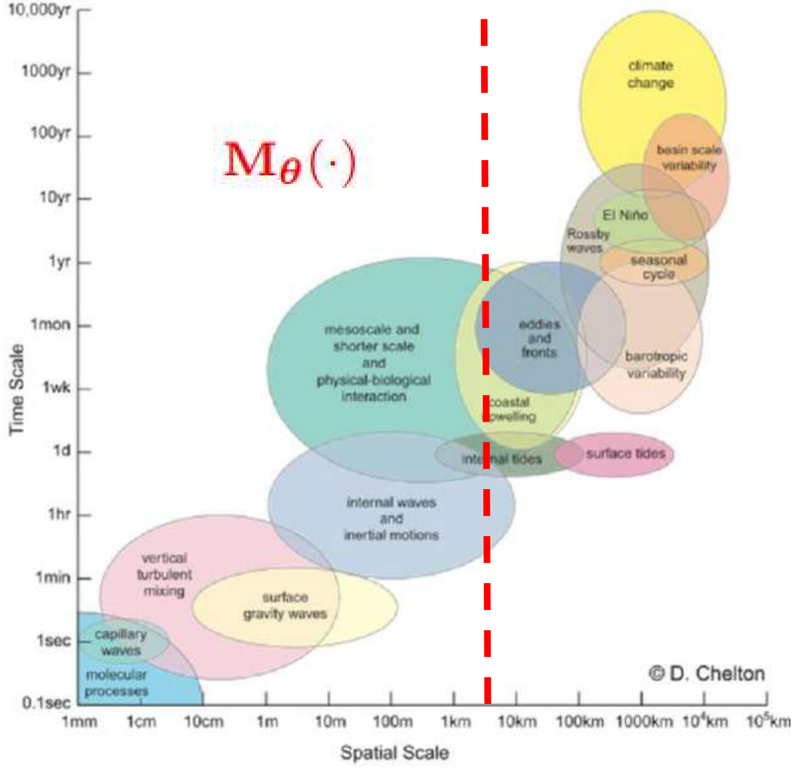

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Online learning with hybrid models ?

Online learning of hybrid models

Training hybrid models

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Online learning of hybrid models

Training hybrid models

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Online learning of hybrid models

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\Psi^n(\mathbf{u}_t) = \mathbf{u}_{t+nh} \approx \mathbf{u}_t + \int_{t_0}^{t0+nh} (\mathbf{F}(\mathbf{u}_t) + \mathbf{M}_{\boldsymbol{\theta}}(\mathbf{u}_t))dt
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- How to calibrate $\boldsymbol{\theta}$ the parameters of the model ?

Online learning of hybrid models

Training hybrid models, offline vs online learning

Training hybrid models, offline vs online learning

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Training hybrid models, offline vs online learning

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- Define and compute the parameterization term: R_t

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- Just an emulator of a parameterization term need to have access to R_t, do not use historical data

Training hybrid models, offline vs online learning

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$$= \underbrace{\frac{\partial Q(\cdot,\cdot,\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}}_{\text{Gradient of the regularization}} + \underbrace{\frac{\partial Q(\cdot, \mathbf{g}(\Psi^n(\mathbf{u}_t)), \cdot)}{\partial \mathbf{g}} \frac{\partial \mathbf{g}}{\partial \Psi}}_{\text{Gradient of the online cost w.r.t. } \Psi} \underbrace{\frac{\partial \Psi^n(\mathbf{u}_t)}{\partial \boldsymbol{\theta}}}_{\text{Gradient of the solver}}$$

Online learning of hybrid models

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  - Derivative free methods ?

Online learning of hybrid models
Euler Gradient Approximation

- Let us consider an explicit Euler solver Ψ_E, a single step integration using Ψ_E can be written as:

$$\mathbf{u}_{t+h} = \Psi(\mathbf{u}_t)$$

where

$$\Psi_E(\mathbf{u}_t) = \mathbf{u}_t + h(\mathbf{F}(\mathbf{u}_t) + \mathbf{M}_{\boldsymbol{\theta}}(\mathbf{u}_t))$$

- Assuming that the solver Ψ has order $p \geq 1$, we can write for any initial condition:

$$\begin{aligned}\mathbf{u}_{t+h} &= \Psi(\mathbf{u}_t) \\ &= \Psi_E(\mathbf{u}_t) + O(h^2)\end{aligned}$$

Online learning of hybrid models
Euler Gradient Approximation

- By using this approximation, we can show that the gradient of the solver can be decomposed as (for a fixed n):

$$\frac{\partial}{\partial \boldsymbol{\theta}}\Psi^n(\mathbf{u}_t) = \sum_{j=1}^{j=n-1}\Big(\prod_{i=1}^{i=n-j}\underbrace{\frac{\partial \Psi(\Psi^{n-i}(\mathbf{u}_t))}{\partial \Psi^{n-i}(\mathbf{u}_t)}}_{\textit{Jacobian of the flow}}\Big) h \underbrace{\frac{\partial}{\partial \boldsymbol{\theta}}\mathbf{M}_{\boldsymbol{\theta}}(\Psi^{j-1}(\mathbf{u}_t))}_{\textit{Gradient of the sub-model}} + h\frac{\partial}{\partial \boldsymbol{\theta}}\mathbf{M}_{\boldsymbol{\theta}}(\Psi^{n-1}(\mathbf{u}_t)) + O(h^2)$$

- If we approximate the Jacobian (we can use a static/ensemble approximation, a TLM if any), we can compute the gradients only using the gradient of the sub-model;
- And for n fixed, the gradients converge to the true ones quadratically in h;

QG turbulence

- The dimensionless governing equations in the vorticity (ω) and stream function (ψ) formulation in a doubly periodic square domain with length L = 2π are:

$$\frac{\partial \omega_t}{\partial t} + \mathcal{A}(\omega_t, \psi_t) = \frac{1}{\mathrm{Re}}\nabla^2 \omega_t - f - r\omega_t$$
$$\nabla^2 \psi_t = -\omega_t$$

- where $\mathcal{A}(\omega_t, \psi_t)$r represents the nonlinear advection term:

$$\mathcal{A}(\omega_t, \psi_t) = \frac{\partial \psi_t}{\partial y}\frac{\partial \omega_t}{\partial x} - \frac{\partial \psi_t}{\partial x}\frac{\partial \omega_t}{\partial y}$$

- and f represents a deterministic forcing:

$$f(x, y) = k_f\left[\cos(k_f x) + \cos(k_f y)\right]$$

QG turbulence, LES

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$$\nabla^2 \psi_t = -\omega_t \qquad\qquad \nabla^2 \bar{\psi}_t = -\bar{\omega}_t$$

- Model the subgrid-scale term $\Pi_t \approx \mathbf{M}_{\boldsymbol{\theta}}$

QG turbulence

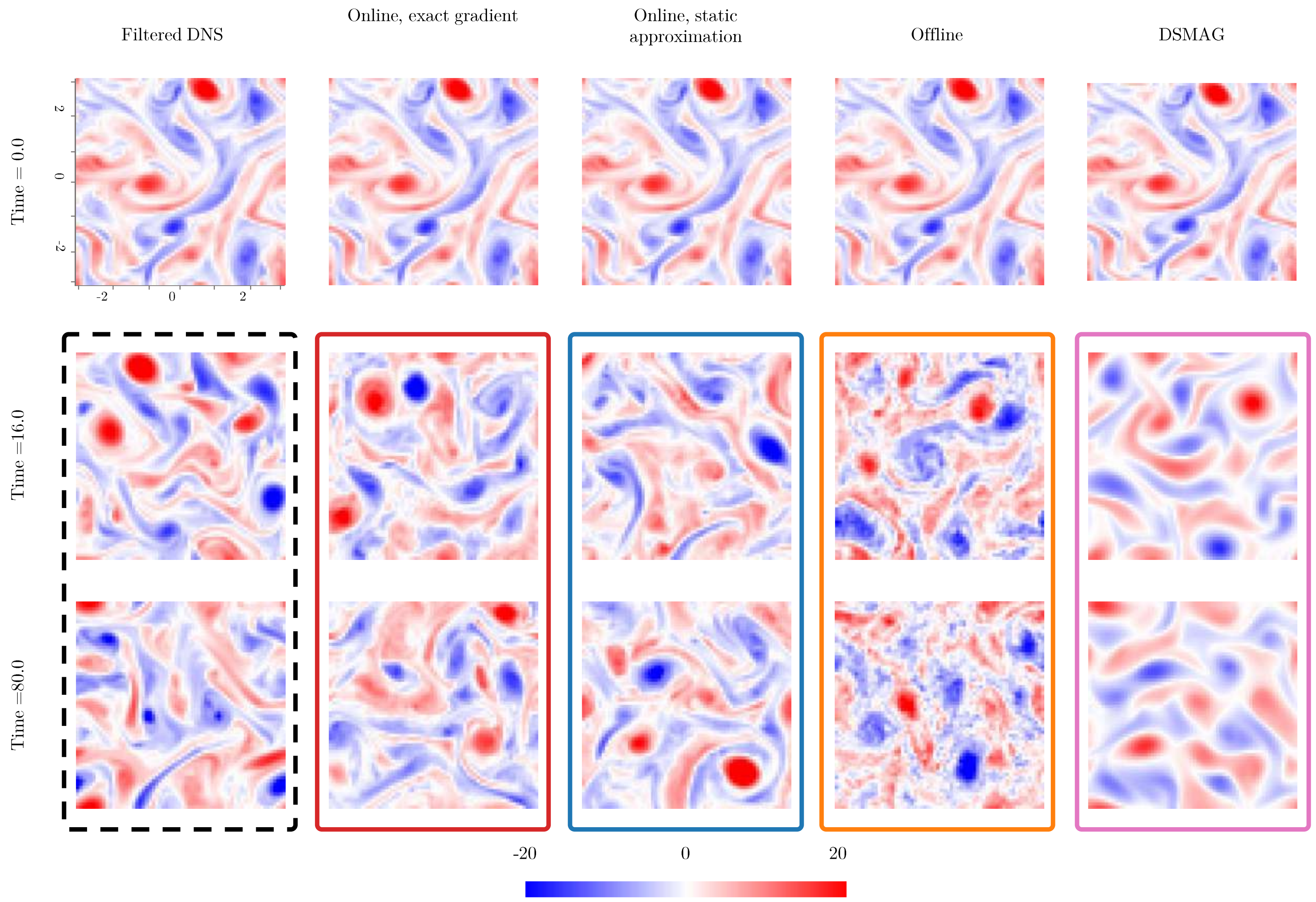
Flow configuration:

- High resolution grid : 1024×1024.
- Low resolution : 64×64.
- Re : 20000, r = 0.1, kf = 4;

Tested models:

- Online learning with exact gradient;
- Online learning with approximate gradient;
- Offline learning;
- Dynamic Smagorinsky (DSMAG)

QG turbulence



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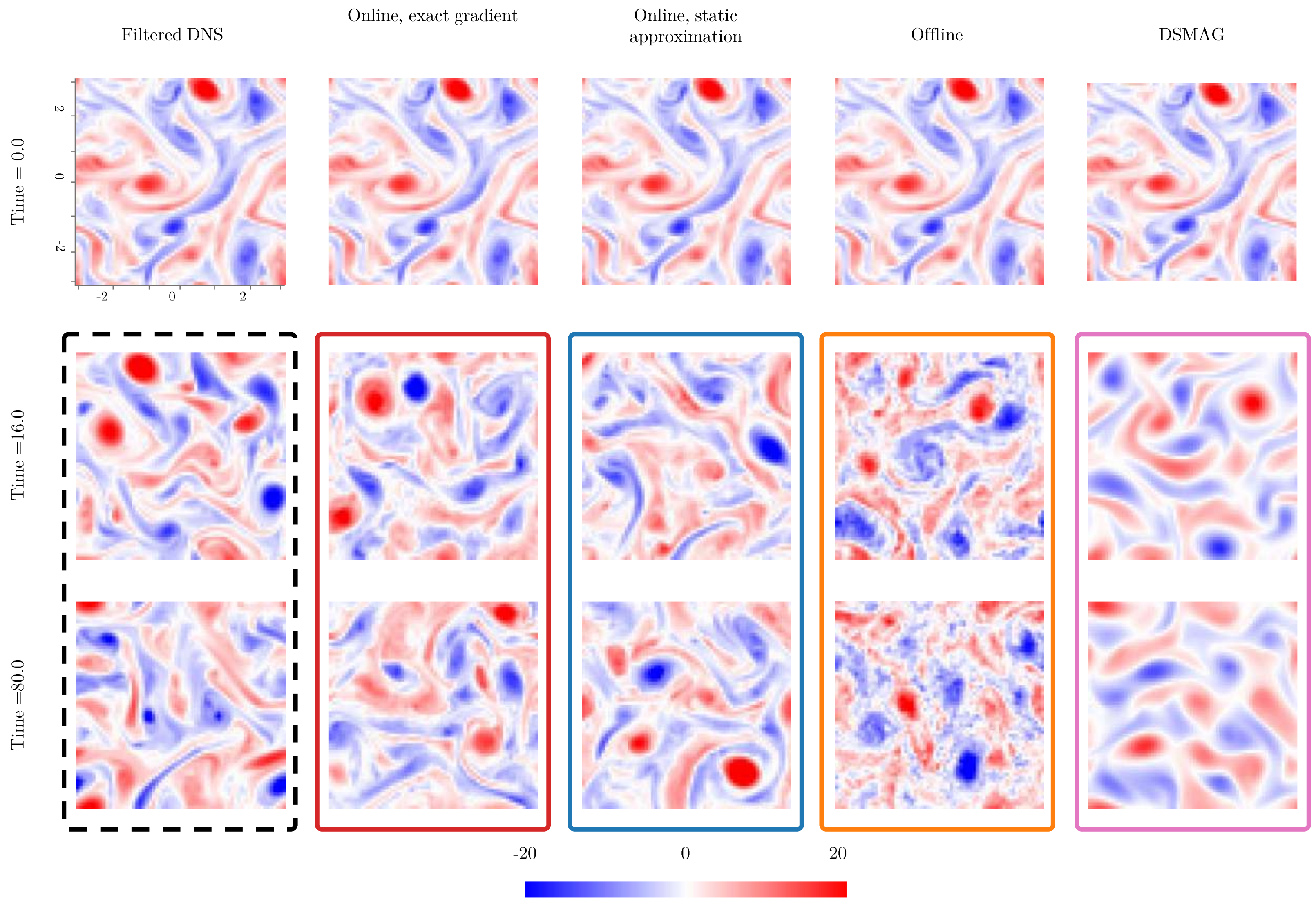

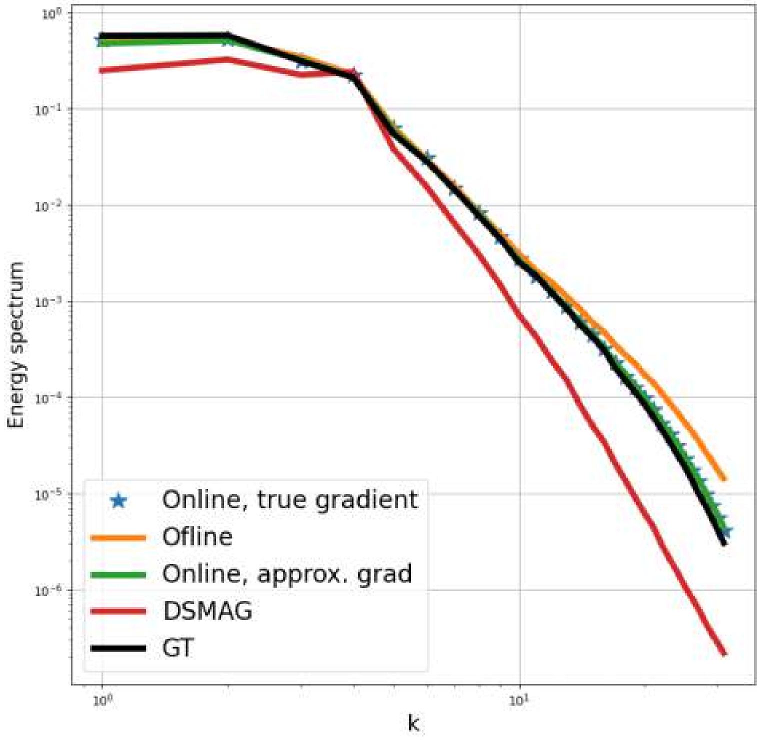

QG turbulence

- We proposed a simple gradient estimator for learning online hybrid models;
- Proposed methodology does not rely on a differentiable physical model, and can (in theory) be applied on non-differentiable CFD/GFD codes;
- Can use better Jacobian approximation and can be extended to definition of non additive correction terms;
- Interpretability/constraining the sub-model ?
- Multiple (stochastic) sub-models ?

Key points and perspectives

- IA can be used to improve models/data
- One of the key points is to formulate the problem we want to solve
- Towards problem standardization, benchmarks based on ocean data ?