

# Lecture #5: Deep Learning and Inverse Problems in Geoscience

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Advanced course on Deep Learning and  
Geophysical Dynamics

Lab-STICC



# Inverse Problems in Geoscience

Mathematical formulation for inverse  
Problems

Inverse problems & Deep learning

Applications to geophysical dynamics

# Inverse Problems in Geoscience

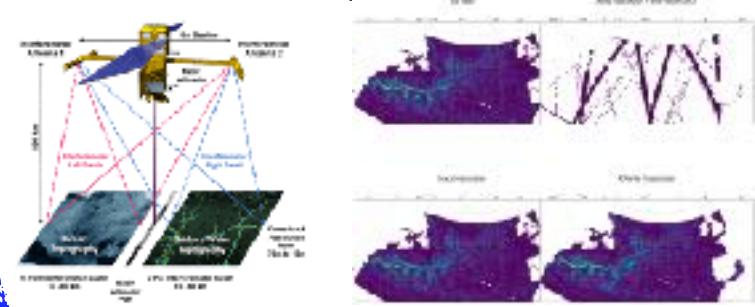
Mathematical formulations for inverse  
Problems

Inverse problems as learning problems

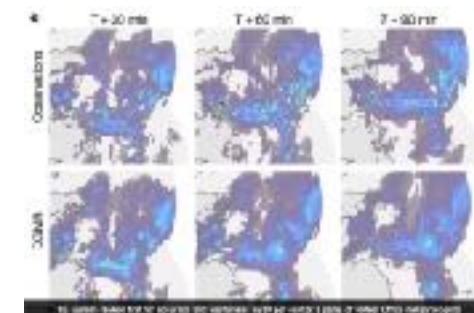
Applications to geophysical dynamics

# Inverse Problems in Geoscience: some examples

# Interpolation

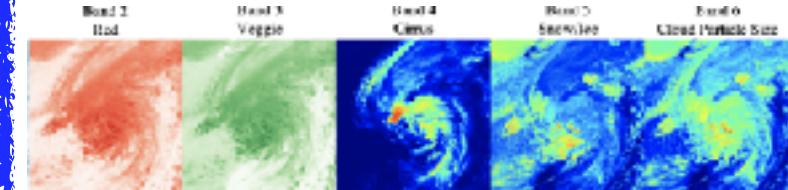


# **Obs.-driven Forecasting**



Deepmind

# Multimodal fusion



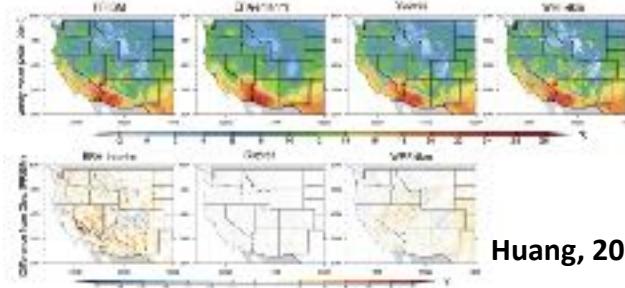
Vandal et al.

## Deconvolution



Carasso et al.

# Downscaling

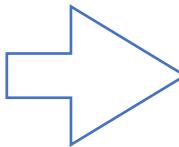
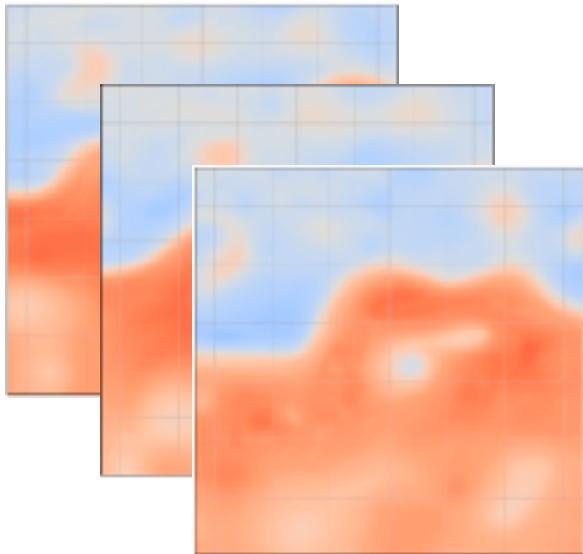


Huang, 2021

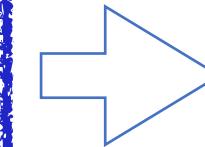
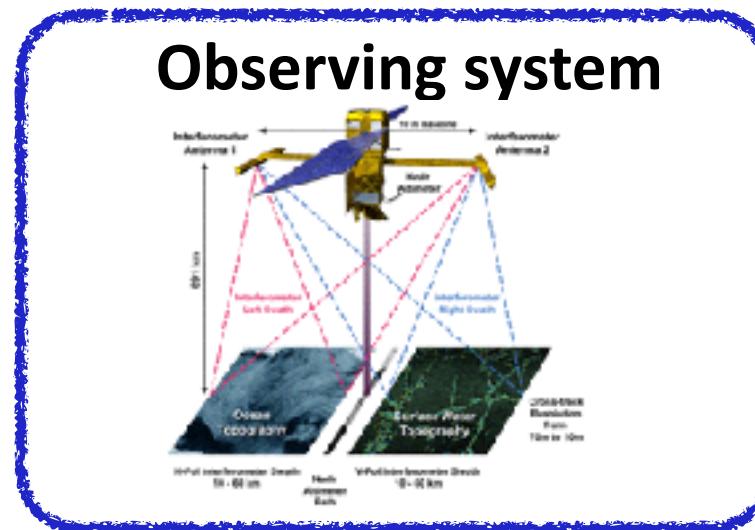


# Inverse Problems in Geoscience: Generic formulation

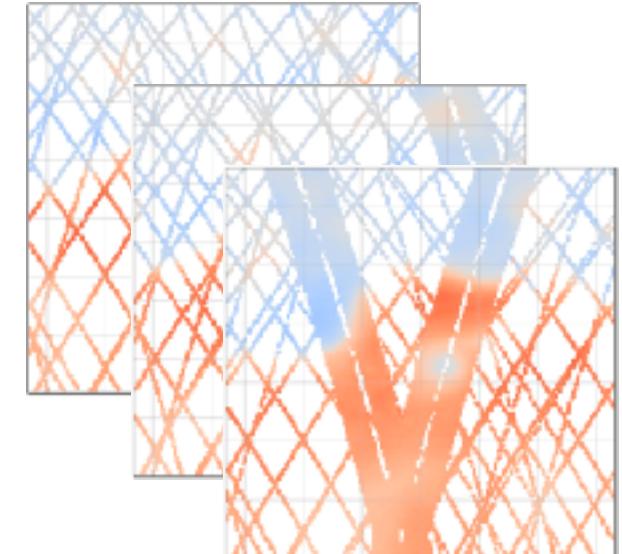
State



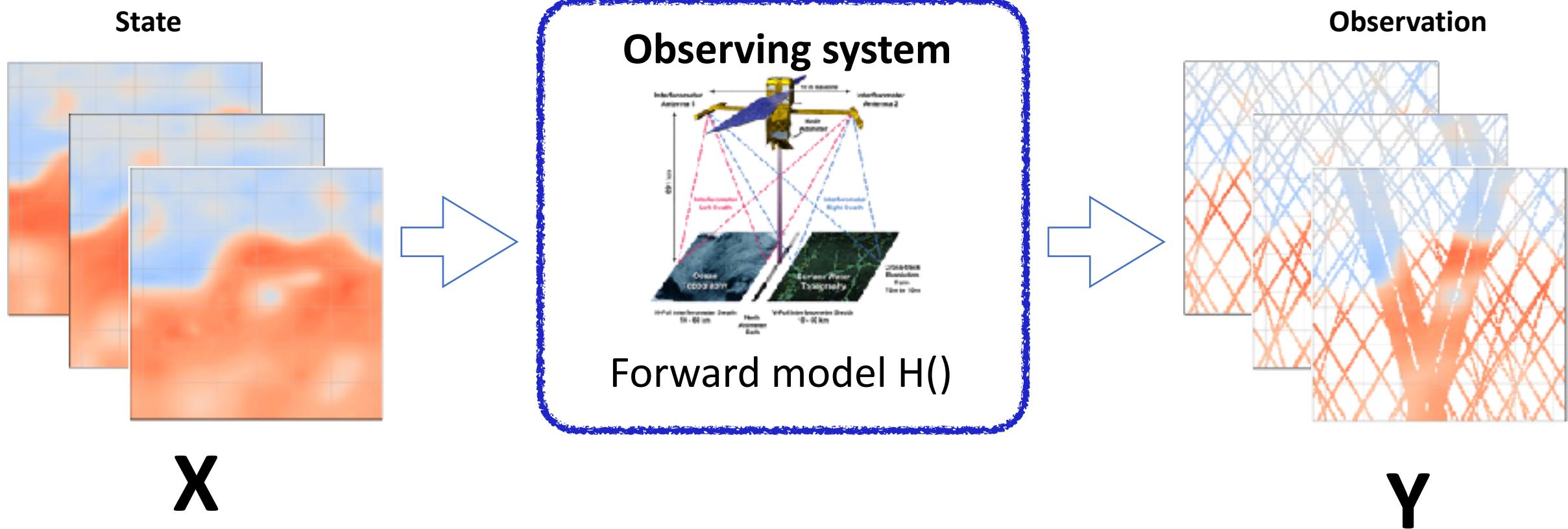
Observing system



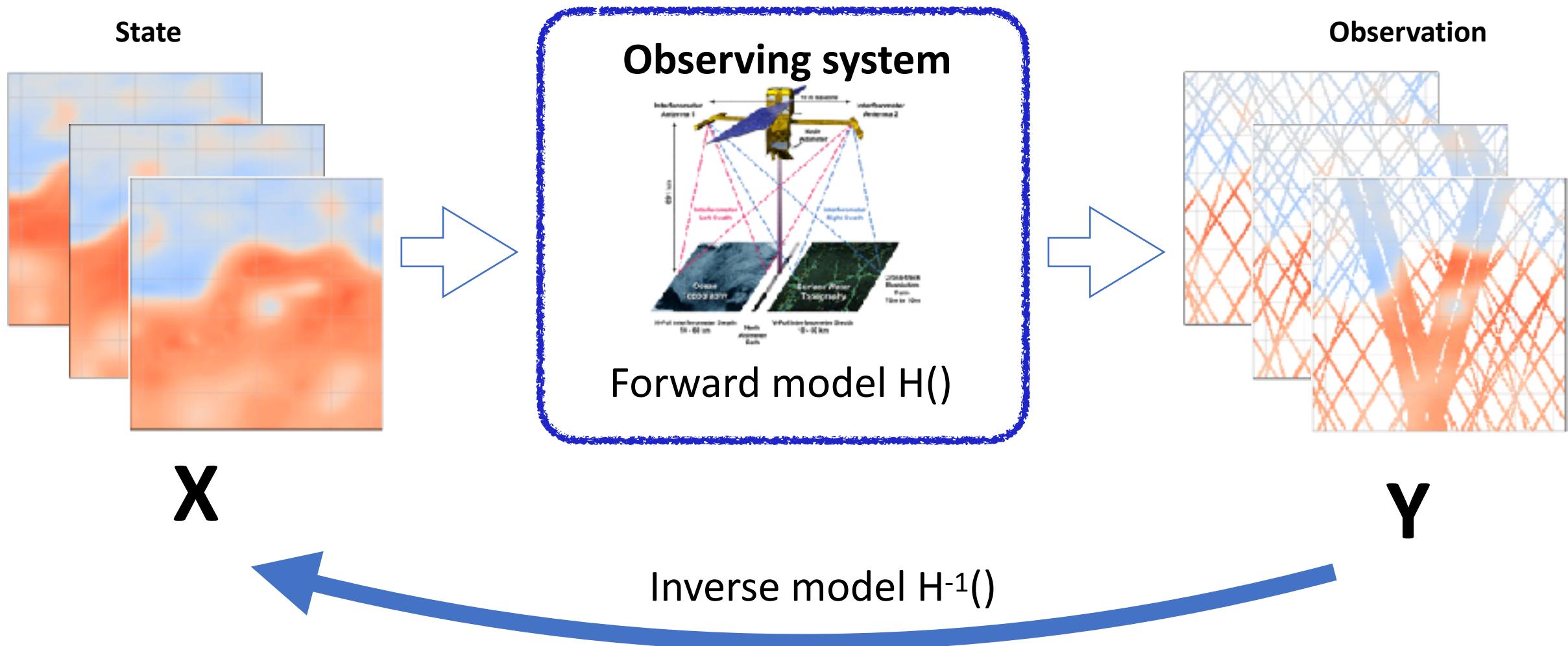
Observation



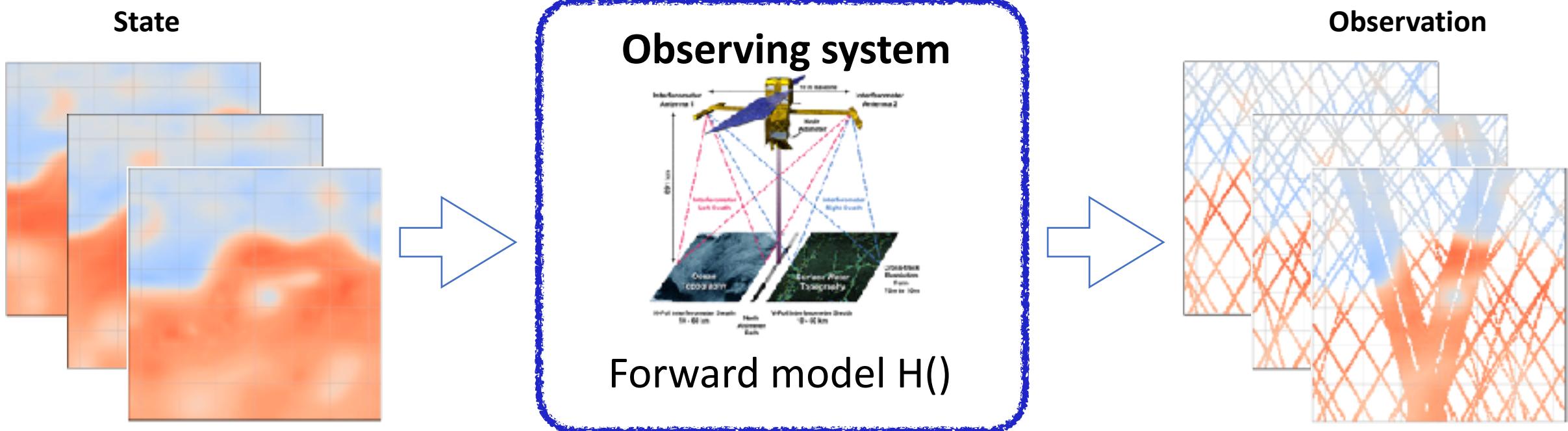
# Inverse Problems in Geoscience: Generic formulation



# Inverse Problems in Geoscience: Generic formulation

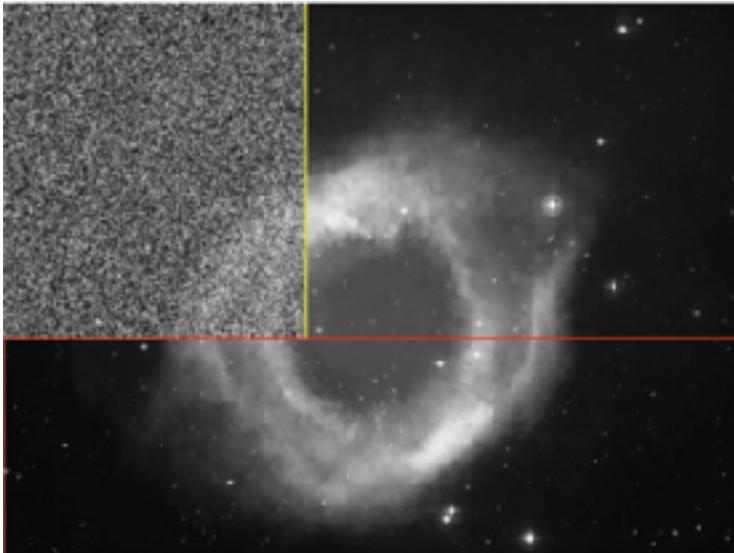


# Inverse Problems in Geoscience: Examples of forward model

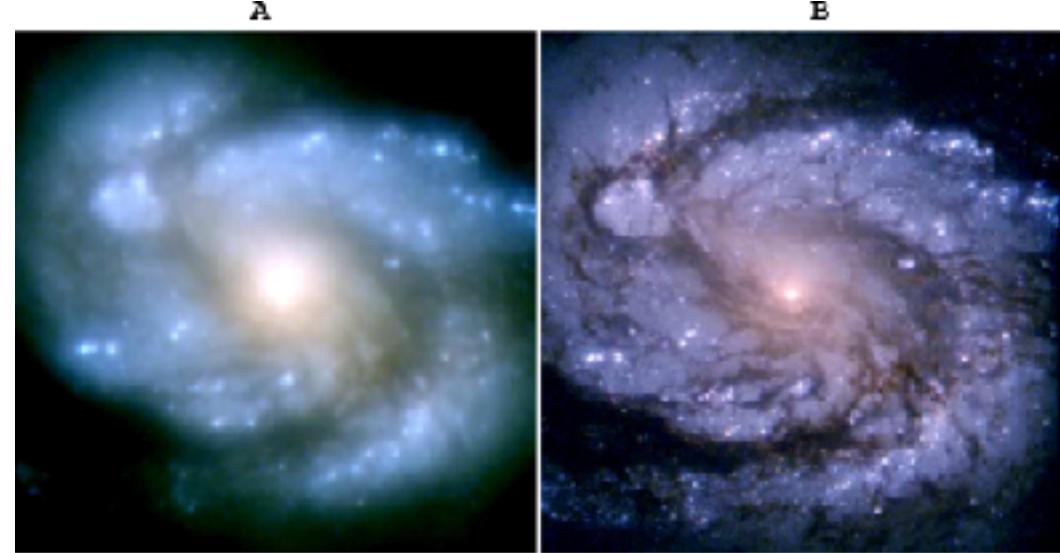


# Inverse Problems in Geoscience: Examples of forward model

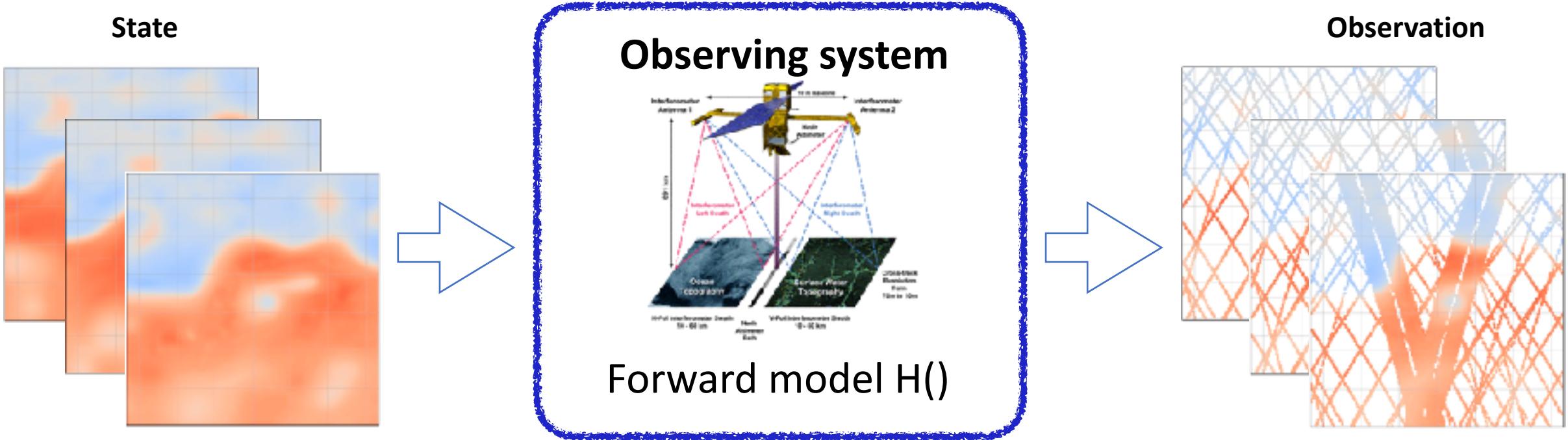
Denoising problem



Downscaling problem

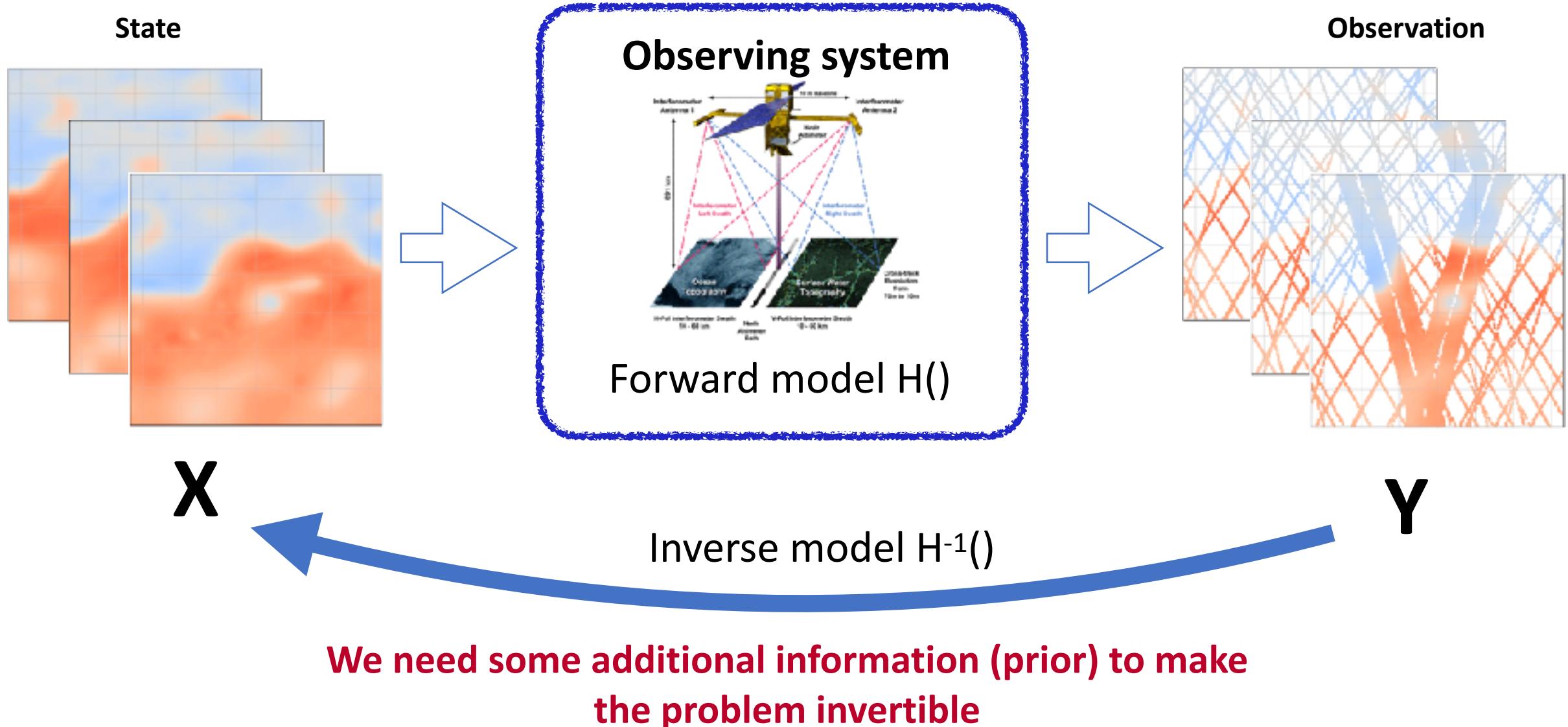


# Inverse Problems and ill-posedness



Why is space-time interpolation an ill-posed problem ?

# Inverse Problems and ill-posedness



# Inverse Problems in Geoscience

**Inverse problems as learning problems**

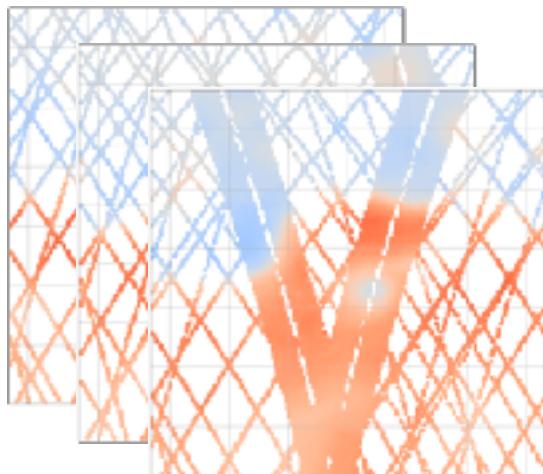
**Mathematical formulations for inverse  
Problems**

**Inverse problems as learning problems**

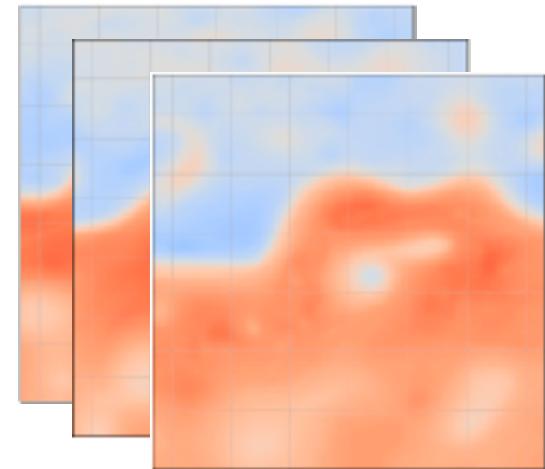
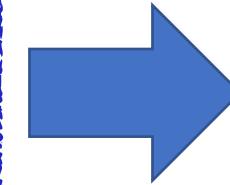
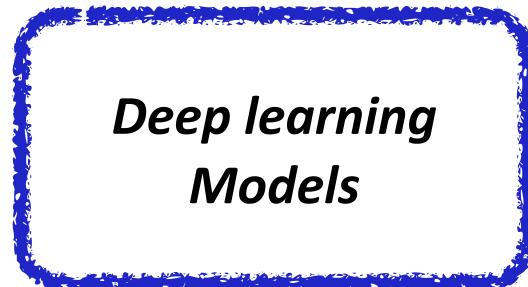
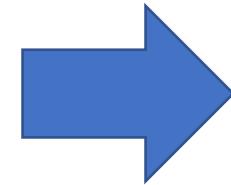
**Applications to geophysical dynamics**

# End-to-end learning for inverse problems

## End-to-end architecture



Partial observations  $y$



True states  $x$

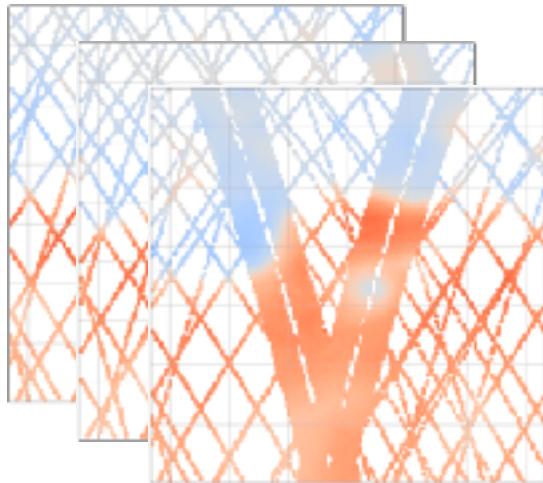
Assuming a dataset of pairs of true states and partial observations is available

Which training loss ?

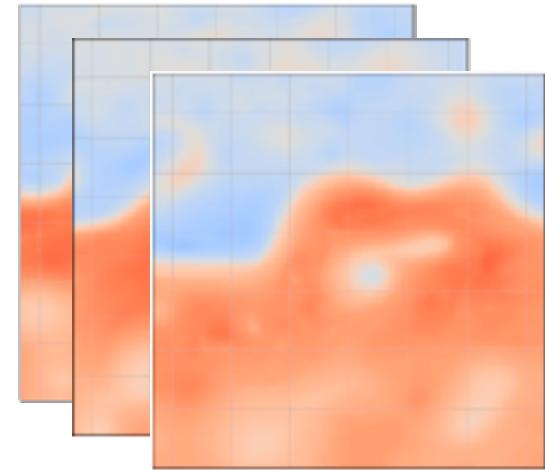
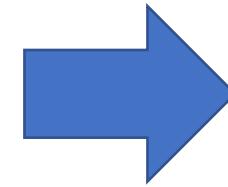
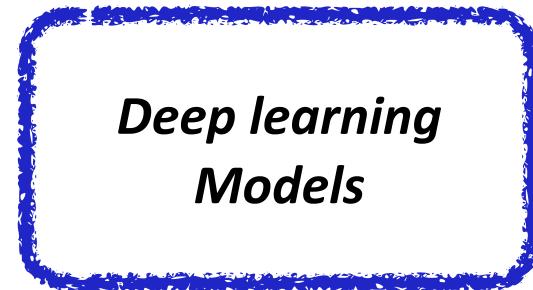
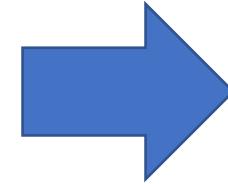
Which models / architectures ?

# End-to-end learning for inverse problems

## End-to-end architecture

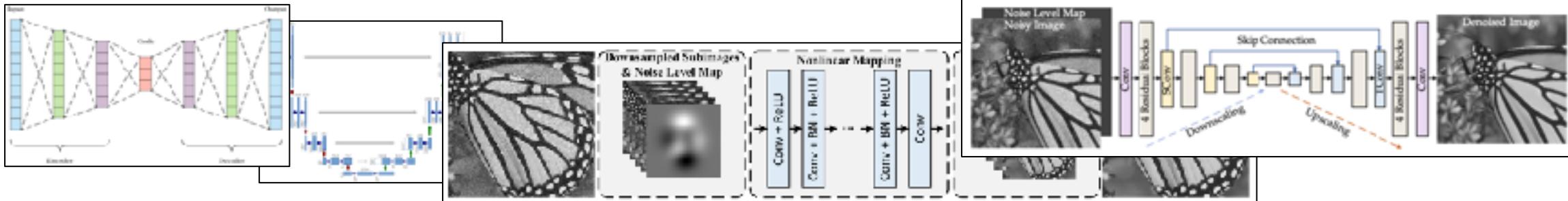


Partial observations  $y$



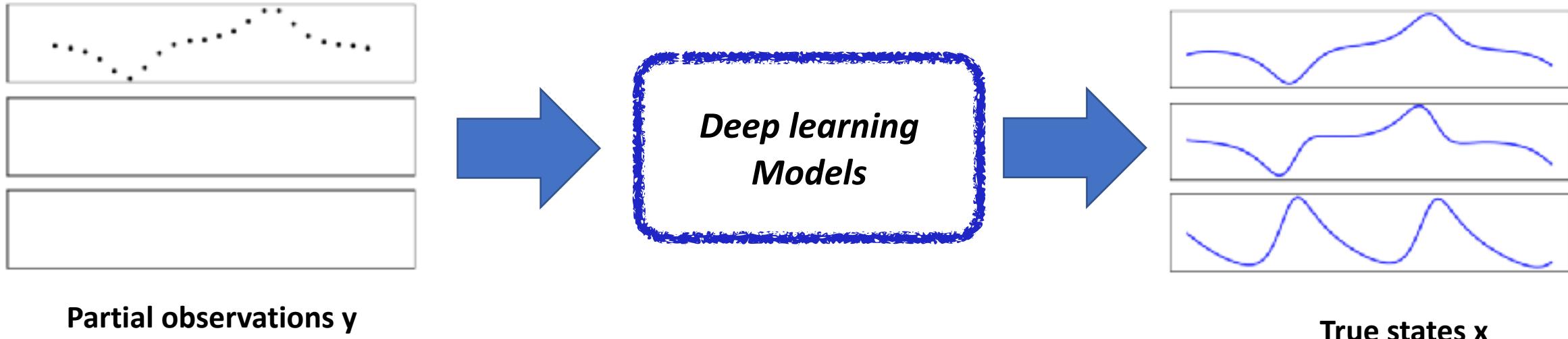
True states  $x$

Which architectures? State-of-the-art CNN architectures?



# End-to-end learning for inverse problems

An illustration for Lorenz-63 dynamics



Colab notebook:

[https://github.com/CIA-Oceanix/DLGD2021/edit/main/lecture-5-inverse-problems/notebookPyTorch\\_InvProb\\_LearningBased\\_UnrollingFixedPoint\\_L63\\_Students.ipynb](https://github.com/CIA-Oceanix/DLGD2021/edit/main/lecture-5-inverse-problems/notebookPyTorch_InvProb_LearningBased_UnrollingFixedPoint_L63_Students.ipynb)

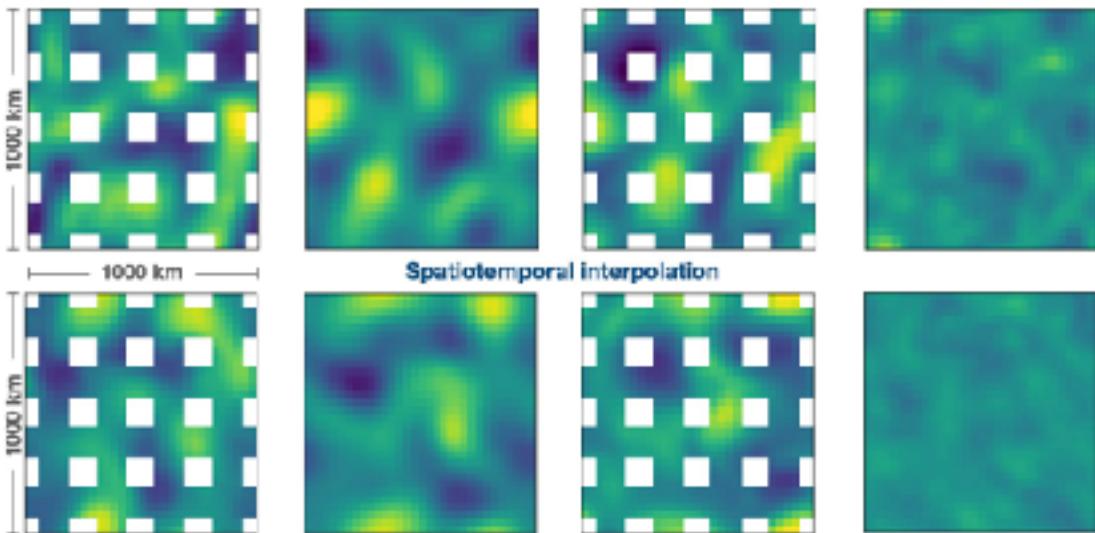
# Example for geoscience problems

JAMES | Journal of Advances in  
Modeling Earth Systems

RESEARCH ARTICLE  
10.1029/2019MS001965

Key Points

- The efficacy of Deep Learning in exploiting sparse sea surface height (SSH) data is demonstrated in a quasigeostrophic model.
- Recurrent Neural Networks are superior to linear and dynamical interpolation techniques for SSH.



## A Deep Learning Approach to Spatiotemporal Sea Surface Height Interpolation and Estimation of Deep Currents in Geostrophic Ocean Turbulence

Georgy E. Manucharyan<sup>1</sup> , Lia Siegelman<sup>2</sup> , and Patrice Klein<sup>2,3,4</sup>

<sup>1</sup>School of Oceanography, University of Washington, Seattle, WA, USA, <sup>2</sup>Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, USA, <sup>3</sup>Laboratoire de Mécanique Dynamique, Ecole Normale Supérieure, CNRS, Paris, France, <sup>4</sup>Laboratoire d'Océanographie Physique et Spatiale, IFREMER, CNRS, Brest, France

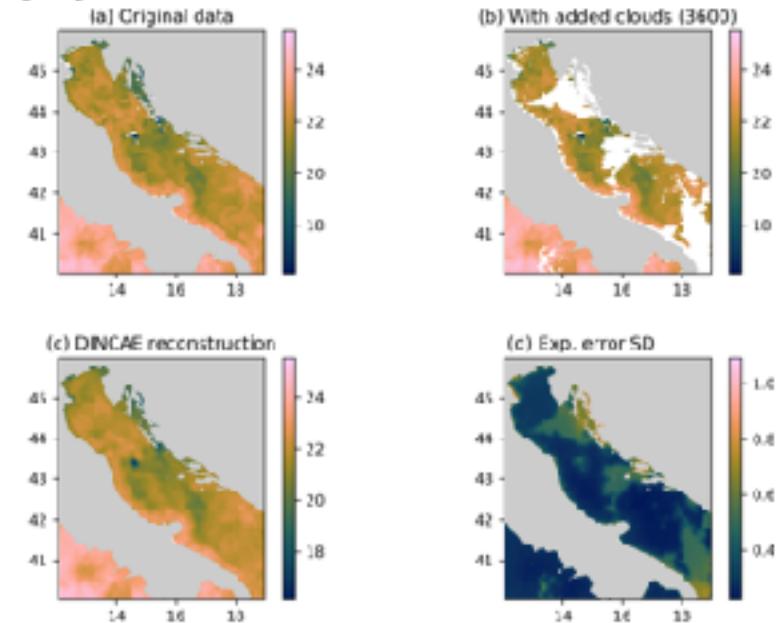
Geosci. Model Dev., 15, 2183–2196, 2022  
<https://doi.org/10.5194/gmd-15-2183-2022>  
© Author(s) 2022. This work is distributed under the Creative Commons Attribution 4.0 License.



Geoscientific  
Model Development

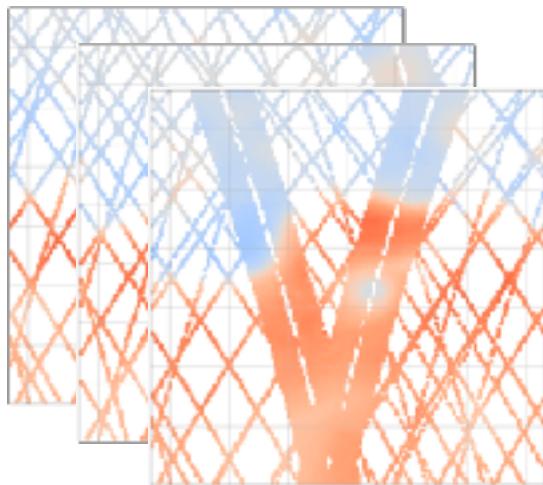
## DINCAE 2.0: multivariate convolutional neural network with error estimates to reconstruct sea surface temperature satellite and altimetry observations

Alexander Barth, Aida Alvern-Axirante, Charles Troupin, and Jean-Marie Becker  
GHER, University of Liège, Liège, Belgium

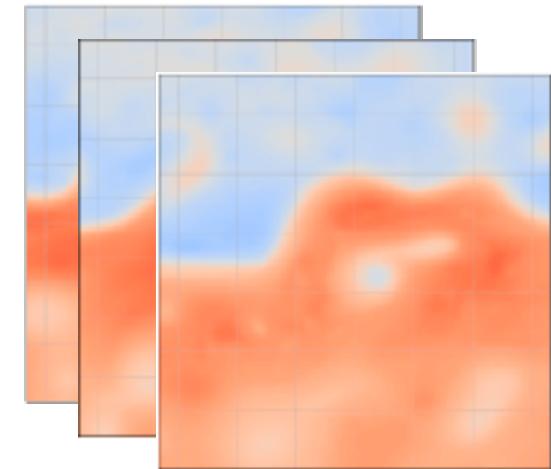
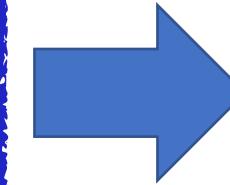
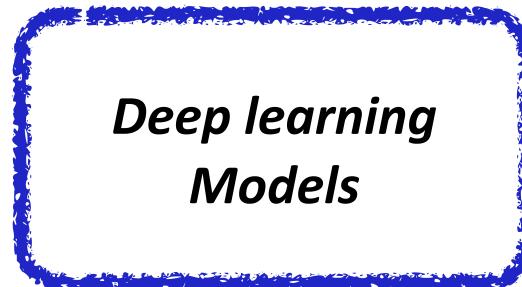
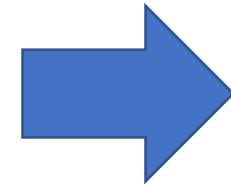


# Deep learning and inverse problems

End-to-end architecture



Partial observations  $y$



True states  $x$

Should we reinvent the wheel ? Or can we benefit from more than 50 years of knowledge and research in signal processing, optimisation, applied math.... ?

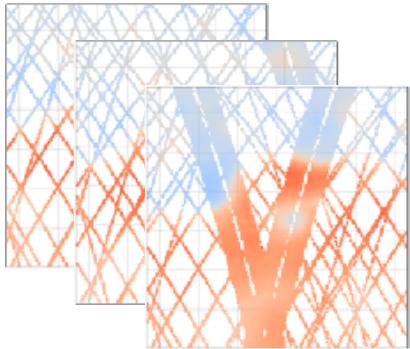
# Inverse Problems in Geoscience

**Mathematical formulations for inverse  
Problems**

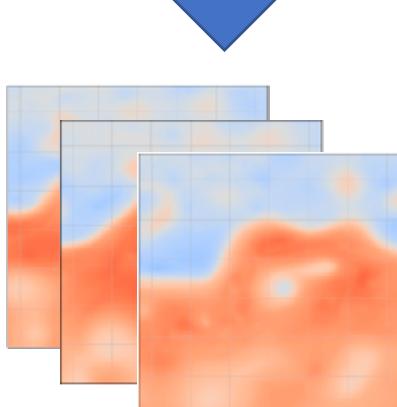
**Inverse problems as learning problems**

**Applications to geophysical dynamics**

# (Variational) Data Assimilation: (Weak-Constraint) 4DVar DA



Partial observations  $y$



True states  $x$

**State-space formulation:**

$$\begin{cases} \frac{\partial x(t)}{\partial t} = \mathcal{M}(x(t)) + \eta(t) \\ y(t, p) = x(t, p) \quad \forall t, \forall p \in \Omega_t \end{cases}$$

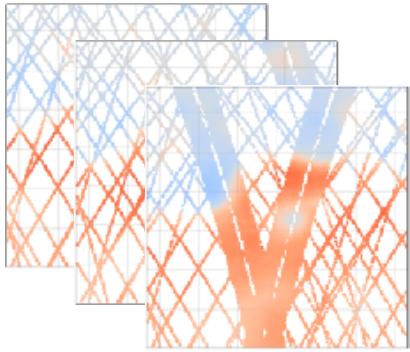
**Associated variational formulation:**

$$\arg \min_x \lambda_1 \sum_i \|x(t_i) - y(t_i)\|_{\Omega_{t_i}}^2 + \lambda_2 \sum_i \|x(t_i) - \Phi(x)(t_i)\|^2$$

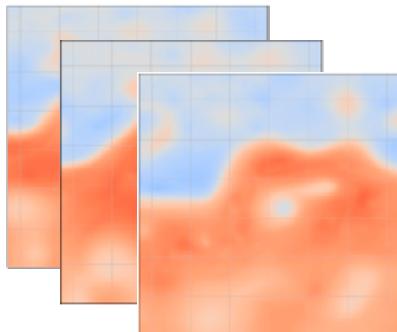
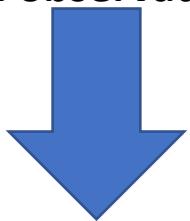
$$\text{with } \Phi(x)(t) = x(t - \Delta) + \int_{t-\Delta}^t \mathcal{M}(x(u)) du$$

$$\boxed{\arg \min_x \lambda_1 \|x - y\|_{\Omega}^2 + \lambda_2 \|x - \Phi(x)\|^2}$$

# (Variational) Data Assimilation: (Weak-Constraint) 4DVar DA



Partial observations  $y$

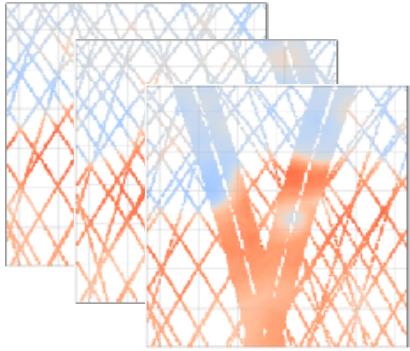


True states  $x$

**State-space formulation:**

$$\begin{cases} \frac{\partial x(t)}{\partial t} = \mathcal{M}(x(t)) + \eta(t) \\ y(t, p) = x(t, p) \quad \forall t, \forall p \in \Omega_t \end{cases}$$

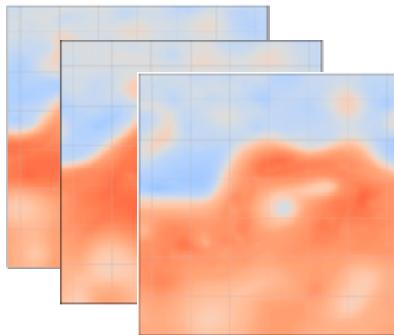
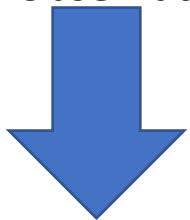
# Inverse problems stated as minimisation problems



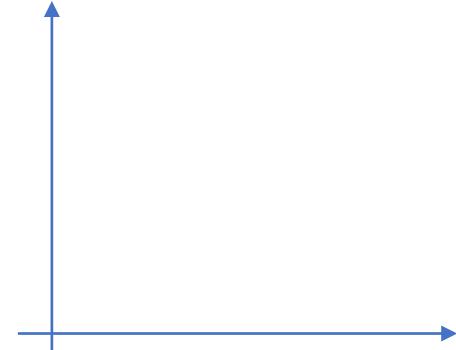
**Minimization problem**

$$X = \arg \min_X \|Y - H(X)\|^2 + \lambda U_{reg}(X)$$

Partial observations  $y$



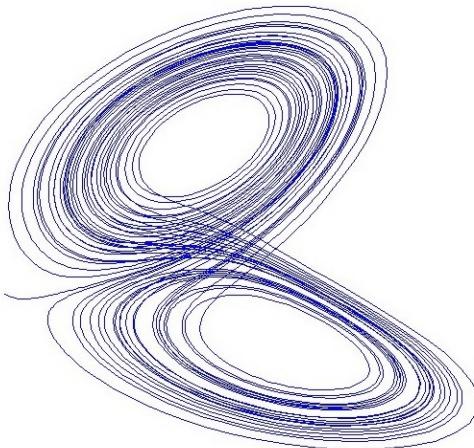
True states  $x$



**How to solve the minimization ?**

**Can we use Pytorch to implement the minimization ?**

# (Variational) Data Assimilation: (Weak-Constraint) 4DVar DA



## Minimization problem

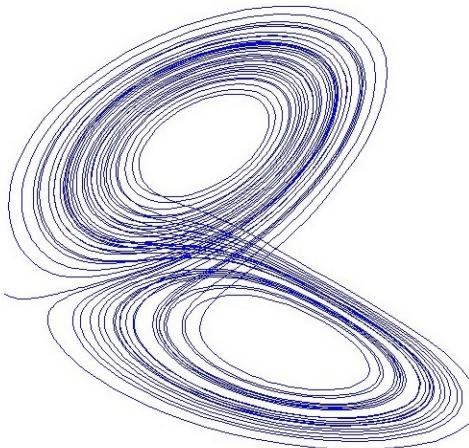
$$\arg \min_x \lambda_1 \|x - y\|_{\Omega}^2 + \lambda_2 \|x - \Phi(x)\|^2$$

with  $\Phi(x)(t) = x(t - \Delta) + \int_{t-\Delta}^t \mathcal{M}(x(u)) du$

$$\begin{aligned}\frac{dx(t)}{dt} &= \sigma(y(t) - x(t)) \\ \frac{dy(t)}{dt} &= x(t)(\rho - z(t)) - y(t) \\ \frac{dz(t)}{dt} &= x(t)y(t) - \beta z(t)\end{aligned}$$

Lorenz-63 equations

# (Variational) Data Assimilation: (Weak-Constraint) 4DVar DA



## Minimization problem

$$\arg \min_x \lambda_1 \|x - y\|_{\Omega}^2 + \lambda_2 \|x - \Phi(x)\|^2$$

with  $\Phi(x)(t) = x(t - \Delta) + \int_{t-\Delta}^t \mathcal{M}(x(u)) du$

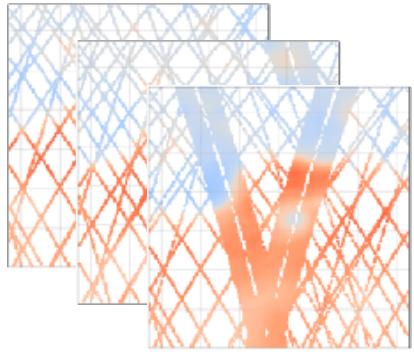
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Lorenz-63 equations

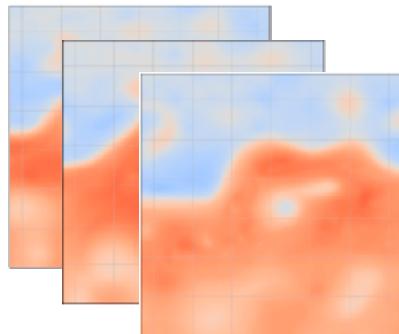
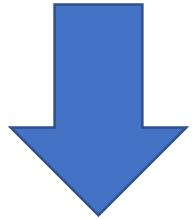
**Let's try to implement this minimisation with Pytorch.**

[https://github.com/CIA-Oceanix/DLGD2021/blob/main/lecture-5-inverse-problems/notebookPyTorch\\_InvProb\\_ModelBased\\_L63\\_Students.ipynb](https://github.com/CIA-Oceanix/DLGD2021/blob/main/lecture-5-inverse-problems/notebookPyTorch_InvProb_ModelBased_L63_Students.ipynb)

# 4DVar Data Assimilation and Optimal Interpolation



Partial observations  $y$

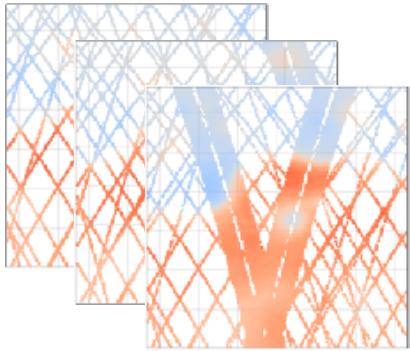


True states  $x$

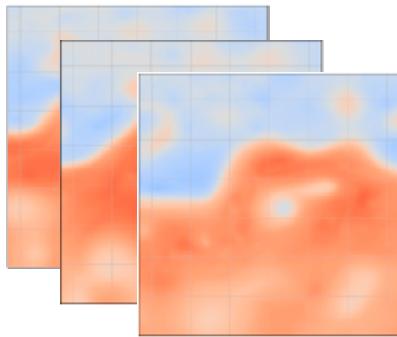
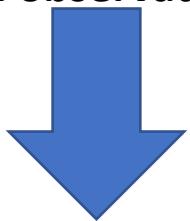
$$\left\{ \begin{array}{l} x \propto \mathcal{N}(\mu, B) \\ y(p, t) = x(p, t) + \epsilon(t, p) \quad \forall t, p \text{ with } p \in \Omega_t \\ \epsilon \propto \mathcal{N}(0, R) \end{array} \right.$$

$$\hat{x} = \arg \min_x \log P(y|x) + \log P(x)$$

# 4DVar Data Assimilation and Optimal Interpolation



Partial observations  $y$



True states  $x$

**(Weak-Constraint) 4DVar formulation**

$$\arg \min_x \lambda_1 \|x - y\|_{\Omega}^2 + \lambda_2 \|x - \Phi(x)\|^2$$

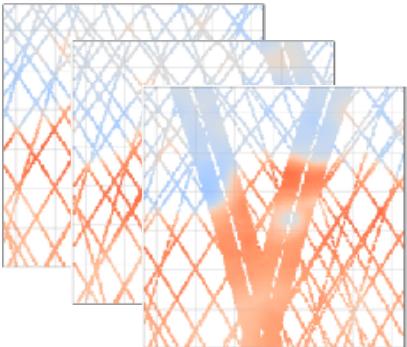
**Optimal interpolation formulation**

$$\arg \min_x \|y - H_{\Omega} \cdot x\|_R^2 + x^t B^{-1} x$$

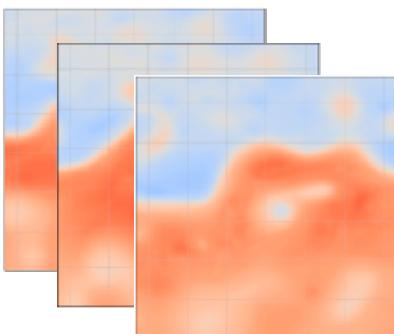
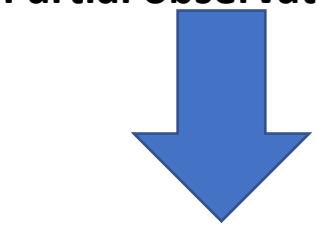
$$\arg \min_x \|y - H_{\Omega} \cdot x\|_R^2 + \|x - (\mathbb{I} - L) \cdot x\|^2 \text{ with } B = L^t L$$

**OI solution**  $\hat{x} = \mu + \mathbf{K} \cdot y$  with  $\mathbf{K} = B H_{\Omega} (H_{\Omega} B H_{\Omega}^t + R)^{-1}$

# Wrap-up on 4DVar DA and OI



Partial observations  $y$



True states  $x$

## Weak-Constraint 4DVar formulation

$$\arg \min_x \|y - H_\Omega \cdot x\|^2 + \lambda \|x - \Phi(x)\|^2 + \nu \|x_0 - \mu_0\|_{B_0}^2$$

$$\Phi(x)(t) = x(t - \Delta) + \int_{t-\Delta}^t \mathcal{M}(x(u)) du$$

## Strong-Constraint 4DVar formulation

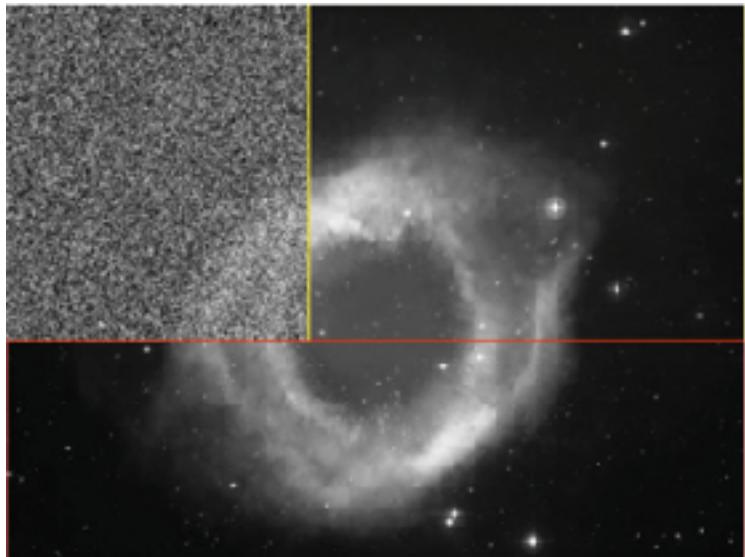
$$\arg \min_{x_0} \|y - H_\Omega \cdot x\|^2 + \nu \|x_0 - \mu_0\|_{B_0}^2 \text{ s.t. } \begin{cases} x(t_0) &= x_0 \\ \frac{dx}{dt} &= \mathcal{M}(x(t)) \end{cases}$$

## OI solution

$$\arg \min_x \|y - H_\Omega \cdot x\|_R^2 + \|x - (\mathbb{I} - L) \cdot x\|^2 \text{ with } B = L^t L$$

# Inverse problems stated as minimisation problems

Denoising problem



$$Y = X + \epsilon \text{ with } \epsilon \sim \mathcal{N}(0, \sigma^2)$$

$$X \sim P_X$$

Probabilistic prior

$$X = \arg \min_X \lambda \|X - Y\|^2 - \log P_X(X)$$

$$X = D.\alpha$$

Dictionary-based prior

$$\hat{x} = \arg \min_{x,\alpha} \|y - x\|^2 + \lambda \|x - D.\alpha\|^2$$

Norm-based prior

$$\hat{x} = \arg \min_x \|y - x\|^2 + \lambda \|\nabla x\|^2$$

Generic formulation

$$\hat{x} = \arg \min_x \|y - H(x)\|^2 + \lambda U_{Reg}(x)$$

# Key message for (variational) Model-based Methods

- *Solution stated as the minimisation of a variational cost*
- *Explicit knowledge of observation model and prior*
- *Implementation of associated minimisation algorithm*
- *Analytical derivation of gradient operator* (e.g., Euler-Lagrange equations, Adjoint Methods)
- *Implementation using DL schemes* (eg, Pytorch) *do not require the analytical gradient operator*

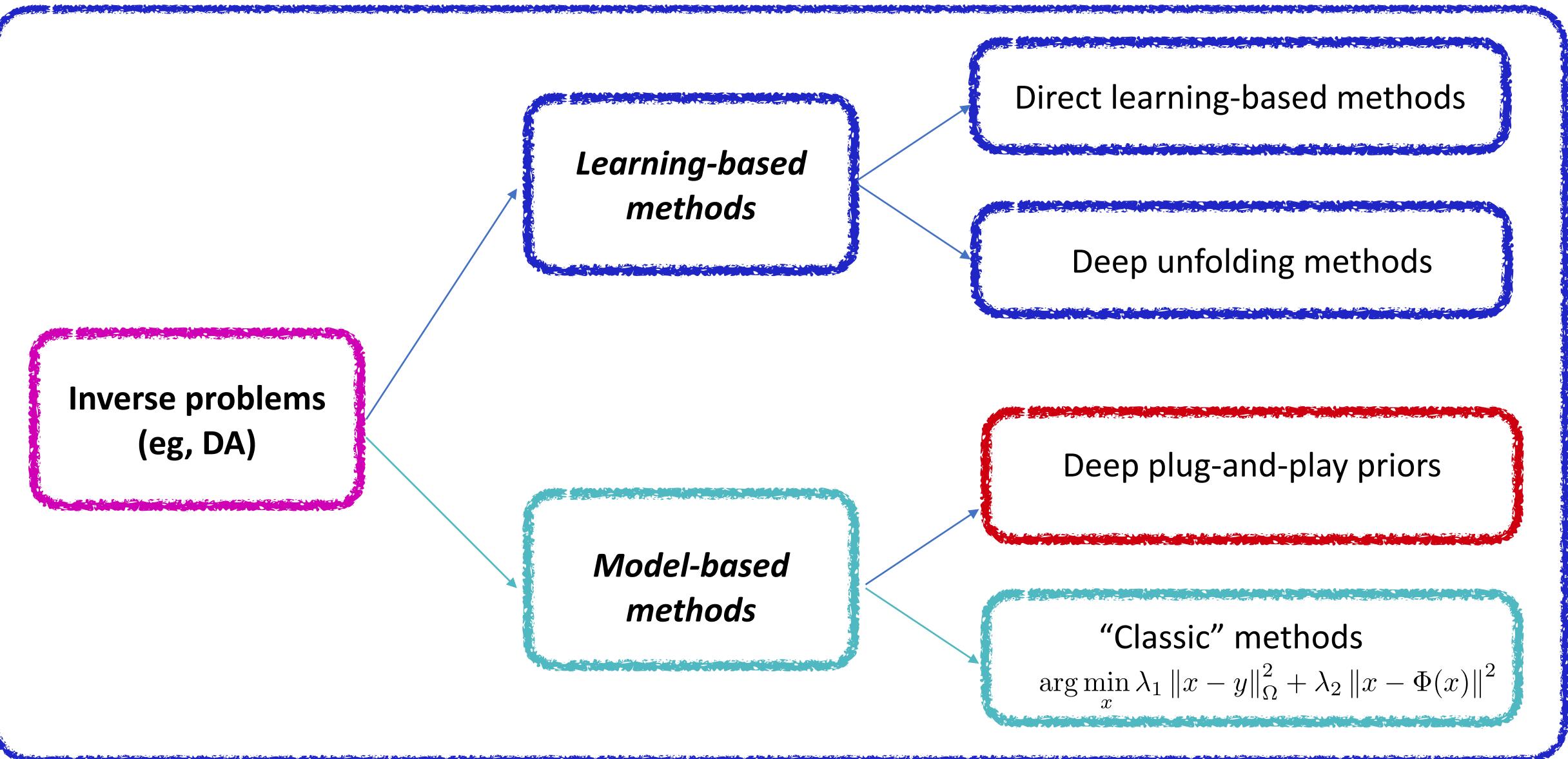
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Mathematical formulations for inverse  
Problems

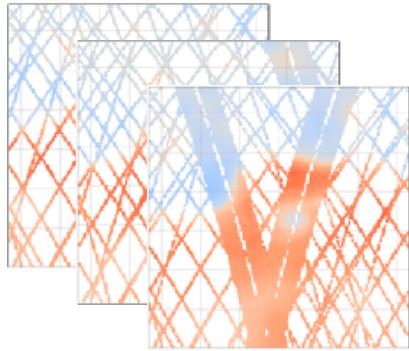
**Inverse problems & Deep learning**

Applications to geophysical dynamics

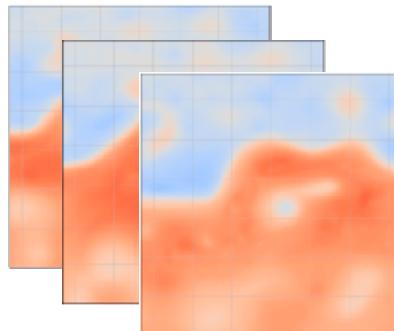
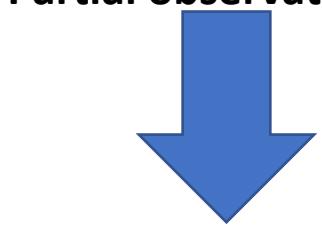
# Model-driven vs. Learning-based approaches



# Inverse problems using Deep plug-and-play priors



Partial observations  $y$

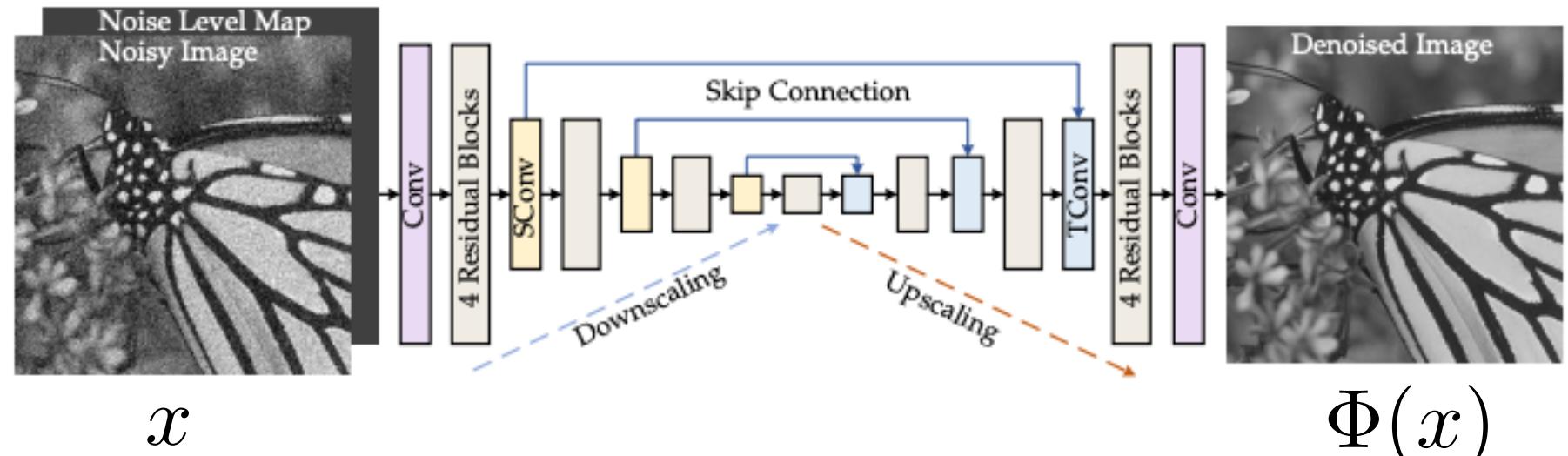


True states  $x$

Model-based formulation with a (deep) learning-based prior

$$\arg \min_x \lambda_1 \|x - y\|_{\Omega}^2 + \lambda_2 \|x - \Phi(x)\|^2$$

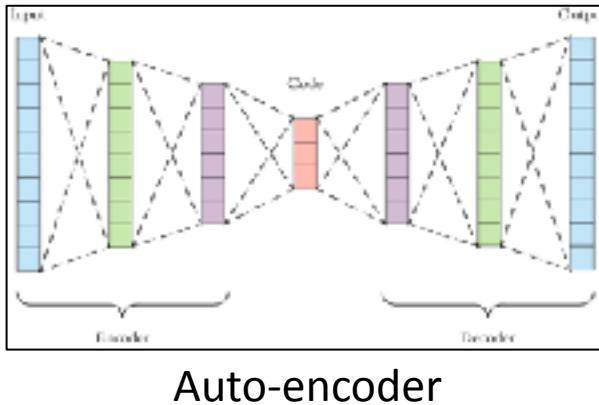
Trainable plug-and-play prior



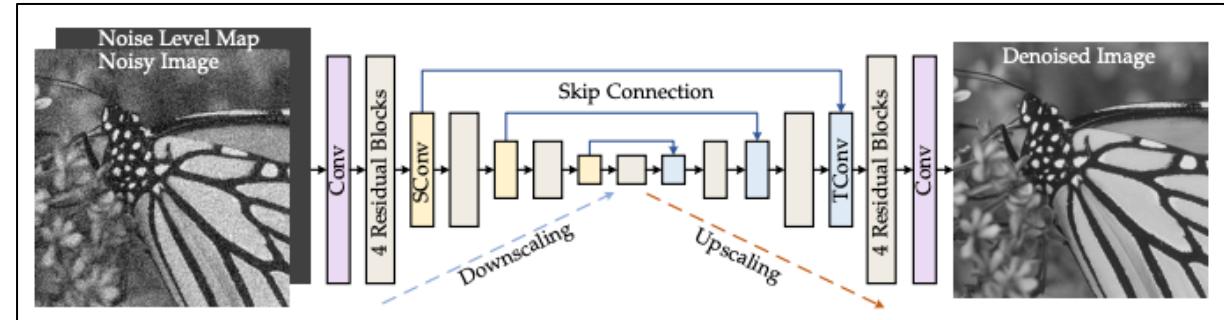
$\Phi(x)$

# Inverse problems using Deep plug-and-play priors

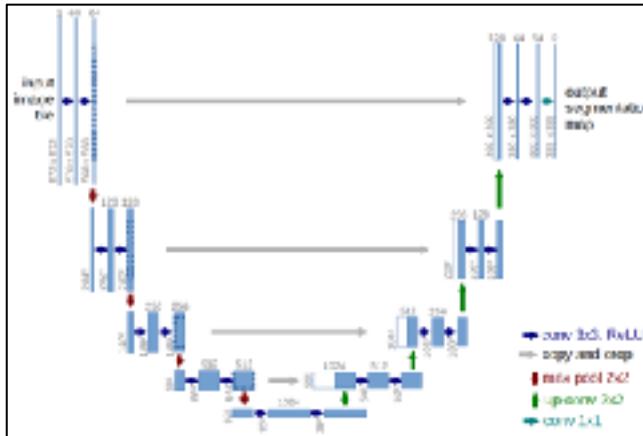
## Examples of plug-and-play priors (denoiser architecture)



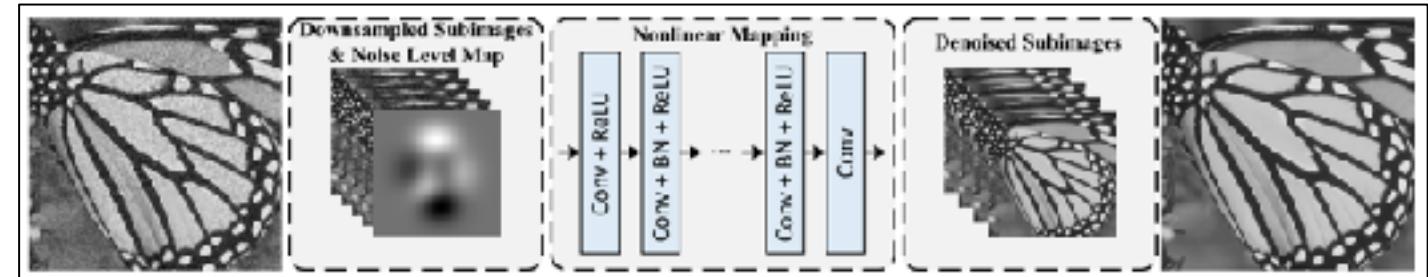
Auto-encoder



DRUNet <https://arxiv.org/pdf/2008.13751.pdf>

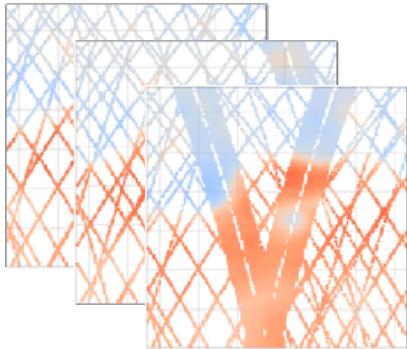


UNet <https://arxiv.org/abs/1505.04597>

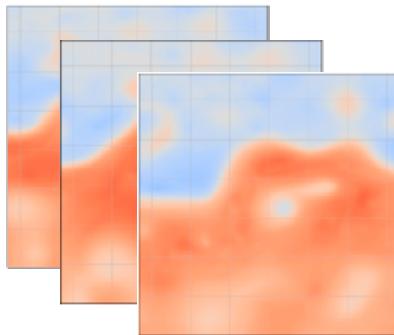


FFDNet <https://arxiv.org/pdf/1710.04026.pdf>

# Inverse problems using Deep plug-and-play priors



Partial observations  $y$



True states  $x$

## Model-based formulation

$$\arg \min_x \lambda_1 \|x - y\|_{\Omega}^2 + \lambda_2 \|x - \Phi(x)\|^2$$

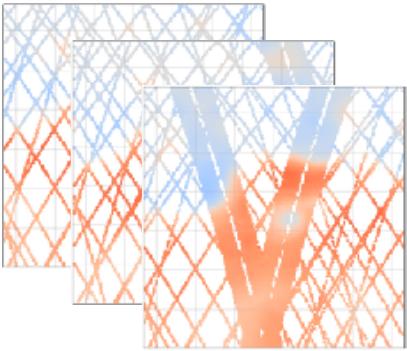
Trainable plug-and-play prior

Use of trainable priors but no actual learning specifically designed for the targeted inverse problem

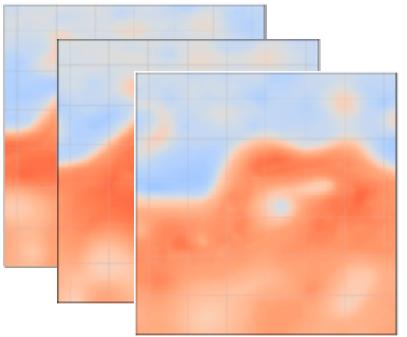
Let's go and test it using a PCA-based prior

[https://github.com/CIA-Oceanix/DLGD2021/blob/main/lecture-5-inverse-problems/notebookPyTorch\\_InvProb\\_ModelBased\\_L63\\_Students.ipynb](https://github.com/CIA-Oceanix/DLGD2021/blob/main/lecture-5-inverse-problems/notebookPyTorch_InvProb_ModelBased_L63_Students.ipynb)

# Inverse problems: from plug-and-play to implicit priors



Partial observations  $y$



True states  $x$

## Inverse problem with plug-and-play priors

$$\arg \min_x \lambda_1 \|x - y\|_{\Omega}^2 + \lambda_2 \|x - \Phi(x)\|^2$$

Trainable plug-and-play prior

## Inverse problem with a prior in latent space

$$\arg \min_z \lambda_1 \|y - x\|_{\Omega}^2 \text{ s.t. } x = \mathcal{D}(z)$$

Pre-trained decoder

## Inverse problem with deep image prior [Ulyanov'17]

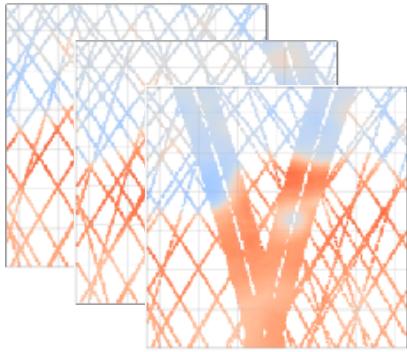
$$\arg \min_{\theta} \lambda_1 \|y - x\|_{\Omega}^2 \text{ s.t. } x = \mathcal{D}_{\theta}(z) \text{ and } z \sim \mathcal{N}(0, \mathbb{I})$$

<https://arxiv.org/abs/1711.10925>

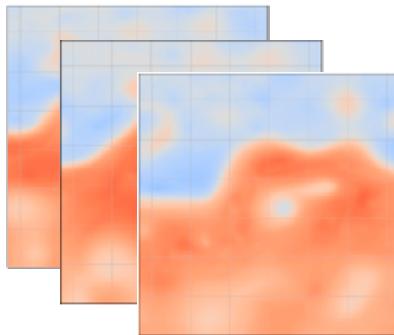
## Inverse problem with implicit neural representation

$$\arg \min_{\theta} \lambda_1 \|y - x\|_{\Omega}^2 \text{ s.t. } \forall p, x(p) = \mathcal{D}_{\theta}(p)$$

# Inverse problems: from plug-and-play to implicit priors



Partial observations  $y$



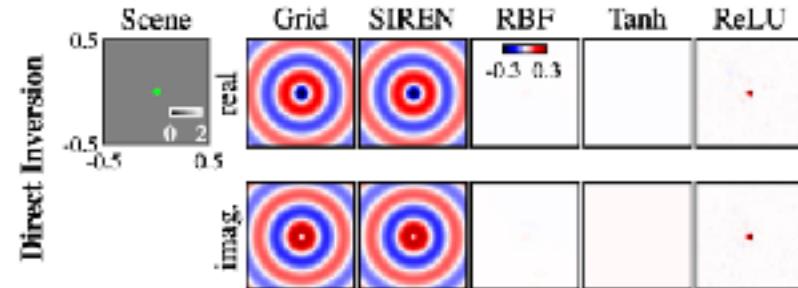
True states  $x$

## Inverse problem with implicit neural representations

$$\forall p, \quad x(p) = \mathcal{D}_\theta(p)$$

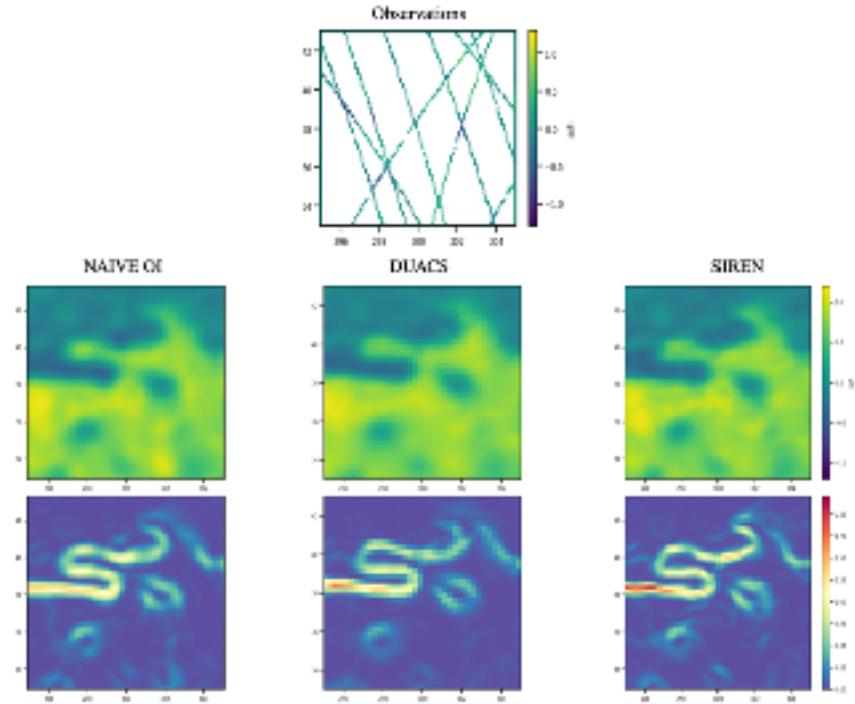
Space-continuous (grid-free)  
representations of nD tensors

SIREN: implicit representations  
with periodic activations



<https://www.vincentsitzmann.com/siren/>

Application to SSH mapping  
SIREN architecture / unsupervised learning



Jhonson et al., ML4PS'22  
<https://arxiv.org/abs/2211.10444>

# Key messages for (variational) Model-based Methods

- *Solution stated as the minimisation of a variational cost*
- *Explicit knowledge of observation model and prior*
- *Implementation of associated minimisation algorithm*
- *Analytical derivation of gradient operator* (e.g., Euler-Lagrange equations, Adjoint Methods)
- *Implementation using DL schemes* (eg, Pytorch) *do not require the analytical gradient operator*
- *Possible extension to pre-trained plug-and-play and implicit priors*

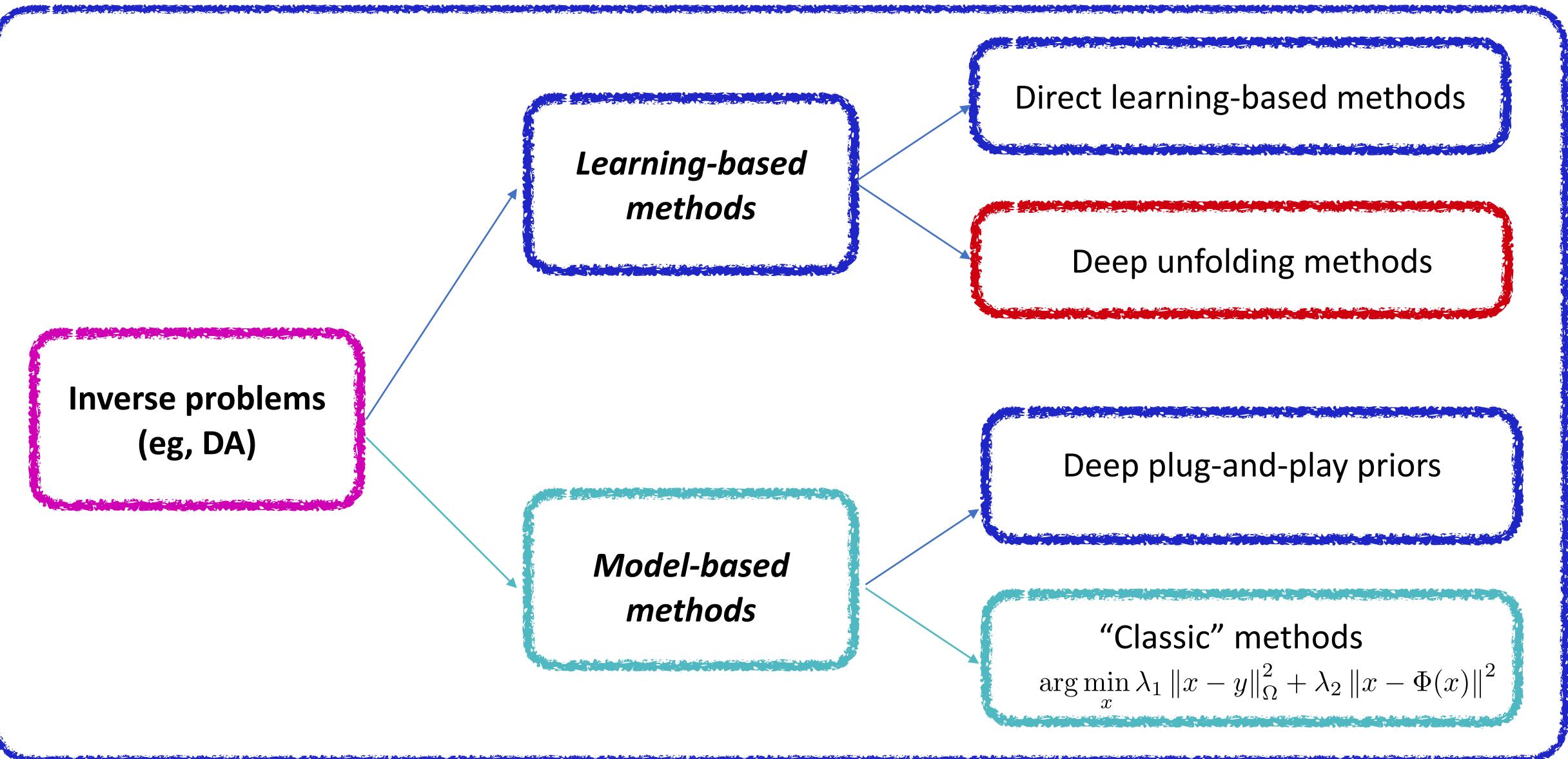
# Inverse Problems in Geoscience

Mathematical formulations for inverse  
Problems

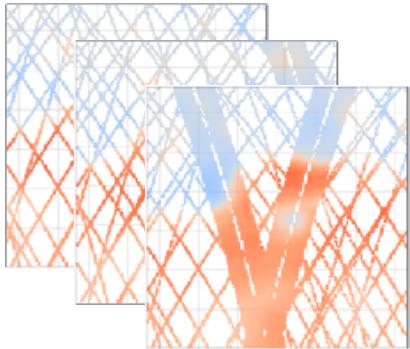
**Inverse problems & Deep learning**

Applications to geophysical dynamics

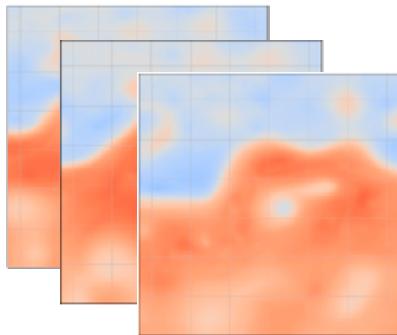
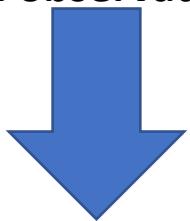
# Model-driven vs. Learning-based approaches



# Can we relate end-to-end learning and model-based schemes?



Partial observations  $y$



True states  $x$

The example of the Optimal Interpolation

$$\arg \min_x \|y - H_\Omega \cdot x\|_R^2 + \|x - (\mathbb{I} - L) \cdot x\|^2 \text{ with } B = L^t L$$

Associated optimality criterion (bi-level formulation)

$$\min_L \mathbb{E} \left( \|\hat{x} - x^{true}\|^2 \right)$$

$$\text{s.t. } \hat{x} = \arg \min_x \|y - H_\Omega \cdot x\|^2 + \|x - \Phi_L(x)\|^2$$

No similar property in general for non-linear/non-quadratic formulations

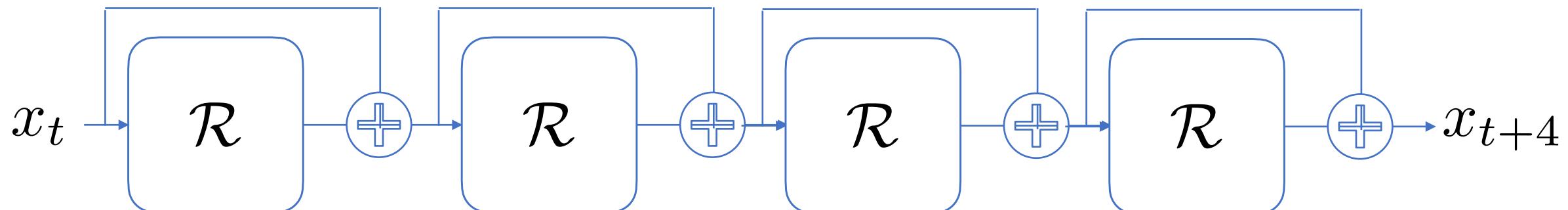
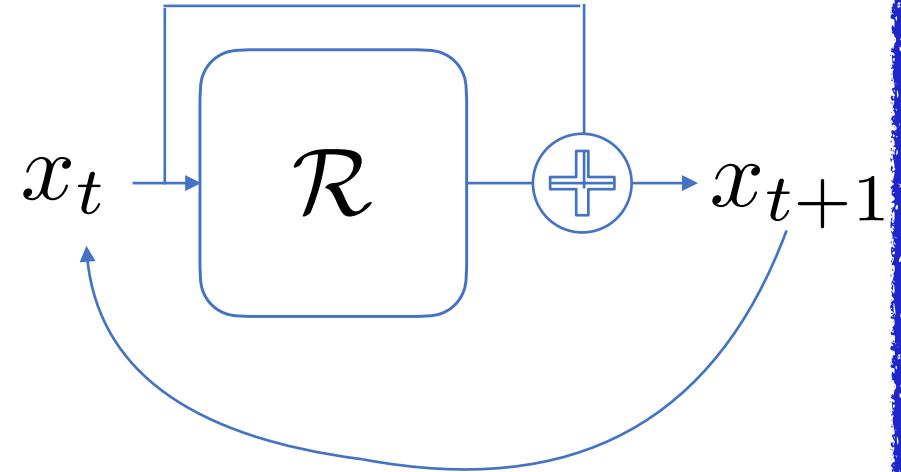
# Folded vs. Unfolded Representations

An example with a ResNet

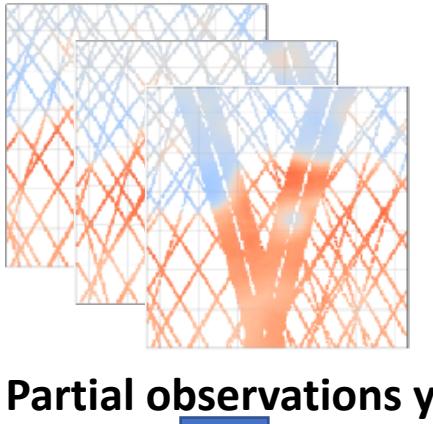
$$x_{t+1} = x_t + \mathcal{R}(x_t)$$

Unfolded  
Representation

Folded  
Representation



# Inverse problems using Deep unfolding schemes



Partial observations  $y$

**Basic idea: exploit knowledge on optimisation algorithms for inverse problems**

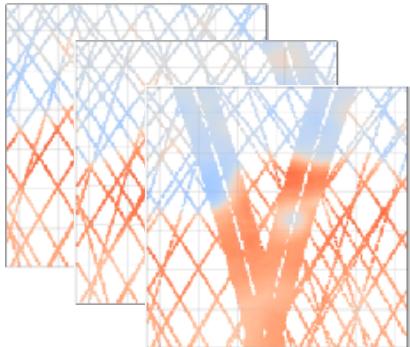
- Many schemes involve iterative algorithms
- One may unfold an iterative procedure to define a deep learning architecture

## Examples

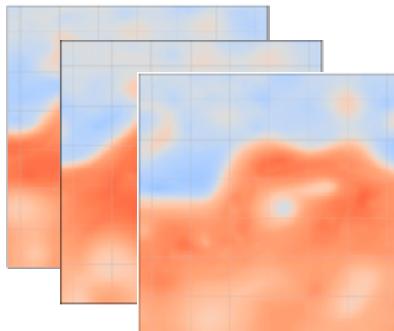
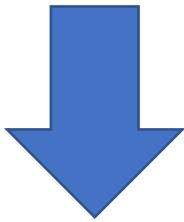
- Image denoising/Unfolding of reaction-diffusion schemes (e.g., Chen et al., 2015)
- Medical imaging/Unfolding of ADMM schemes (e.g., Yang et al., 2016)
- Interpolation/Unfolding of fixed-point algorithms (e.g., Fablet et al., 2020)
- DA/Deep unfolding of sequential DA algorithms (e.g., Boudier et al., 2020)

True states  $x$

# Data Assimilation using Deep unfolding schemes



Partial observations  $y$



True states  $x$

Deep unfolding of Sequential DA filters (e.g., EnKF) [Boudier et al., 2020]

- **Forecasting step:** samples states at time  $t$  given the posterior at time  $t-1$

$$x_t | y_{0:t-1} \text{ given } x_{t-1} | y_{0:t-1}$$

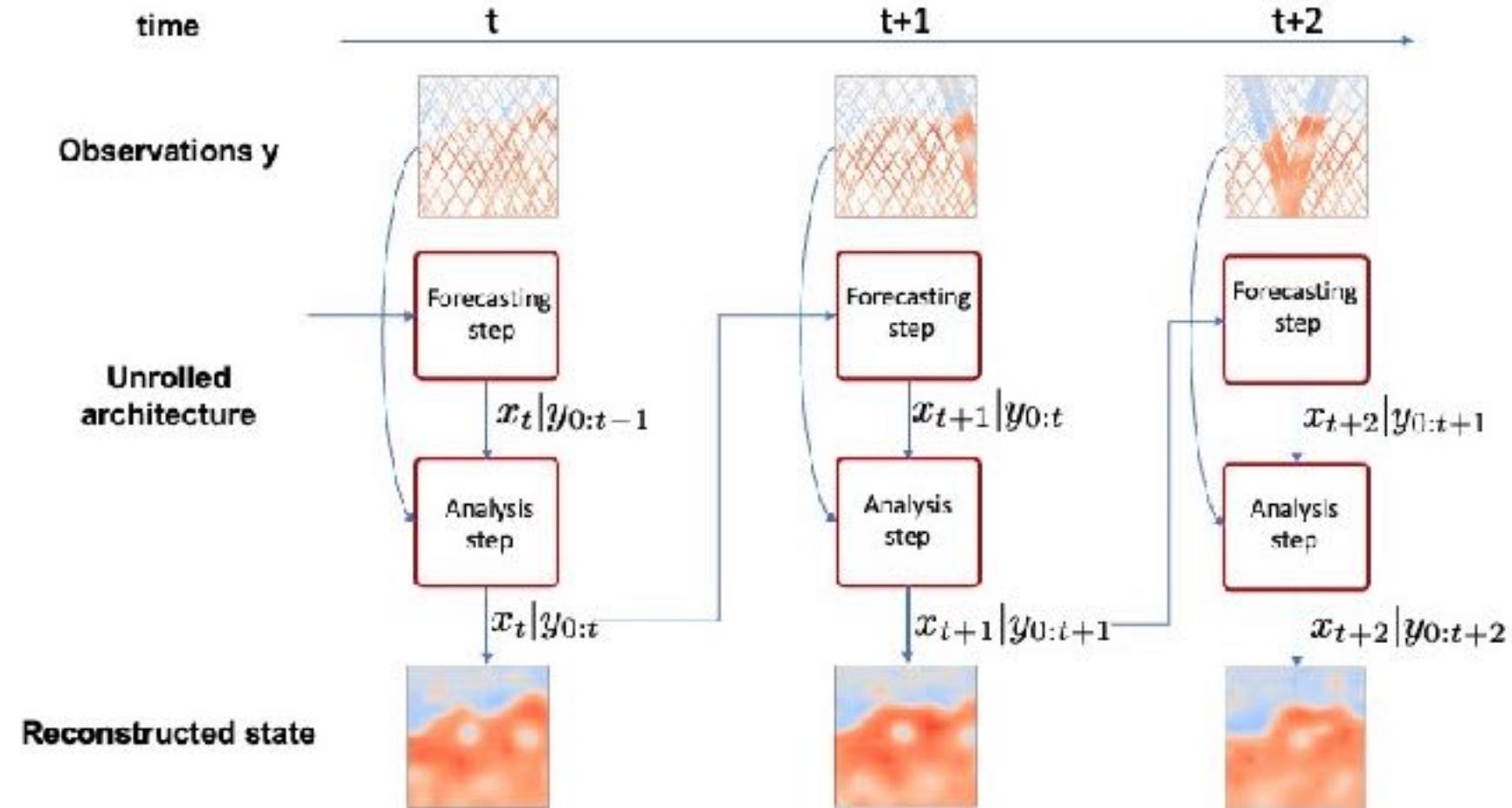
- **Analysis step:** update the posterior at time  $t$  given the new observations at time  $t$

$$x_t | y_{0:t} \text{ given } y_t \text{ and } x_t | y_{0:t-1}$$

# Data Assimilation using Deep unfolding schemes

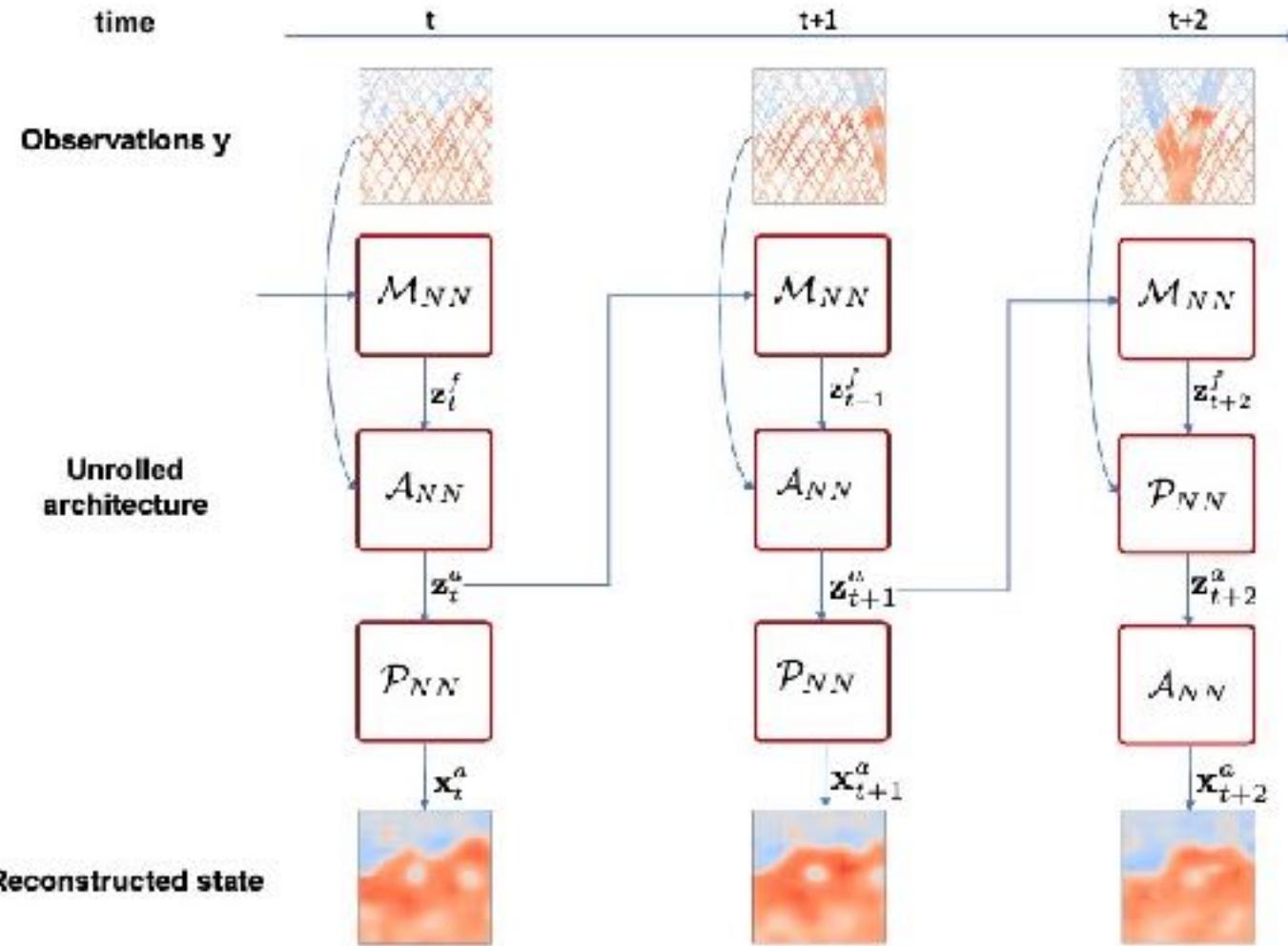
Deep unfolding of Sequential DA filters (e.g., EnKF) [Boudier et al., 2020]

*Unfolded  
architecture of  
Sequential DA  
schemes*



# Data Assimilation using Deep unfolding schemes

Deep unfolding of Sequential DA filters (e.g., EnKF) [Boudier et al., 2020]



**Generalization of the sequential DA schemes with:**

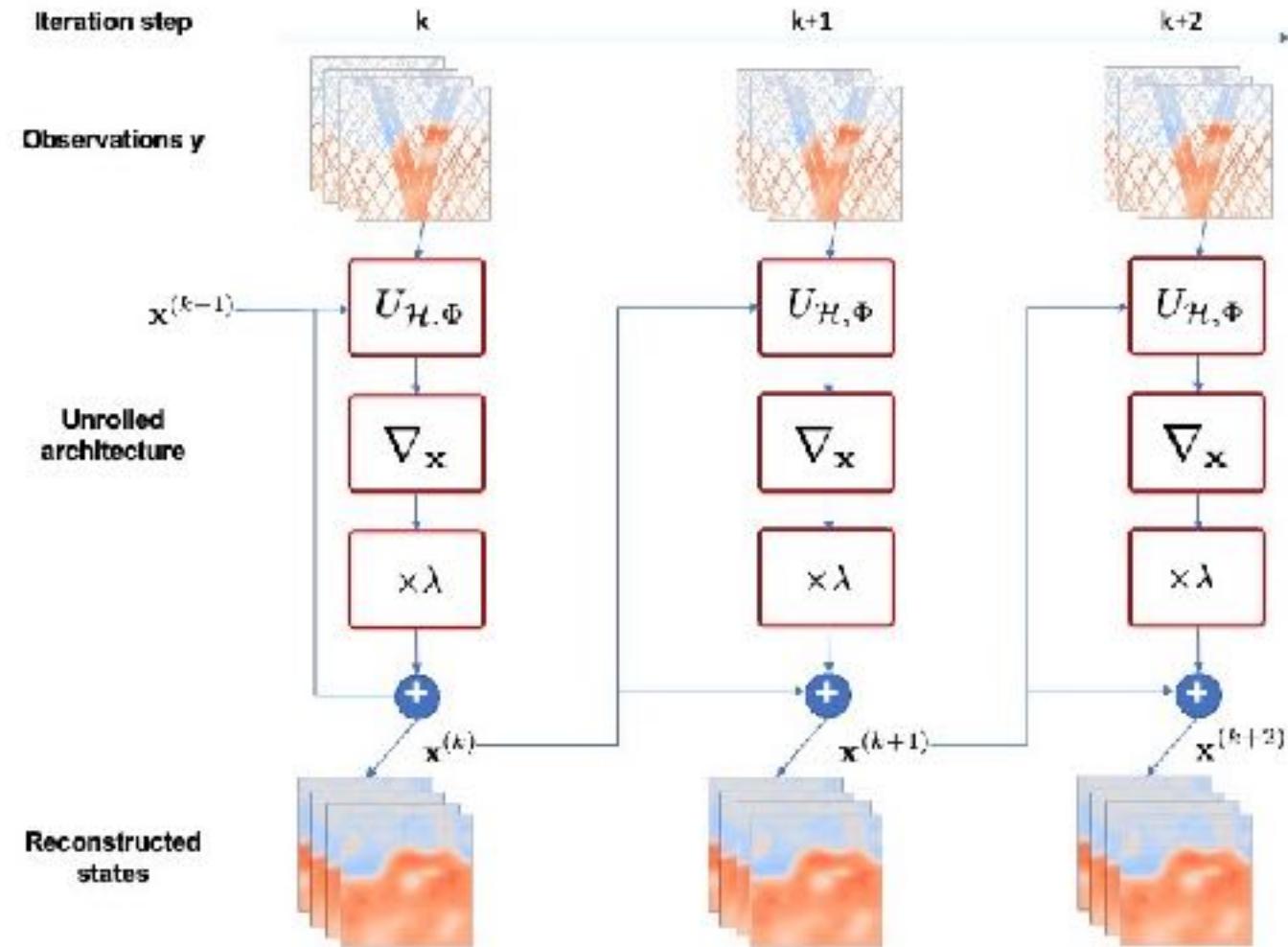
- A latent representation of the posteriors
- NNs to generalize/replace the forecasting and analysis step

# Data Assimilation using Deep unfolding schemes

Deep unfolding of 4DVar DA schemes (e.g., 4DVar-WC) [Fablet et al., 2021]

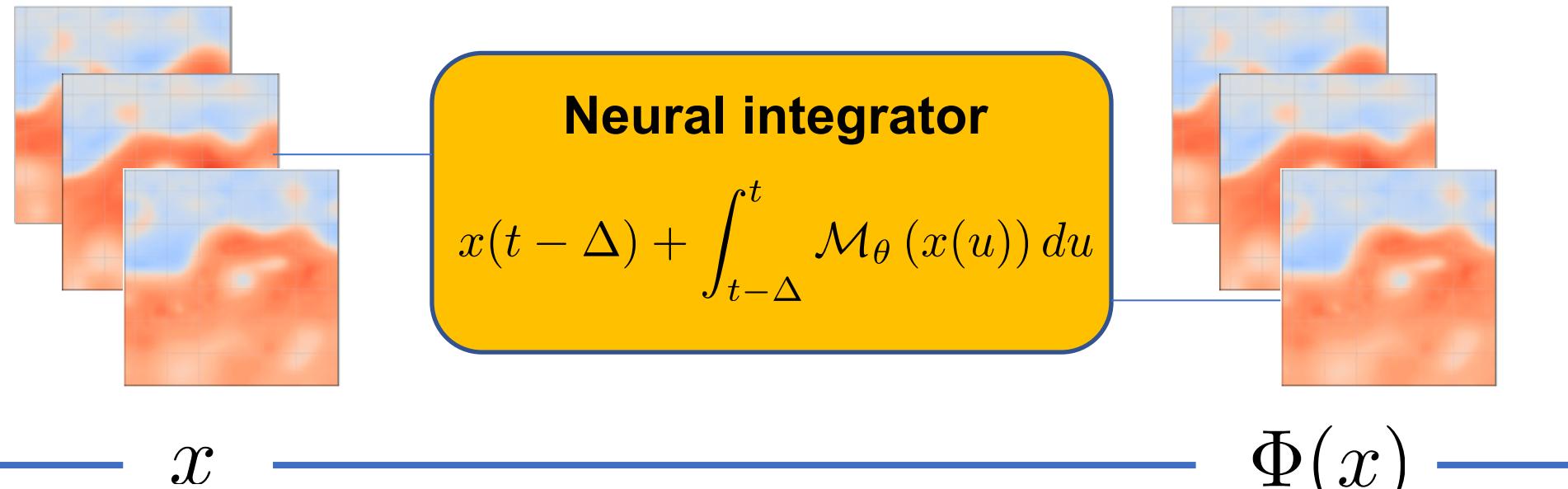
*Unfolded  
architecture of a  
4DVar-WC scheme*

$$\min_{\mathbf{x}} \underbrace{\|\mathbf{x} - \mathcal{H}(\mathbf{x})\|^2 + \nu \|\mathbf{x} - \Phi(\mathbf{x})\|^2}_{U_{\mathcal{H}, \Phi}}$$

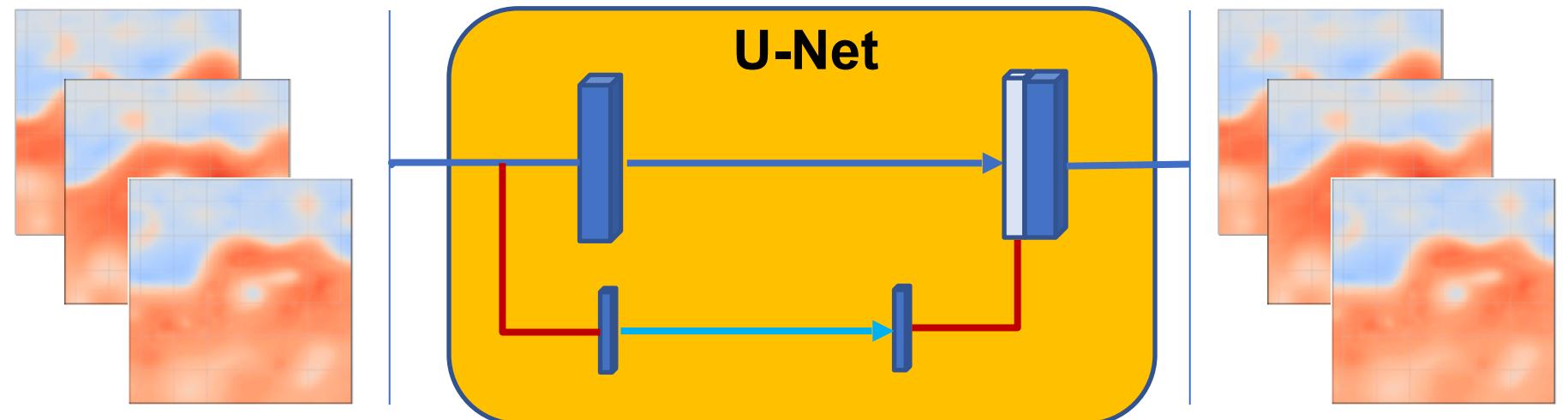


# End-to-end learning for 4DVar DA: projection operator $\Phi$

Parameterization using (learnable) ODE operator

$$\frac{\partial x(t)}{\partial t} = \mathcal{M}_\theta(x(t))$$


Two-scale U-Net-like Parameterization (Gibbs Field)



# Data Assimilation using Deep unfolding schemes

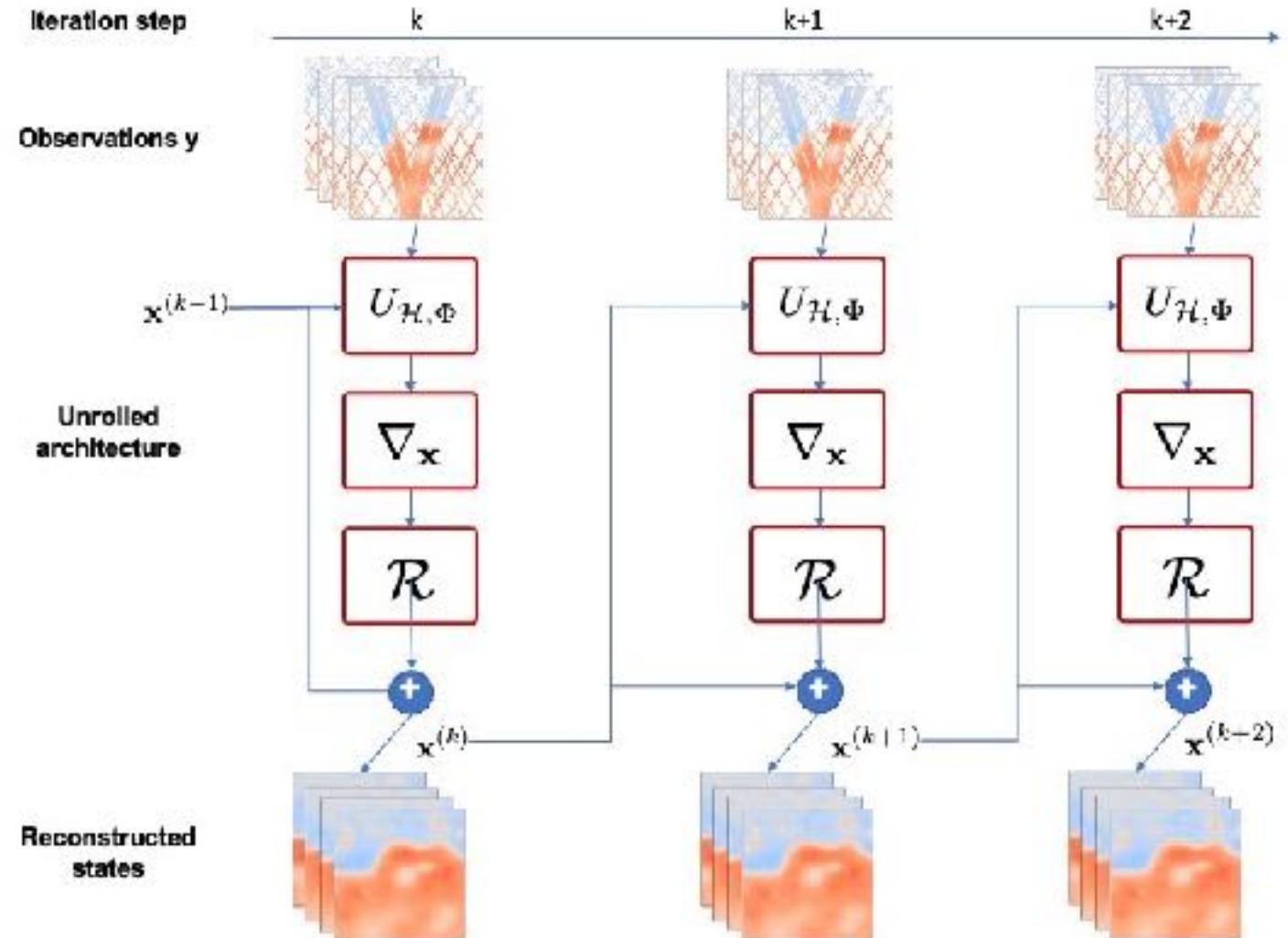
Deep unfolding of 4DVar DA schemes (e.g., 4DVar-WC) [Fablet et al., 2021]

*Unfolded architecture of a  
4DVarNet scheme*

$$\min_{\mathbf{x}} \underbrace{\|\mathbf{x} - \mathcal{H}(\mathbf{x})\|^2 + \nu \|\mathbf{x} - \Phi(\mathbf{x})\|^2}_{U_{\mathcal{H}, \Phi}}$$

*Iterative gradient-based update*

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \mathcal{R}(\nabla_{\mathbf{x}} U_{\mathcal{H}, \Phi}(\mathbf{x}, \mathbf{y}))$$



# Data Assimilation using Deep unfolding schemes

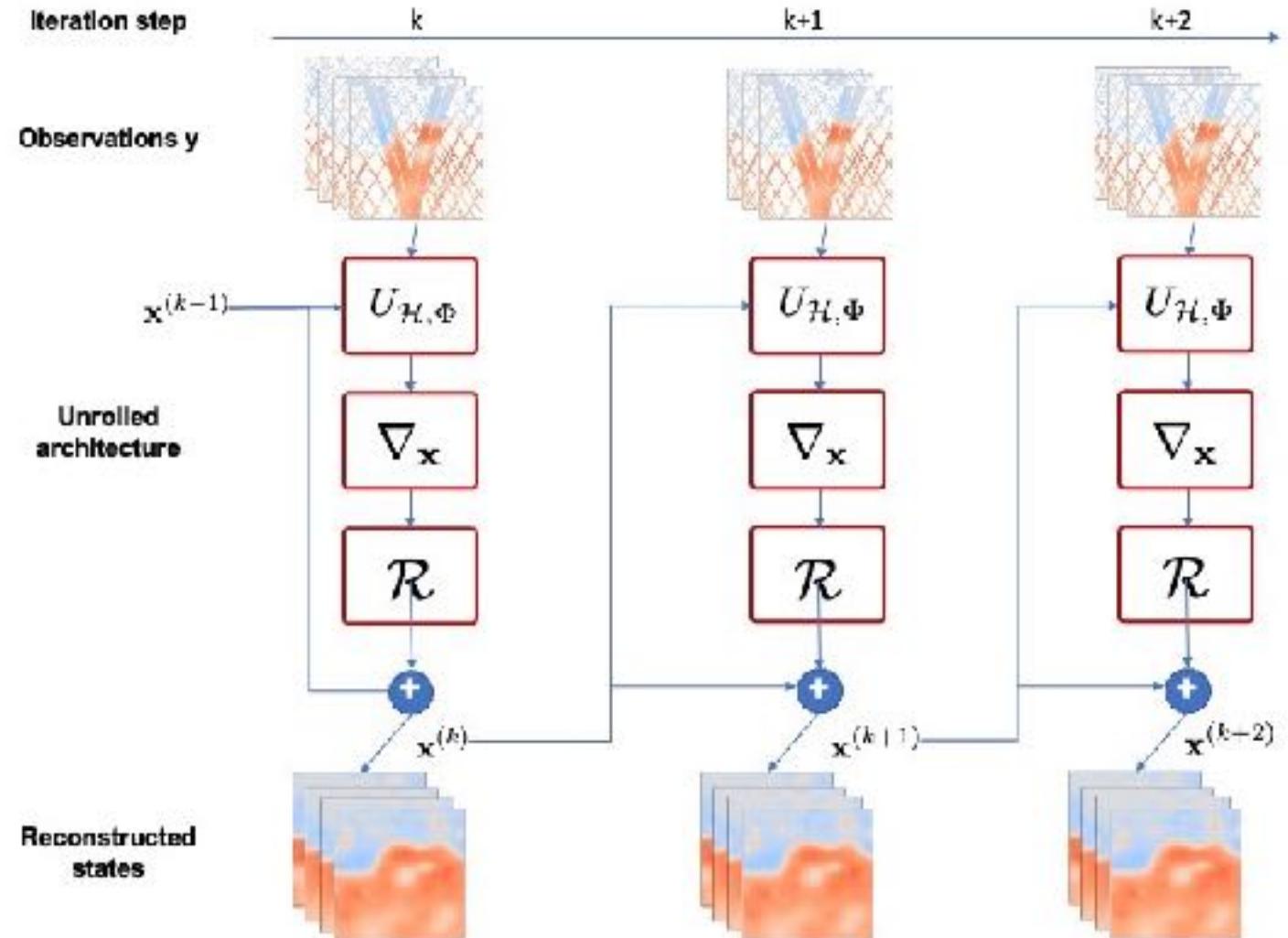
Deep unfolding of 4DVar DA schemes (e.g., 4DVar-WC) [Fablet et al., 2021]

*Unfolded architecture of a  
4DVarNet scheme*

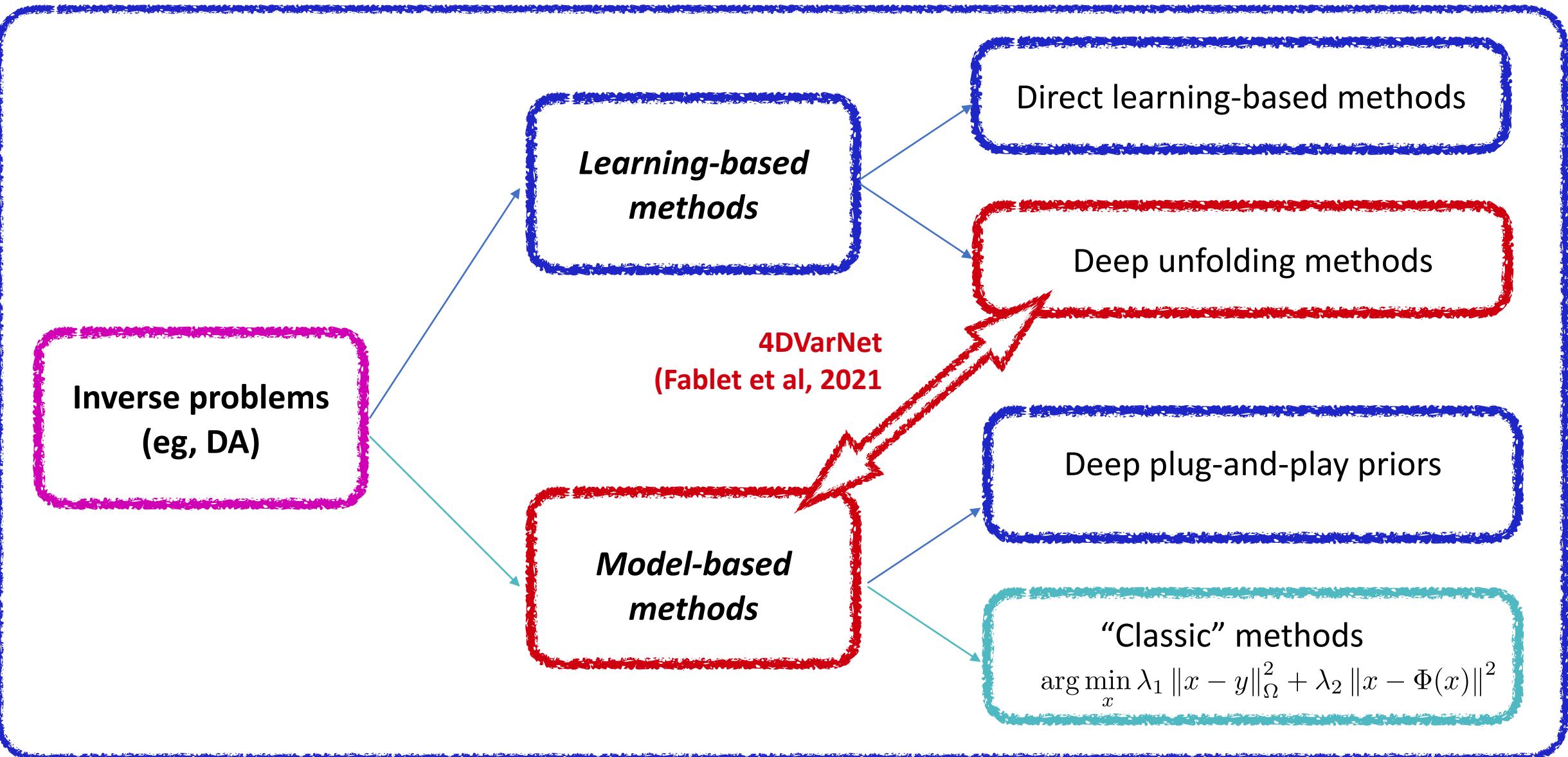
$$\min_{\mathbf{x}} \underbrace{\|\mathbf{x} - \mathcal{H}(\mathbf{x})\|^2 + \nu \|\mathbf{x} - \Phi(\mathbf{x})\|^2}_{U_{\mathcal{H}, \Phi}}$$

*Iterative gradient-based update*

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \mathcal{R}(\nabla_{\mathbf{x}} U_{\mathcal{H}, \Phi}(\mathbf{x}, \mathbf{y}))$$



# Model-driven vs. Learning-based approaches



# 4DVarNet: Trainable 4DVar Models and Solvers

From a Variational DA formulation

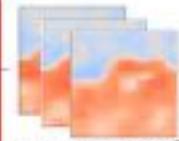
$$\hat{x} = \arg \min_x \|y - H(x)\|^2 + \lambda \|x - \Phi(x)\|^2$$

Trainable variational model

Trainable gradient-based solver

Associated end-to-end scheme

$$x^{(k)} = x^{(k-1)} + \mathcal{R} \left( V_x U \left[ x^{(k)}, y, \Omega \right] \right)$$



Underlying variational formulation

$$\hat{x} = \arg \min_x U [x, y, \Omega]$$

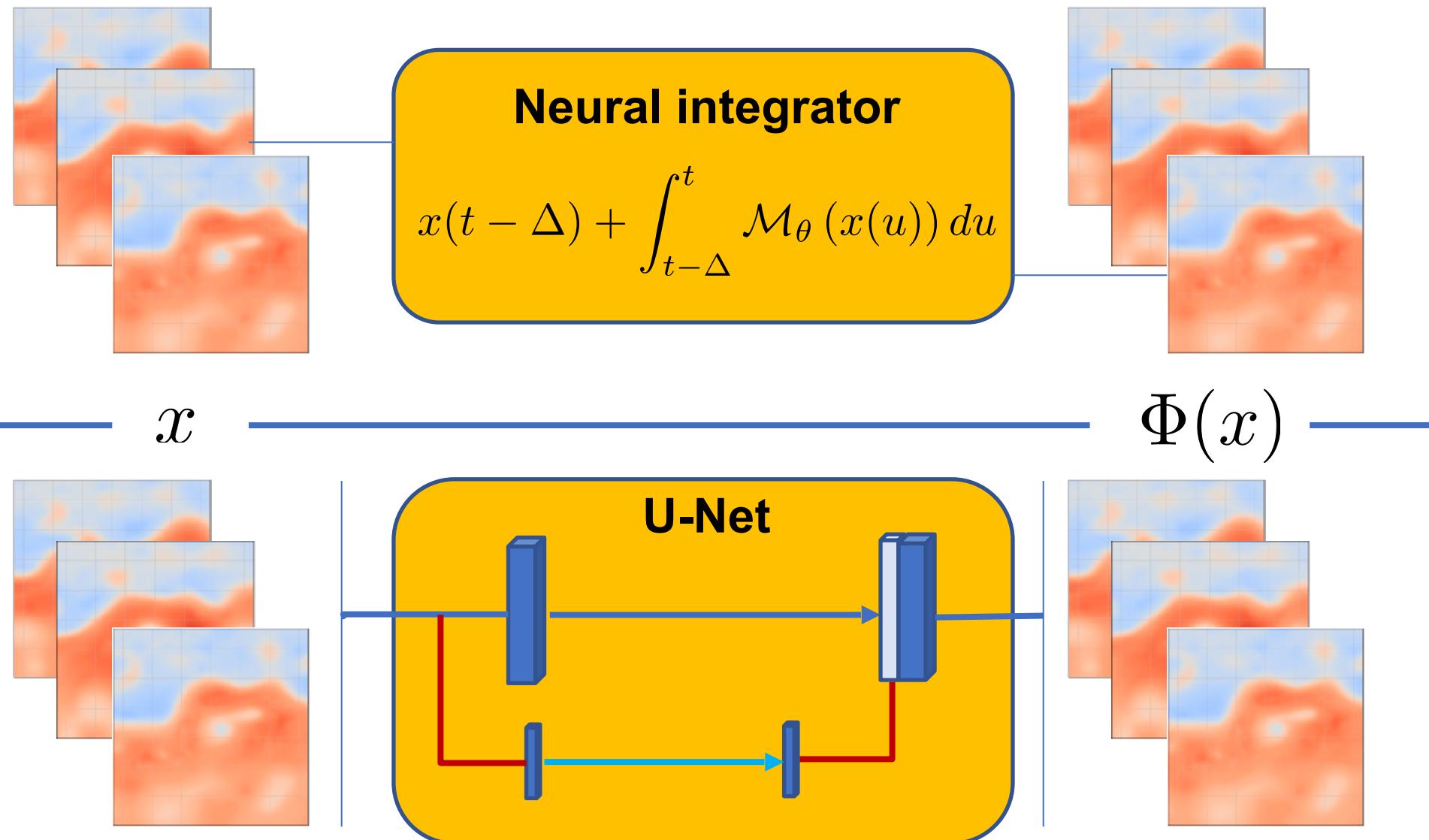
$$\text{with } U [x, y, \Omega] = \|x - y\|_0^2 + \lambda \|x - \Phi(x)\|^2$$

Which training loss ?

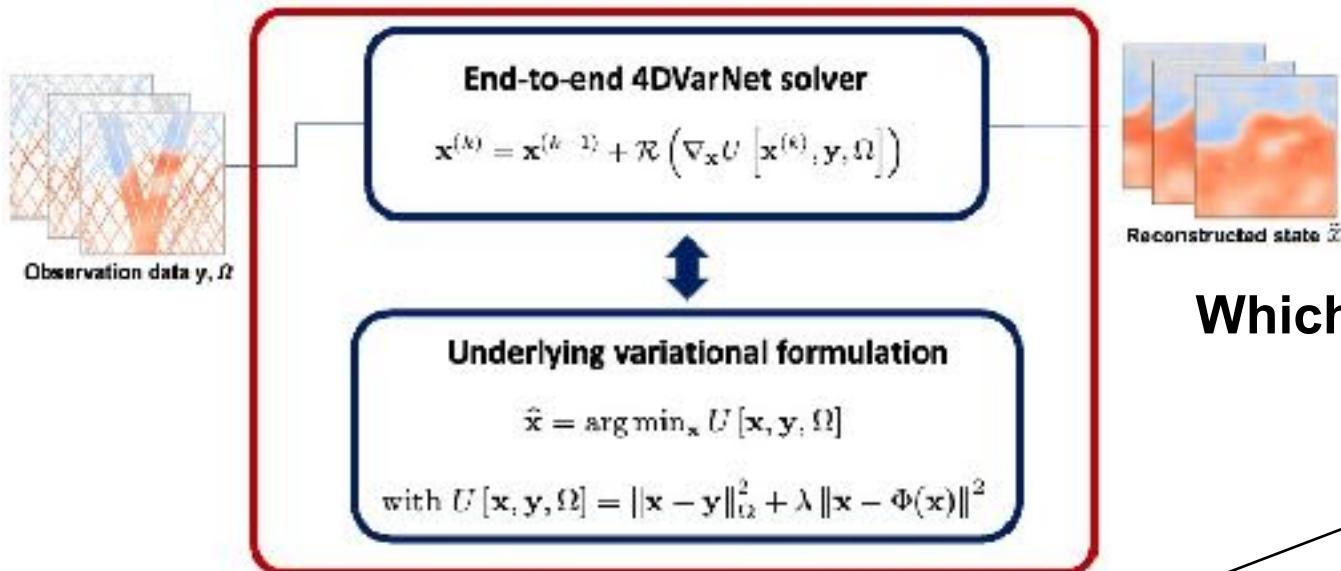
Which parameterisation for operator  $\Phi$  ?

# 4DVarNet architecture: projection operator $\Phi$

Parameterization using (learnable) ODE operator

$$\frac{\partial x(t)}{\partial t} = \mathcal{M}_\theta(x(t))$$


# Model-based vs. Learning-based 4DVar DA: Unsupervised vs. Supervised scheme



**Which training loss for 4DVarNet scheme ?**

**Unsupervised loss**

$$\mathcal{L}(x, y) = \|x - y\|^2 + \lambda \|x - \Phi(x)\|^2$$

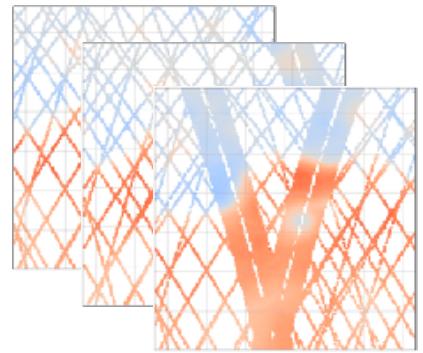
**Supervised loss**

$$\mathcal{L}(x, x^{true}) = \|x - x^{true}\|^2$$

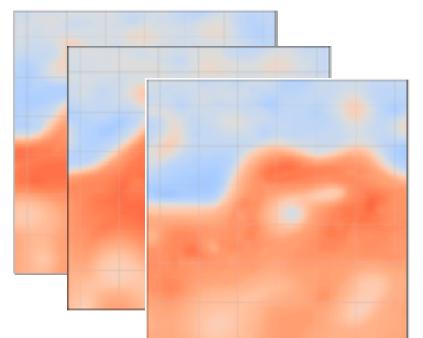
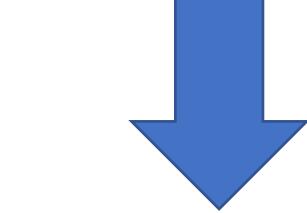
**Regularisation loss**

$$\mathcal{L}_{Reg}(x, x^{true}) = \|x - \Phi(x)\|^2 + \|x^{true} - \Phi(x^{true})\|^2$$

# Model-based vs. Learning-based 4DVar DA



Partial observations  $y$



True states  $x$

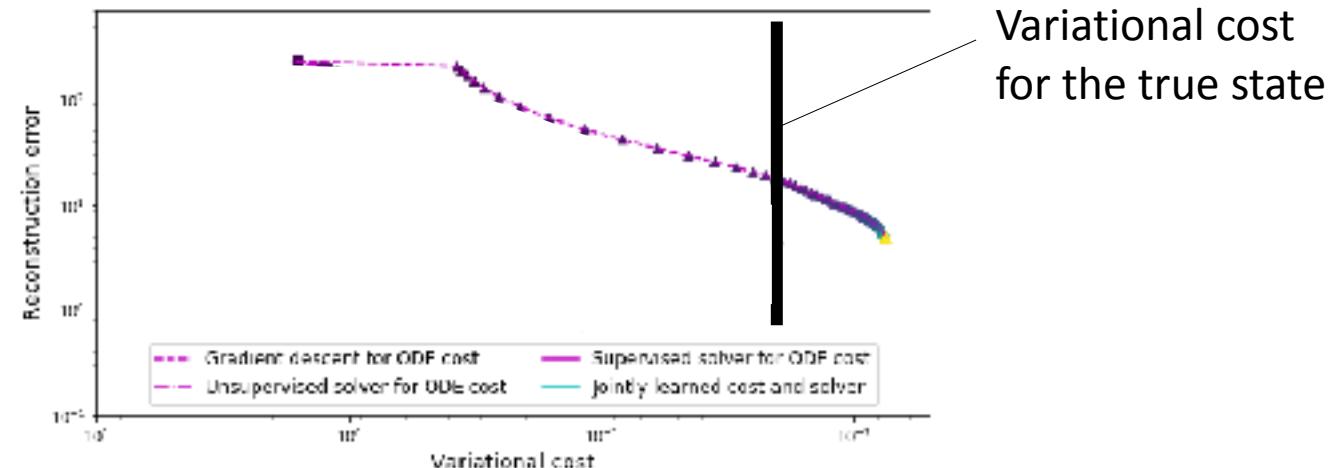
**Model-driven schemes:**  $\widehat{x} = \arg \min_x \underbrace{\lambda_1 \|x - y\|_{\Omega}^2 + \lambda_2 \|x - \Phi(x)\|^2}_{U_{\Phi}(x^{(k)}, y, \Omega)}$

**Gradient-based solver (adjoint/Euler-Lagrange method):**  $U_{\Phi}(x^{(k)}, y, \Omega)$

$$x^{(k+1)} = x^{(k)} - \alpha \nabla_x U_{\Phi}(x^{(k)}, y, \Omega)$$

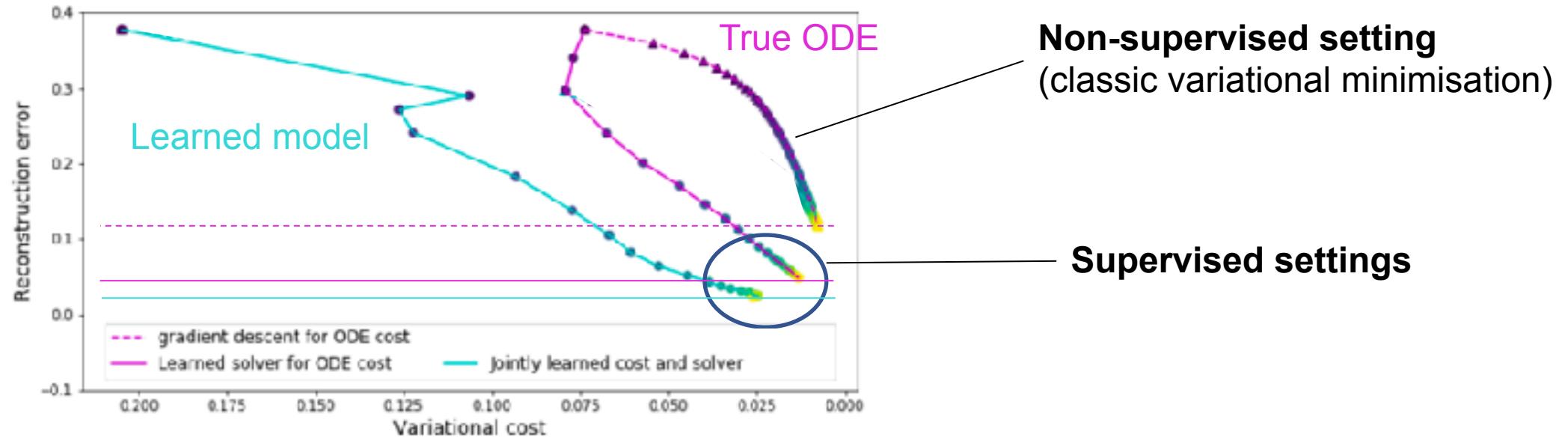
No control on the reconstruction error

$$x^{true} \neq \arg \min_x U_{\Phi}(x^{(k)}, y, \Omega)$$

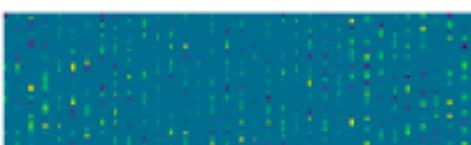
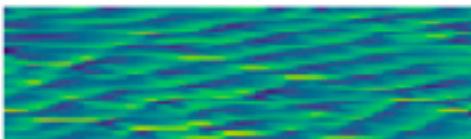


# End-to-end learning for inverse problems (Fablet et al., 2020)

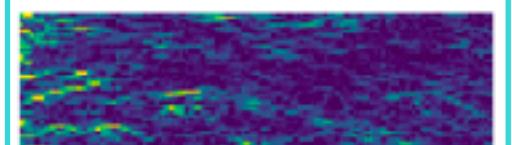
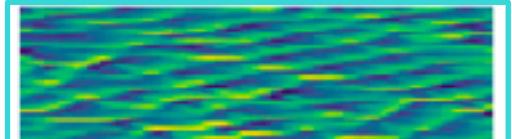
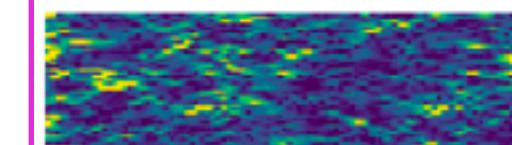
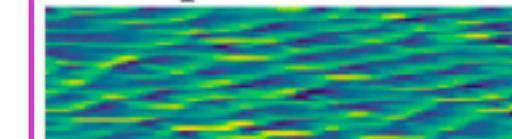
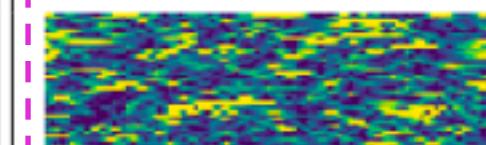
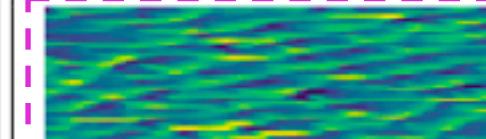
Illustration on Lorenz-96 dynamics (Bilinear ODE)



True and observed states

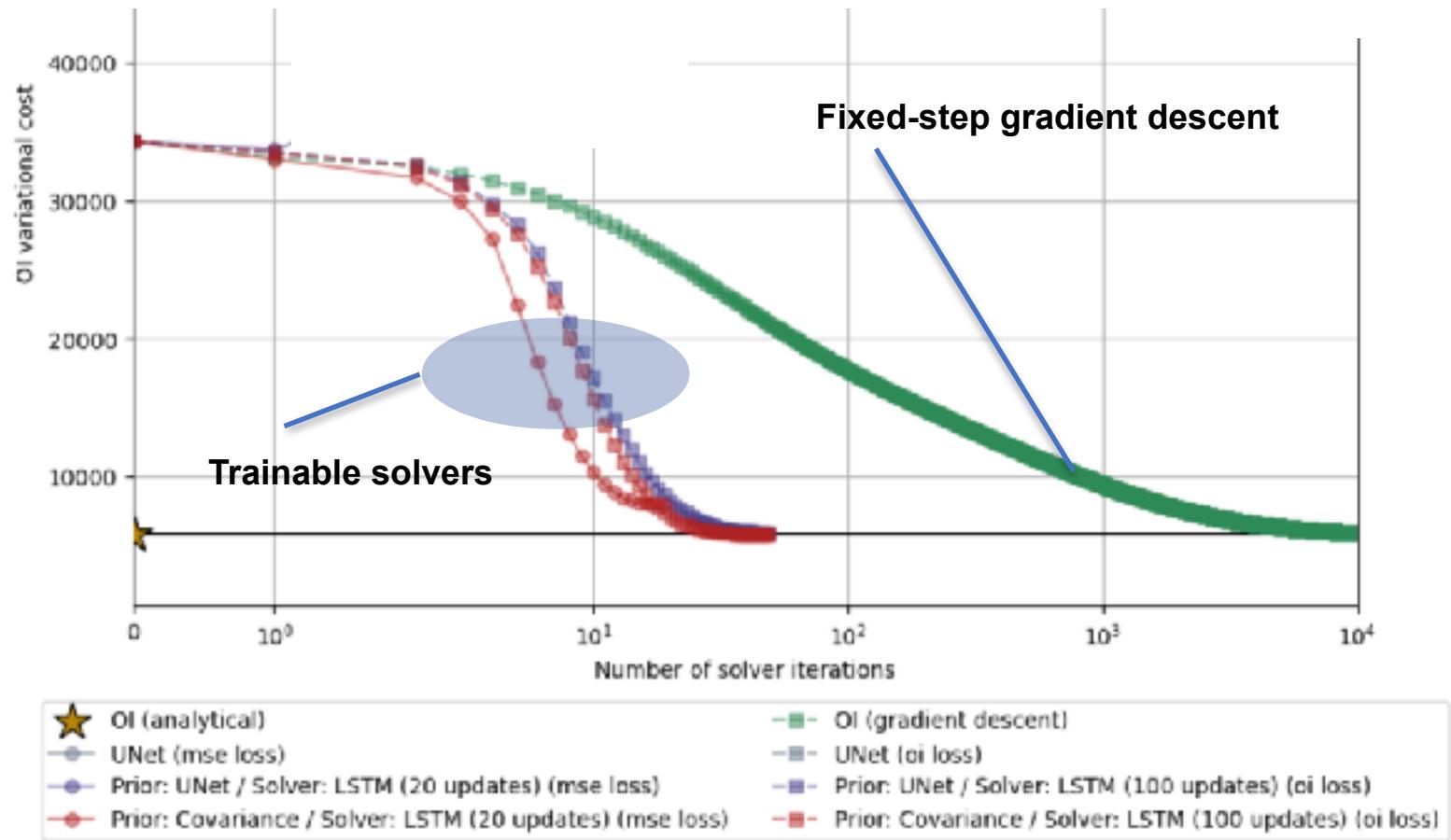
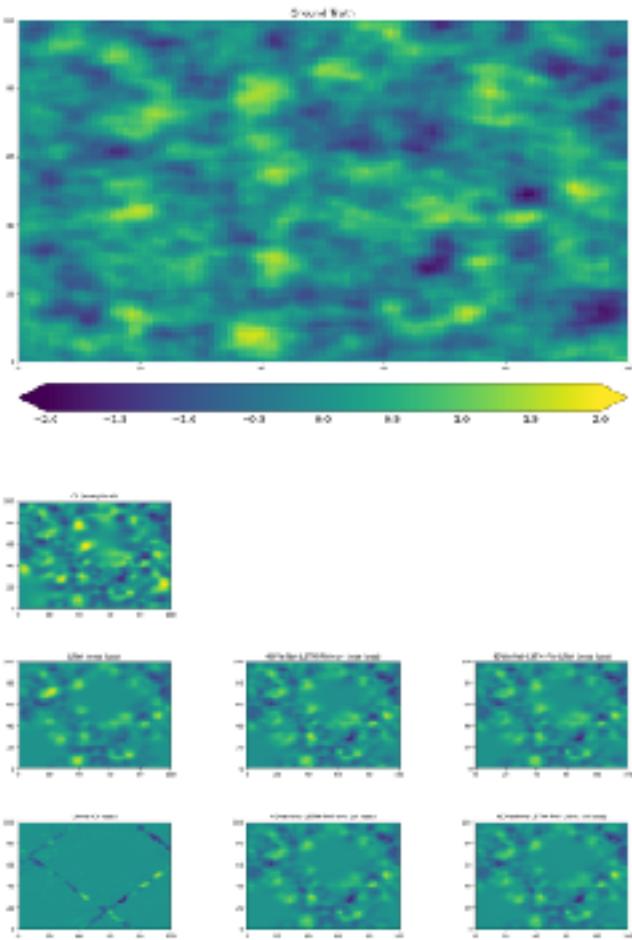


Reconstruction examples and associated error maps



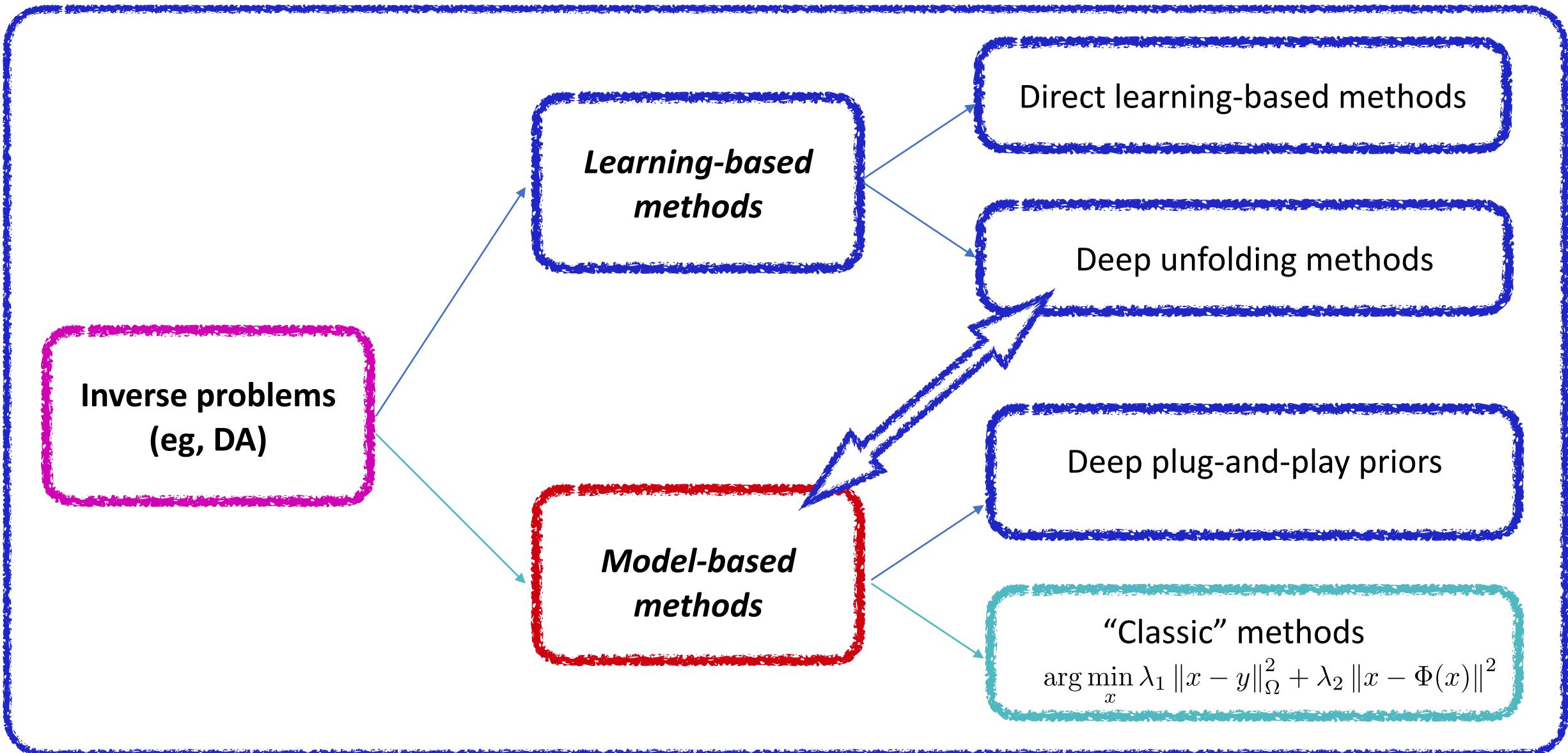
# 4DVarNet and Optimal Interpolation

## Case-study for an isotropic Gaussian Process



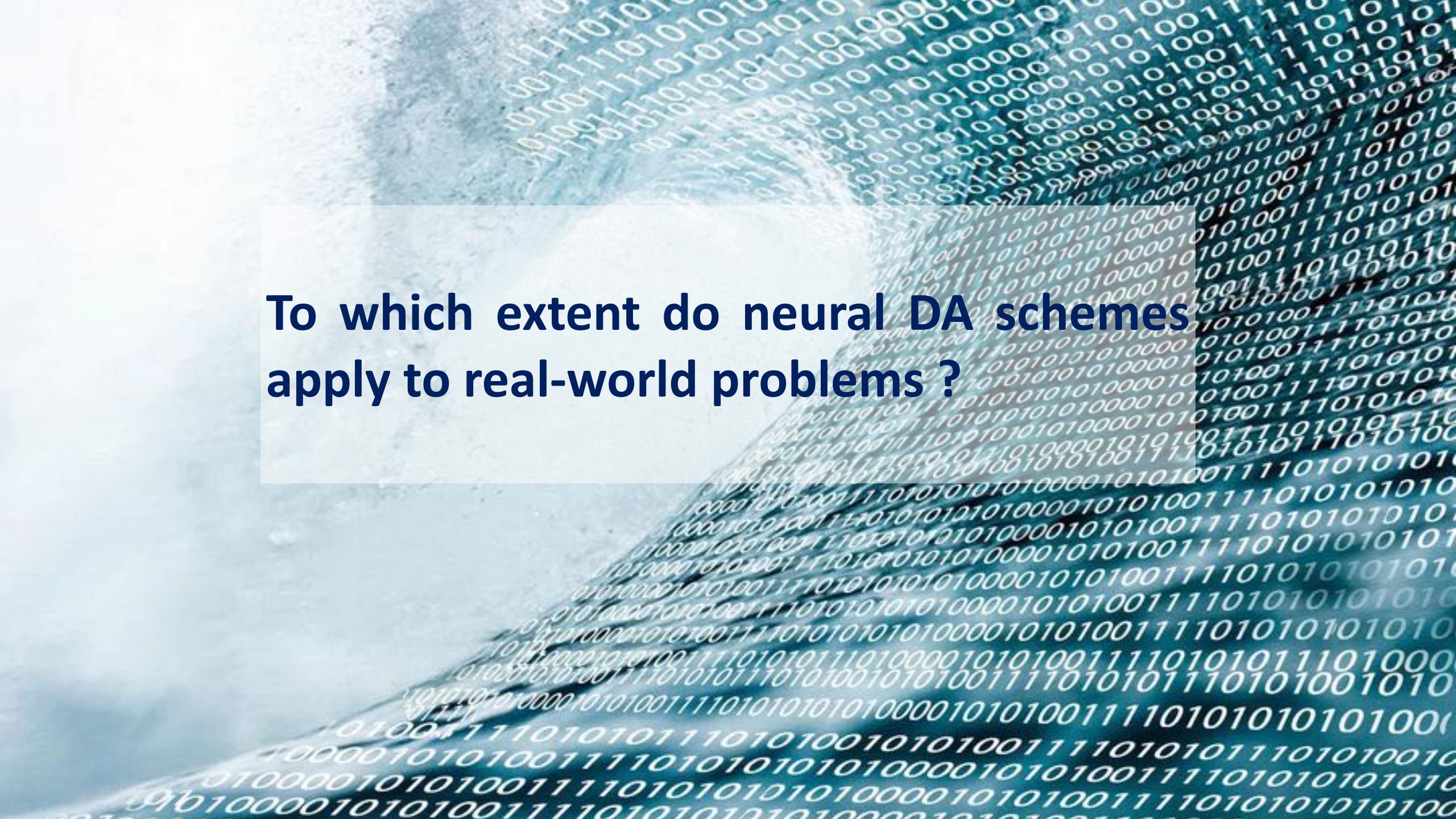
# Summary on Inverse Problems and Deep Learning

# Model-driven vs. Learning-based approaches



# Summary

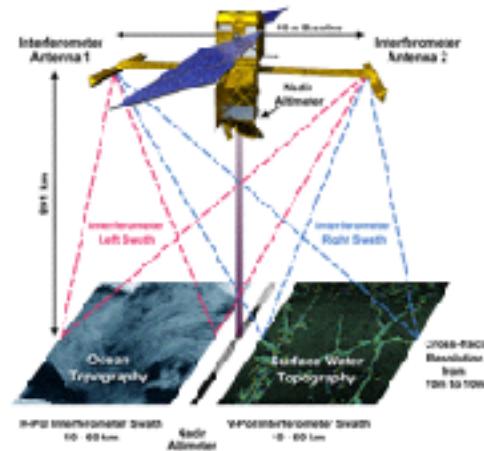
- *NNs as numerical schemes for ODE/PDE/variational representations of geophysical dynamics*
- *NN plug-and-play priors*
- *End-to-end architecture for jointly learning a representation (eg, ODE or NN prior) and a solver*
- *Requirement for differential implementations*
- *The true prior might not be the optimal choice to solve inverse problems*



# To which extent do neural DA schemes apply to real-world problems ?

# 4DVarNet as end-to-end DA schemes for space oceanography

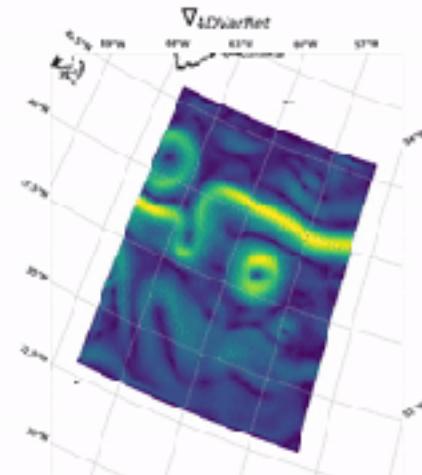
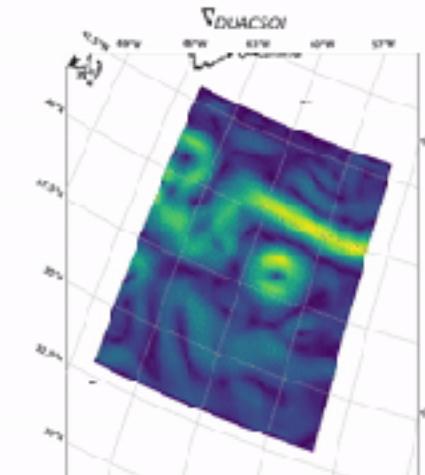
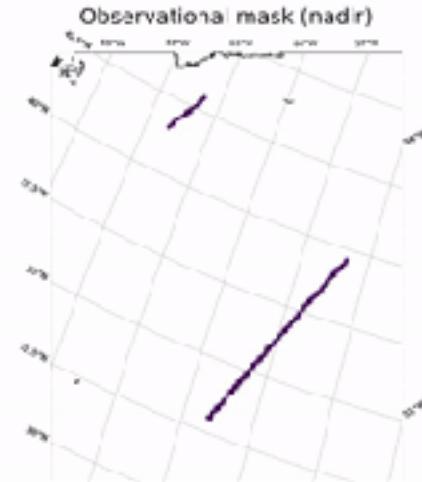
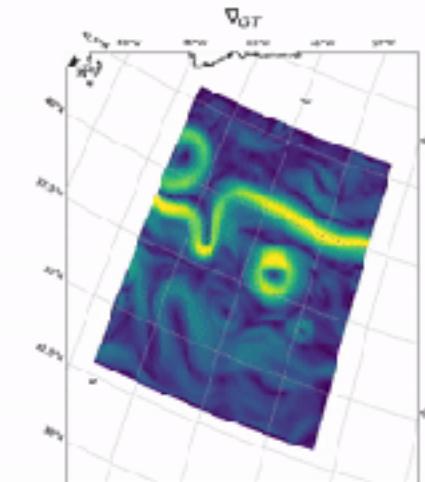
## Satellite altimetry



### Best score for BOOST-SWOT SLA Data Challenge

duacs 1 swot + 4 nadirs	0.92	0.02	1.22	11.15	Covariances DUACS	eval_duacs.ipynb
bfn 1 swot + 4 nadirs	0.93	0.02	0.8	10.09	CG Nudging	eval_bfn.ipynb
dymos: 1 swot + 4 nadirs	0.93	0.02	1.2	10.07	Dynamic mapping	eval_dymos.ipynb
mios: 1 swot + 4 nadirs	0.94	0.01	1.18	10.14	Multiscale mapping	eval_mios.ipynb
<b>4DVarNet 1 swot + 4 nadirs</b>	<b>0.96</b>	<b>0.01</b>	<b>0.70</b>	<b>4.15</b>	4DVarNet mapping	eval_4dvarnet.ipynb

[https://github.com/ocean-data-challenges/2020a\\_SSH\\_mapping\\_NATL60](https://github.com/ocean-data-challenges/2020a_SSH_mapping_NATL60)

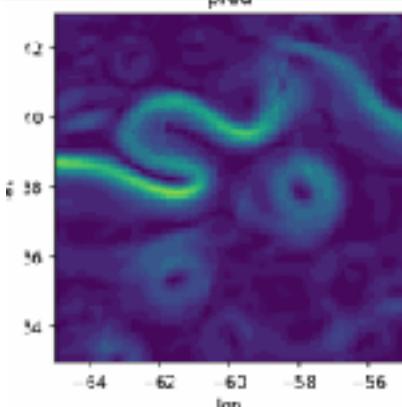


0.00 0.02 0.04 0.06 0.08 0.10 0.12 0.14 0.16

# Application to real satellite-derived datasets

## SLA mapping OSE Data Challenge

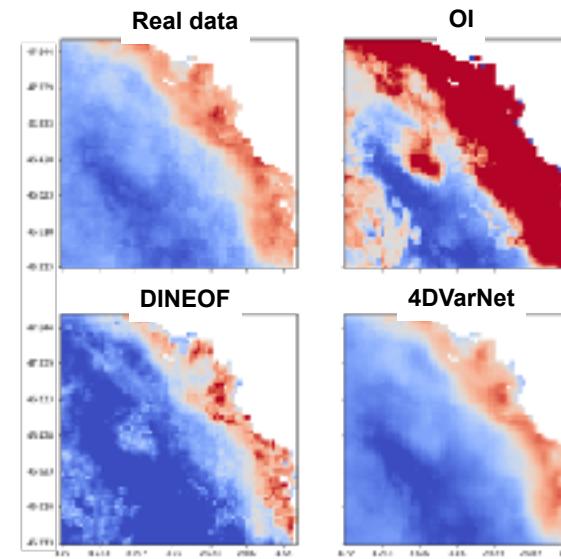
Method	$\mu$ (RMSE)	$\sigma$ (RMSE)	$\lambda x$ (km)	Notes
BASELINE	0.85	0.09	140	Covariances BASELINE OI
DUACS	0.88	0.07	152	Covariances DUACS DT2018
MIOST	0.89	0.08	139	Multiscale mapping
DYMOST	0.89	0.06	129	Dynamic mapping
BNF	0.88	0.06	122	BNF mapping
<b>4DVarNet</b>	<b>0.89</b>	<b>0.06</b>	<b>102</b>	<b>4DVarNet mapping</b>



[https://github.com/ocean-data-challenges/2021a\\_SSH\\_mapping\\_OSE](https://github.com/ocean-data-challenges/2021a_SSH_mapping_OSE)

## Sea surface suspended sediments

Metric	Dataset	Unit	Samp. Strat	OI	DinEOF	4DVarNet
RMSE	OSSE	$\log_{10}[\text{g/L}]/\text{m}$	-	0.176	0.167	<b>0.104</b>
	MODIS	$\log_{10}[\text{g/L}]/\text{m}$	Random	0.304	0.237	<b>0.156</b>
	MODIS	$\log_{10}[\text{g/L}]/\text{m}$	Patch	0.346	0.253	<b>0.168</b>
R-score	OSSE	%	-	90.4	91.3	<b>96.6</b>
	MODIS	%	Random	60.5	76.4	<b>89.5</b>
	MODIS	%	Patch	56.5	73.8	<b>87.3</b>



Simulation and real data

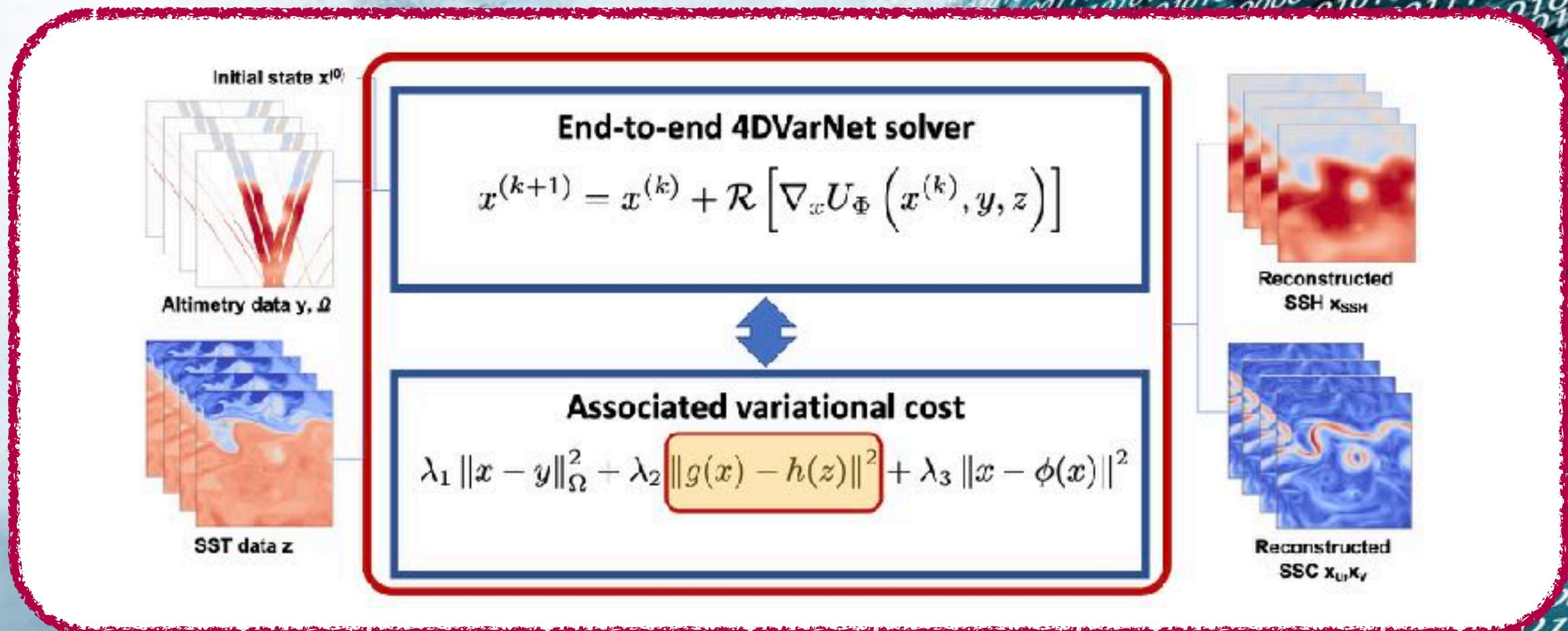
Learning from real gappy data only

Vient et al., 2022

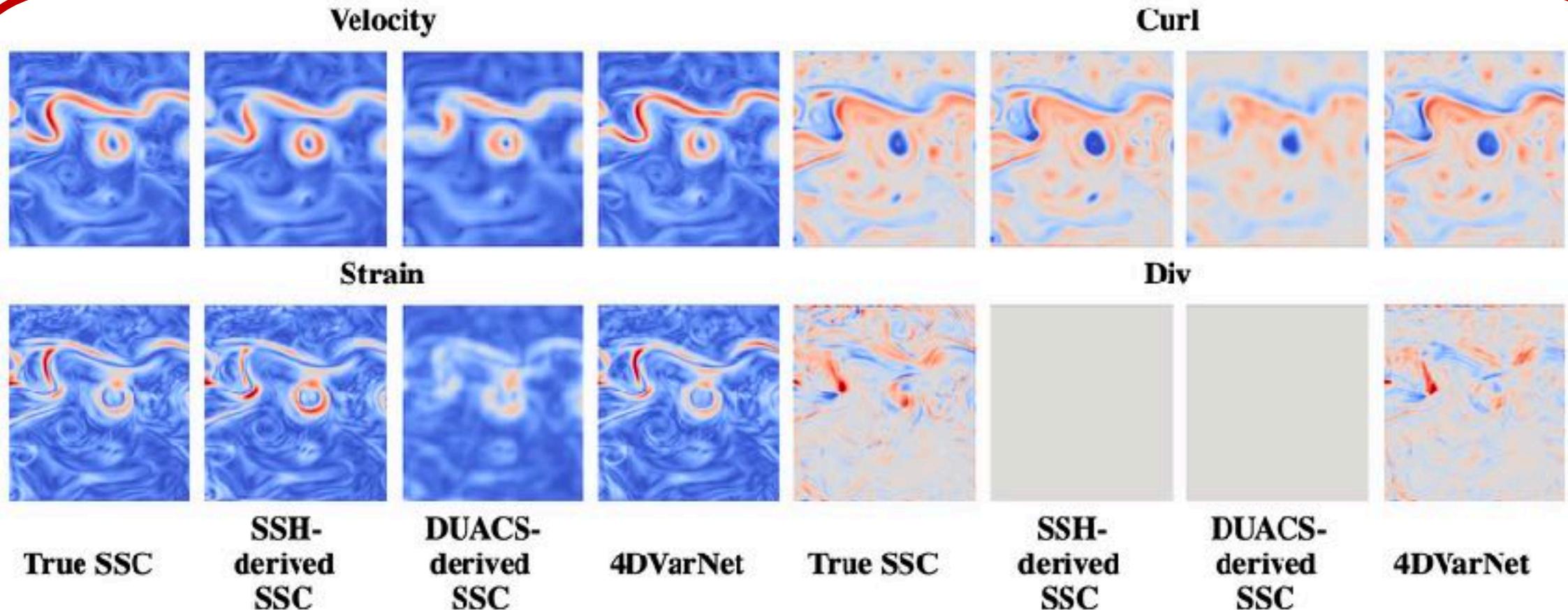
<https://doi.org/10.3390/rs14164024>

Mean gradient norm

# Can we inform sea surface dynamics which are never directly observed ?



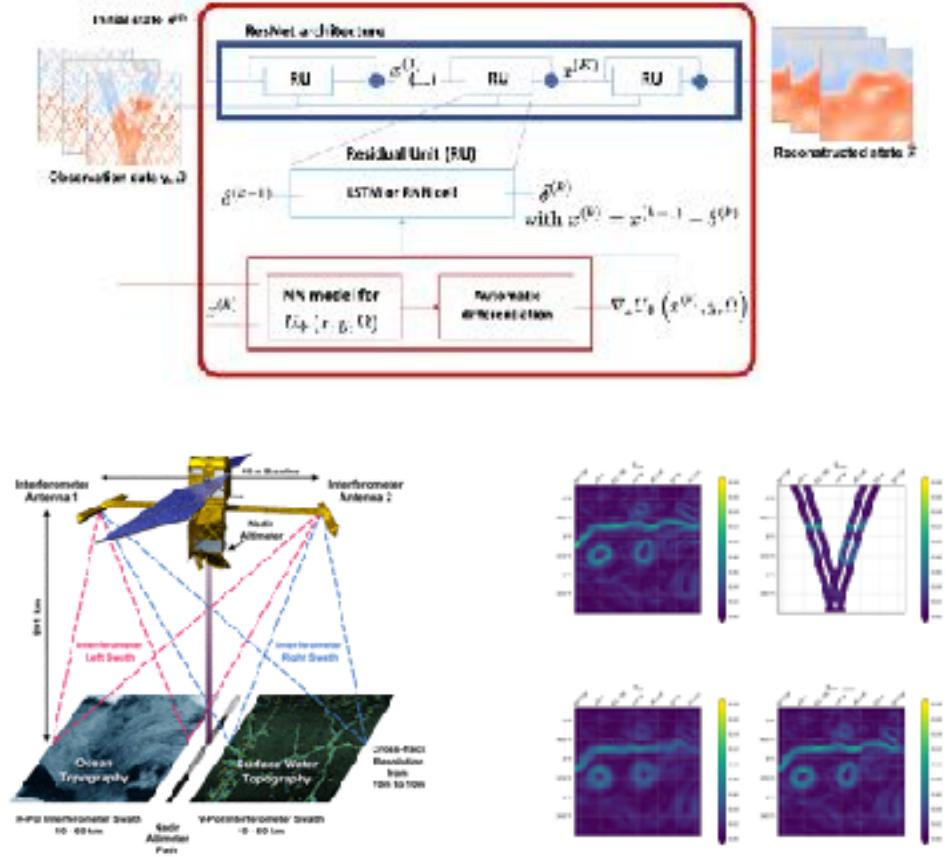
# 4DVarNet to inform sea surface currents (Fablet et al., arXiv 2022)



4DVarNet to recover a significant fraction of the unobserved agesotropvhic (divergent) currents

# Key messages

- Physics-informed learning for satellite ocean remote sensing
- Trainable variational DA models (observation model, prior, solver)
- Application to interpolation, forecasting sampling and multimodal synergies
- Generic framework beyond space oceanography
- Objective-specific vs. Generic priors and DA schemes ?



Preprint: <https://doi.org/10.1029/2021MS002572>  
Code: <https://github.com/CIA-Oceanix/4dvarnet-core>

**Thank you.**

# AI Chair OceaniX 2020-2024

Physics-informed AI for Observation-  
Driven Ocean AnalytiX

PI: R. Fablet, Prof. IMT Atlantique, Brest

Web: <https://cia-oceanix.github.io/>



# References

- **Meta-learning:**
  - Andrychowicz, et al (2016). Learning to learn by gradient descent by gradient descent. NIPS, 2016
  - Hospedales et al. (2020). Meta-learning in neural networks: A survey. arXiv preprint arXiv:2004.05439.
- **End-to-end learning for Inverse Problems:**
  - Dieleman et al. End-to-end learning for music audio. IEEE ICASSP 2014. doi: 10.1109/ICASSP.2014.6854950
  - Lucas et al. (2018). Using Deep Neural Networks for Inverse Problems in Imaging: Beyond Analytical Methods. IEEE SPM, 35(1), 20–36. doi: 10.1109/MSP.2017.2760358
- **Inverse problems with Plug-and-play priors:**
  - McCann et al. (2017). Convolutional Neural Networks for Inverse Problems in Imaging: A Review. IEEE SPM, 34(6), 85–95. doi: 10.1109/MSP.2017.2739299
  - Zhang et al. (2020). Plug-and-Play Image Restoration with Deep Denoiser. <https://arxiv.org/abs/2008.13751>
- **Deep unfolding methods:**
  - Chen et al. (2015). On Learning Optimized Reaction Diffusion Processes for Effective Image Restoration. In Proc. IEEE CVPR (pp. 5261–5269).
  - Yan et al. Deep ADMM-Net for Compressive Sensing MRI. NIPS, 2016.
  - Boudier et al. DAN -- An optimal Data Assimilation framework based on machine learning Recurrent Networks. Preprint, 2020.
  - Fablet et al. Learning Variational Data Assimilation Models and Solvers. JAMES, 2021.