OceaniX-Melody Sandbox: Deep Learning and Data Assimilation (Melody WP3)

OceaniX-Melody Sandbox, April 2021

OceaniX-Melody sandbox, April 9th, 10am-12am

Program

- 4DVarNN@OceaniX: current status and new applications (**Ronan F.**), 10am-10.30am
- Data Assimilation for SSH mapping (**Emmanuel C.**), 10.30am-10.50am
- SSH mapping Data Challenge (**Quentin F.**), 10.50am-11.00am
- Learning physical parameterizations using DA and EM (**Pierre T.**), 11.00am-11.20am
- Discussion on end-to-end learning, DA and uncertainty propagation (**Said O.**), 11.20am-11.40am
- Discussion on future work, 11.40am-12.00am

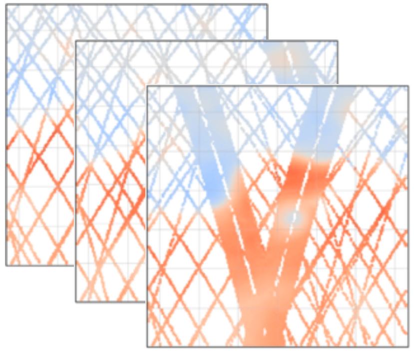
4DVarNN@OceaniX: current status and new applications

OceaniX team

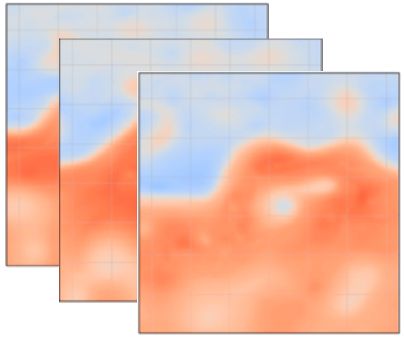
Webpage: https://cia-oceanix.github.io/
Code: https://github.com/CIA-Oceanix/DinAE_4DVarNN_torch

OceaniX-Melody Sandbox, April 2021

(Weak constraint) **4DVar Data Assimilation (DA) formulation**



Partial observations y



True states x

State-space formulation:

$$\left\{\begin{array}{lcl} \dfrac{\partial x(t)}{\partial t} & = & \mathcal{M}\left(x(t)\right) \\ \\ y(t) & = & x(t)+\epsilon(t), \forall t \in \{t_0, t_0+\Delta t, \ldots, , t_0+N\Delta t\} \end{array}\right.$$

Associated variational formulation:

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

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

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

4DVarNN: Learning 4DVar models and solvers

Trainable Variational DA formulation

$$\widehat{x} = \arg\min_{x} \|x - y\|^2_\Omega + \lambda \|x - \Phi(x)\|^2$$

Predefined

Observation model

Trainable prior

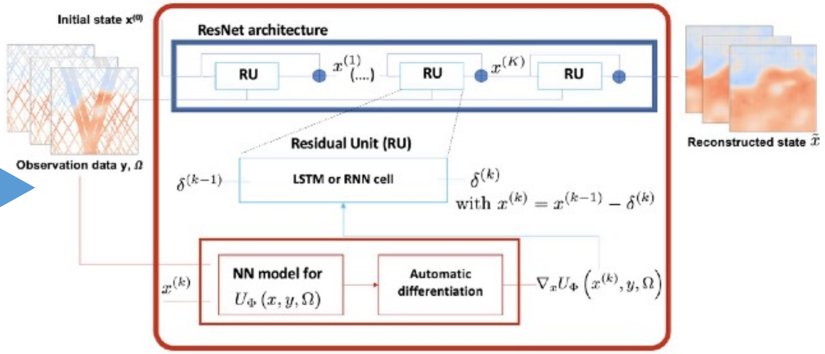
ODE-based

U-Net

AE

Variational model implemented in a differentiable framework (eg, pytorch)

End-to-end architecture



Trainable gradient-based solver

Learning criterion

Variational cost (non-supervised)

Reconstruction error (supervised)

Preprint: https://arxiv.org/abs/2006.03653
Code: https://github.com/CIA-Oceanix/DinAE_4DVarNN_torch

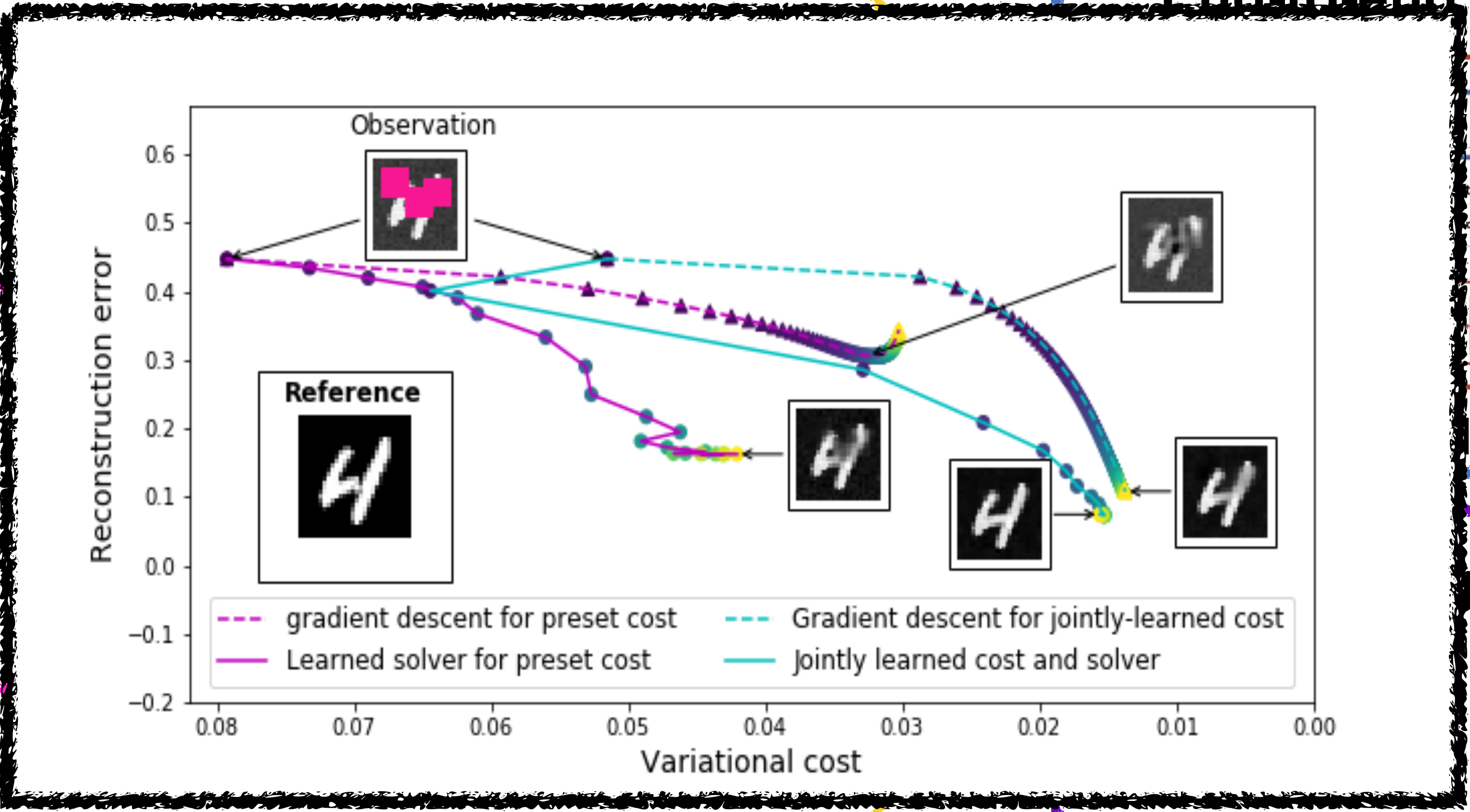
4DVarNN: Learning 4DVar models and solvers

Trainable

$\widehat{x} = \arg\min_{x}$

Prede

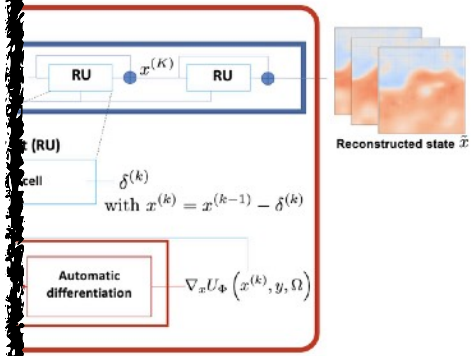
Observati



Variatio

differentiable framework (eg, pytorch)

End-to-end architecture



ient-based solver

criterion

(non-supervised)

error (supervised)

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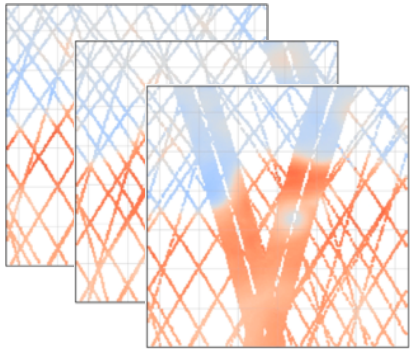
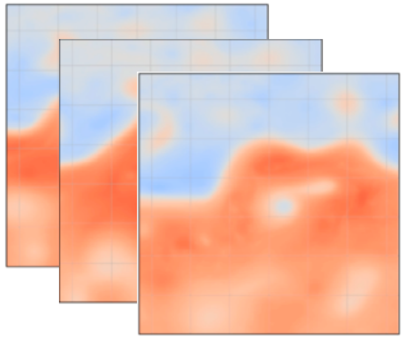
Code: https://github.com/CIA-Oceanix/DinAE_4DVarNN_torch

4DVarNN: Application to satellite-derived SSH mapping



Partial observations y



True states x

Considered formulation:

$$x = (\overline{x}, \delta x)$$

Coarse-scale (for $\overline{x}$) — Fine-scale anomaly (for δx)

$$y = (\overline{y}, y_{alt})$$

OI field (for $\overline{y}$) — Altimeter data (for y_{alt})

Variational model:

$$\sum_t \lambda_{1,t} \|\overline{y}(t) - \overline{x}(t)\|^{\alpha_1} + \lambda_{2,t} \|y_{alt}(t) - \overline{y}(t) - \delta x(t)\|^{\alpha_2}_{\Omega_t}$$

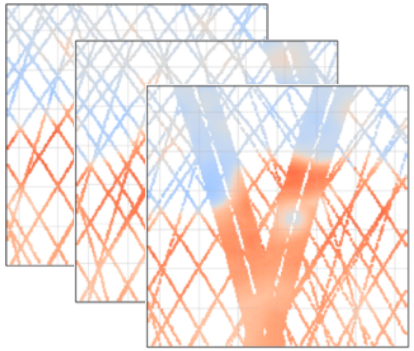
$$+\lambda_3 \|x - \Phi(x)\|^{\alpha_3}$$

Trainable prior: U-Net prior (not ODE-based, cf. L63/L96 experiments)

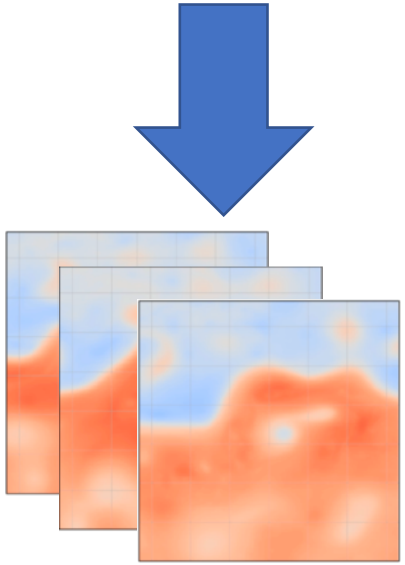
Solver: iterative gradient-based LSTM solver

Training criterion: MSE for the SSH and its gradient norm (supervised learning)

4DVarNN: Application to satellite-derived SSH mapping



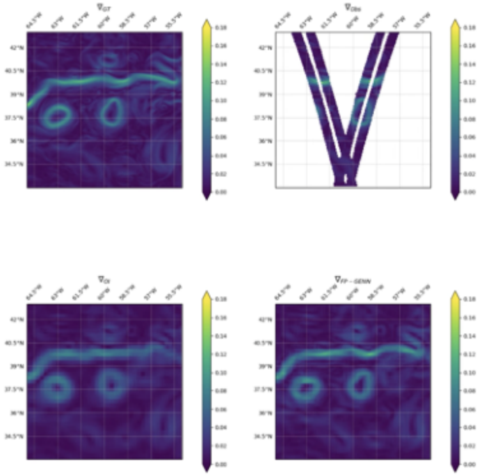
Partial observations y



True states x

OSSE:

- NATL60 data / Gulf Stream region (10°x10°)
- Noise-free SWOT+4-nadir observation dataset
- Test period on 20 days (remaining data used for training)



Results

Models	4DVarNN-L2-LSTM	4DVarNN-L1-LSTM	4DVarNN-L2-FP
relative MSE gain vs. OI for SSH	53 %	52 %	37 %
Relative MSE gain vs. OI for gSSH	45 %	45 %	30 %

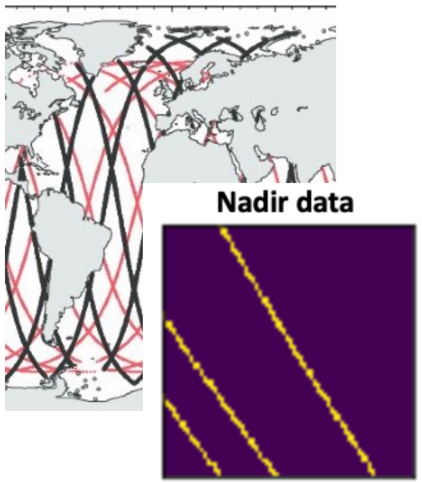
Resolved horizontal scale ~70km
(To be checked for these results)

Lower to no improvement if the prior model to a ConvAE

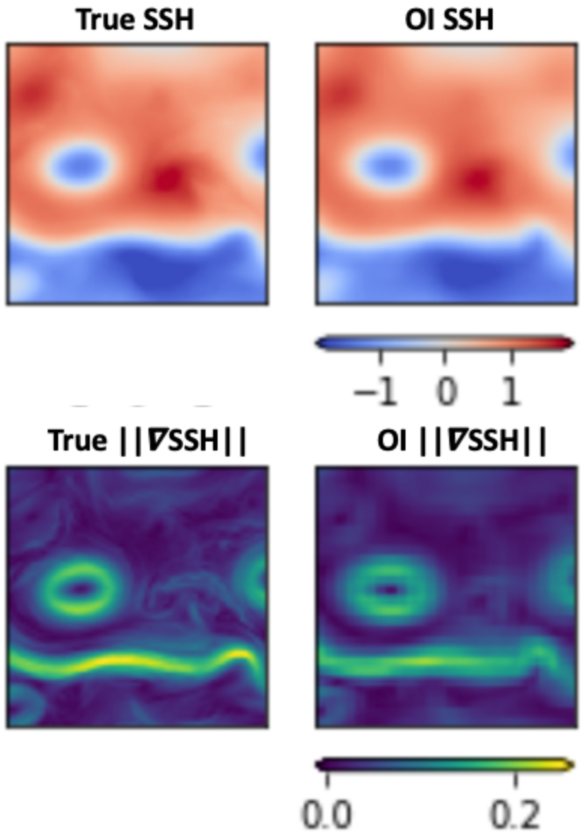
Trained models also apply to nadir-only observation data (with a lower improvement)

4DVarNN #2: New applications

Learning where to sample ?



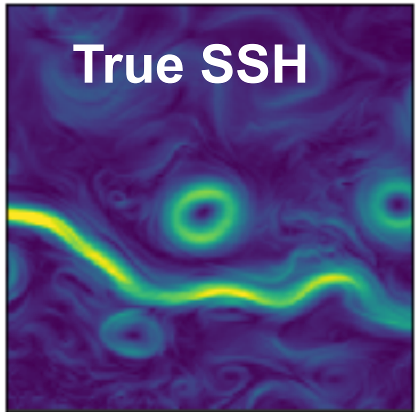
Available sampling pattern (nadir satellite altimeter)

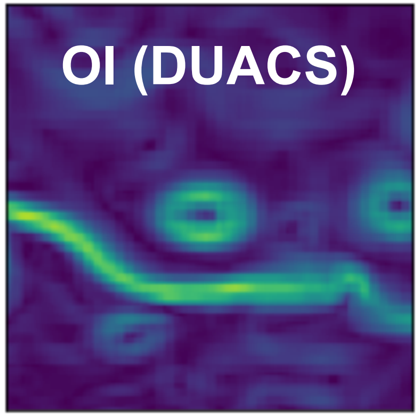


Where to collect new altimetry/ current data to improve the reconstruction of the SSH field and of its gradient ?

4DVarNN #2: New applications

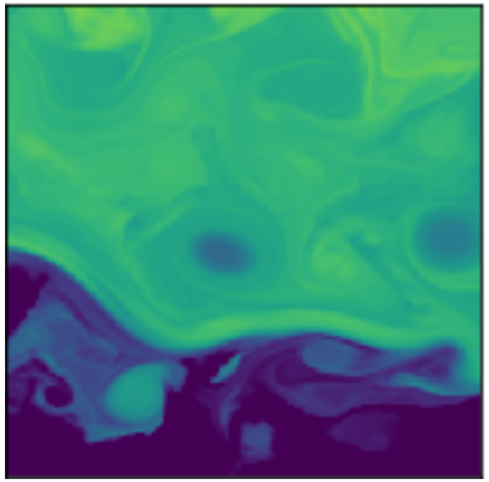
Learning what to measure or extract?





Nadir and SWOT altimeter data mask

What to extract from sea surface fields to improve the reconstruction of the SSH field and of its gradient ?



SST data

4DVarNN #2: New applications

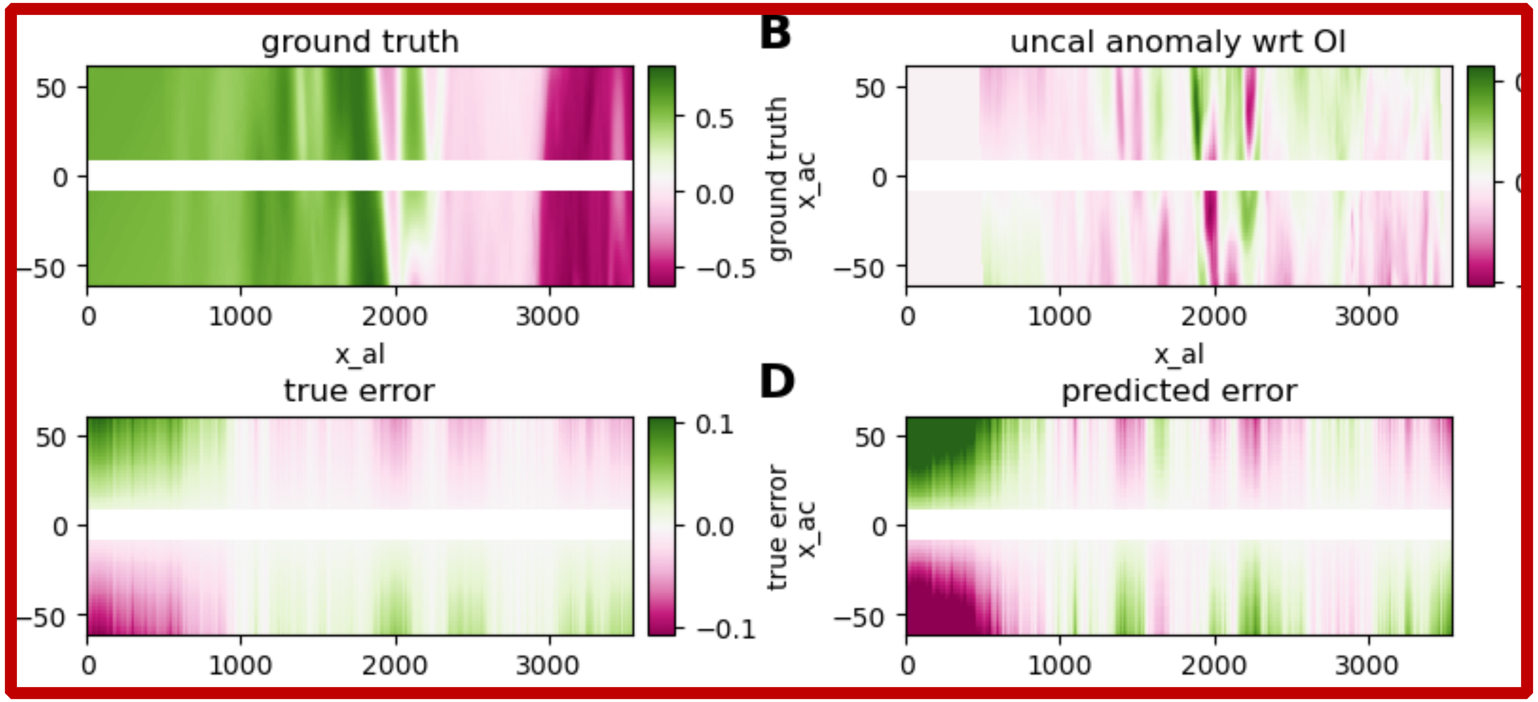
Unsupervised SWOT Calibration

OSSE with NATL60 data + Roll Error signal from SWOT simulator

4-nadir-altimeter + SWOT + DUACS baseline

Gulf Stream area (10°x10°)

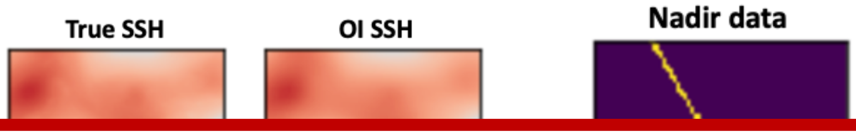
In the 4DVarNN framework we can learn the calibration operator as an observation model jointly with the prior operator



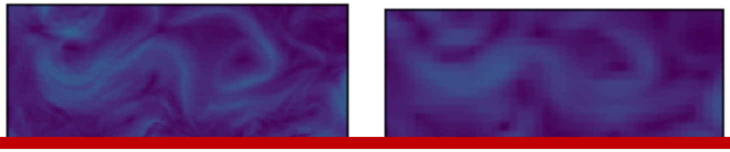
PhD Q. Febvre

4DVarNN #2: New applications

Learning where to sample ?



Learning what to measure ?



4DVarNet models with trainable observation models

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

Sparse sampling operator

$$\|H(z) * (x - y)\|^2$$

$$\text{s.t. } \forall z, \ \|H(z)\|_1 < \epsilon$$

Multimodal observation

$$\|x - y\|^2 + \alpha \|G * x - F * z\|^2$$

SWOT calibration

$$\|H(y) - x\|_\Omega^2$$

4DVarNN #2: New applications

4DVarNet models with trainable observation models

Spase sampling operator

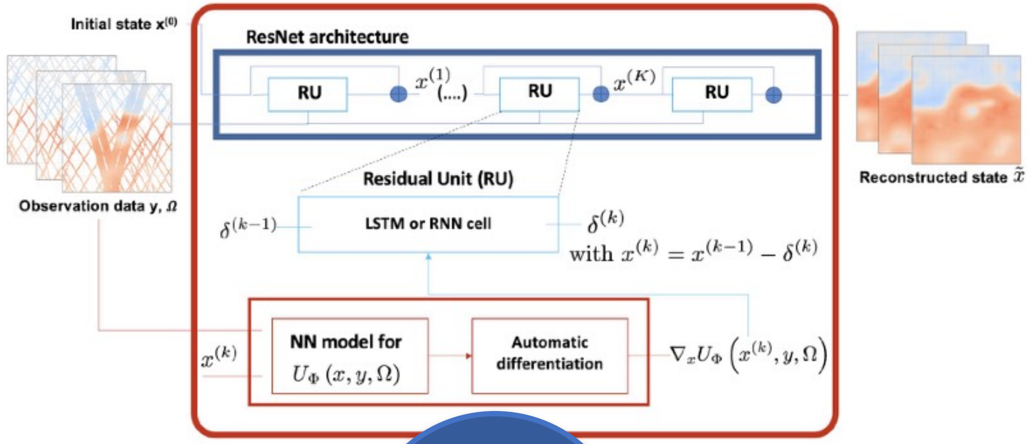
$$\|H(z) * (x - y)\|^2$$

$$\text{s.t. } \forall z, \ \|H(z)\|_1 < \epsilon$$

Multimodal observation

$$\|x - y\|^2 + \alpha\|G * x - F * z\|^2$$

End-to-end 4DVarNet



Supervised training loss

(under sparsity constraint for the optimal sampling case)

4DVarNN #2: Preliminary results

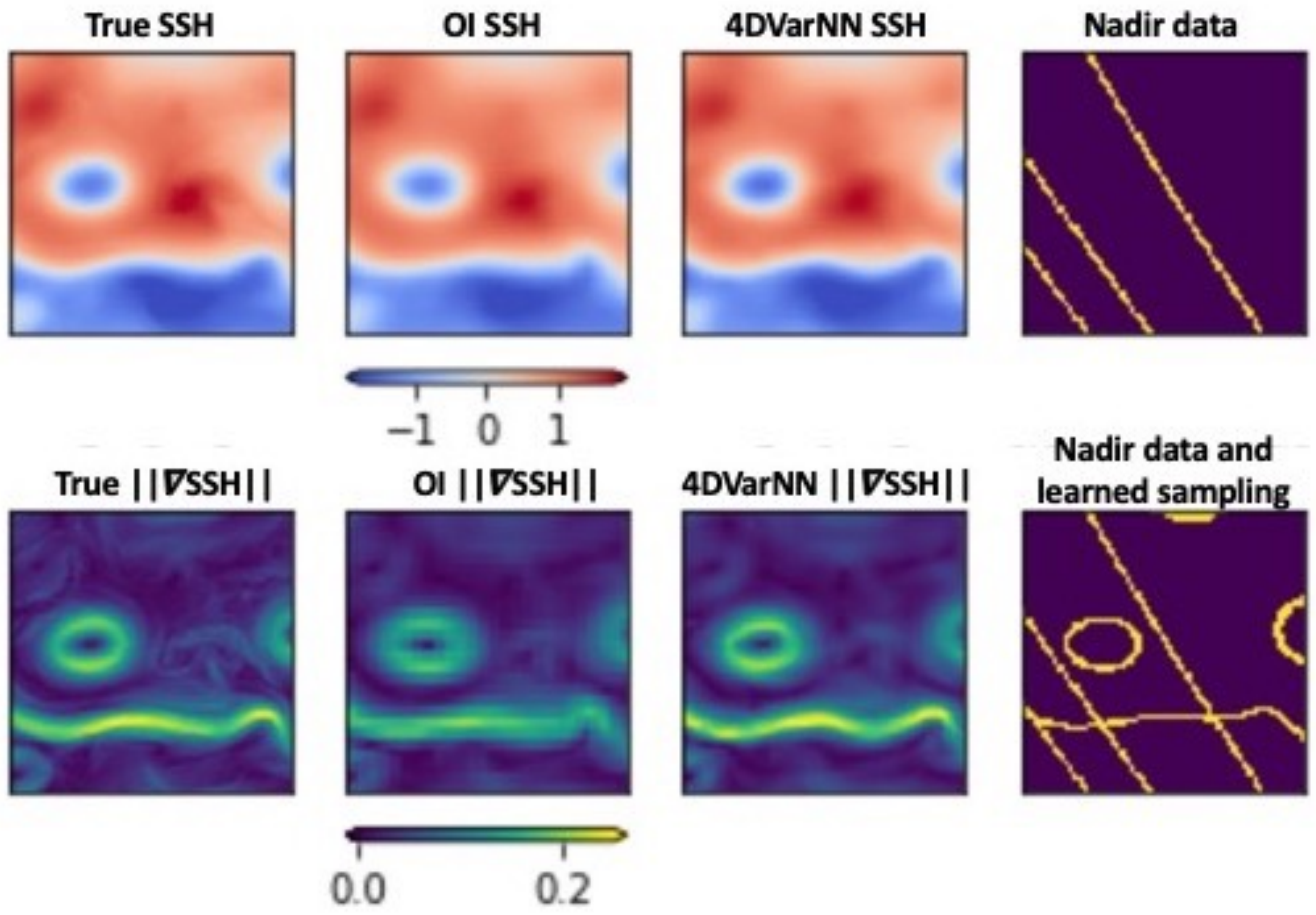
Optimal sampling

OSSE with NATL60 data

4-nadir-altimeter + DUACS baseline

Gulf Stream area (10°x10°)

Mean relative gain of 60% in the reconstruction of the SSH using the learned sampling (~6% of the pixels vs. 1.3% for nadir altimeters)



4DVarNN #2: Preliminary results

Multimodal DA

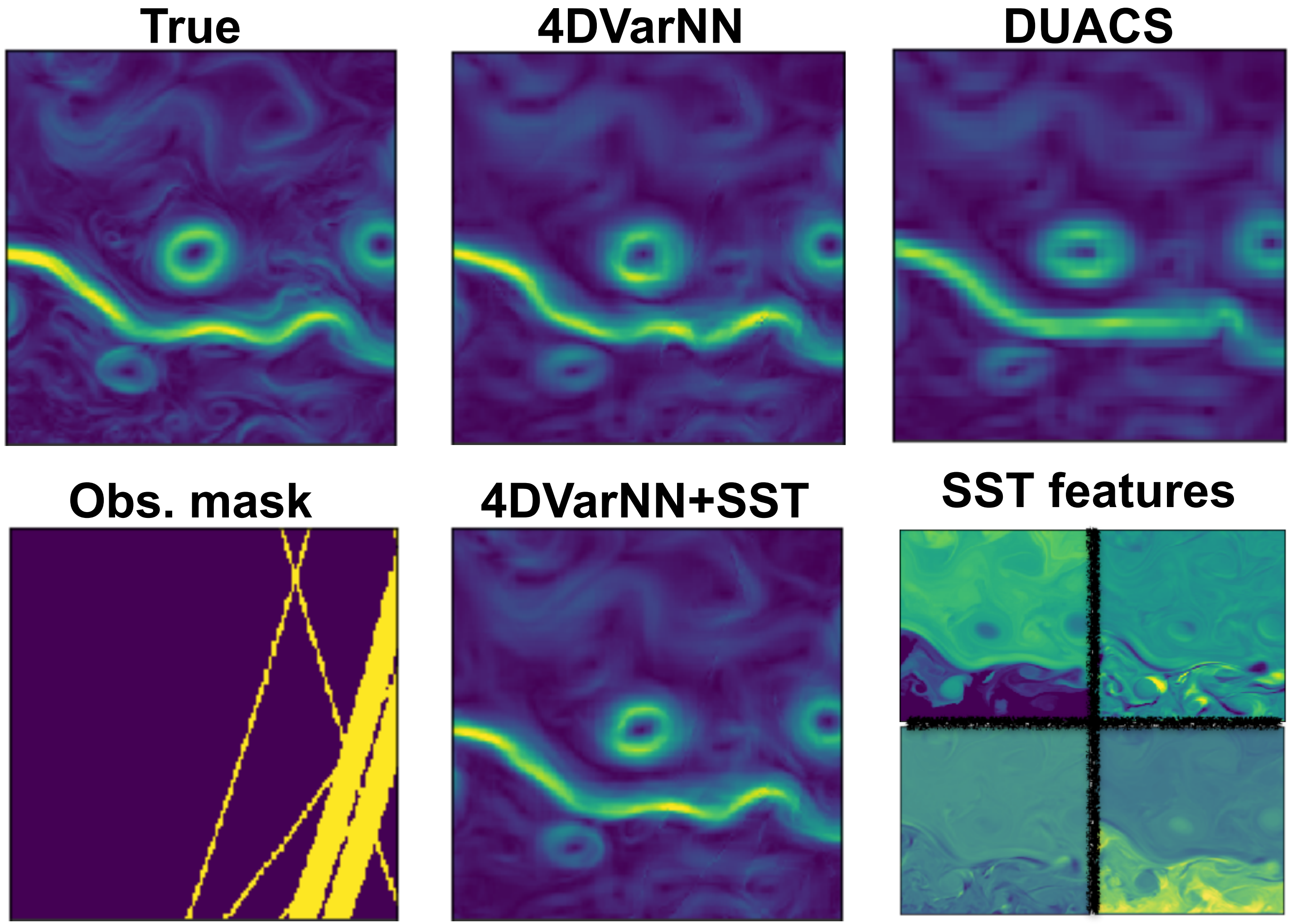
OSSE with NATL60 data

4-nadir-altimeter + SWOT + DUACS baseline

Gulf Stream area (10°x10°)

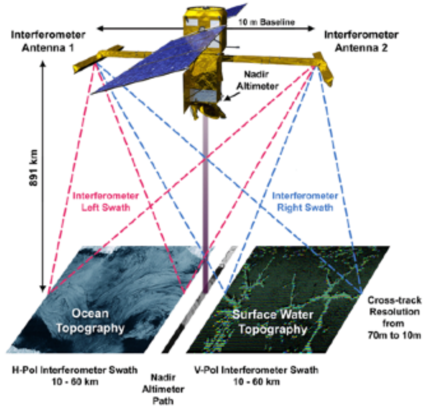
63% vs. 53% gain in SSH MSE w.r.t. DUACS with/ without SST (Winter period)

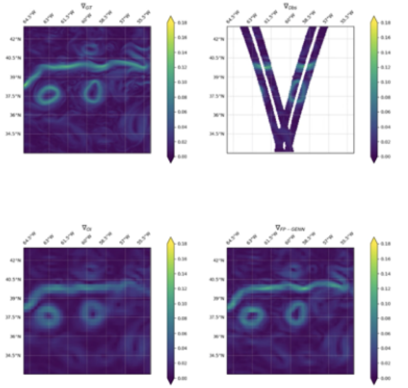
50% vs. 13% gain in SSH MSE w.r.t. DUACS using nadir altimeter data only

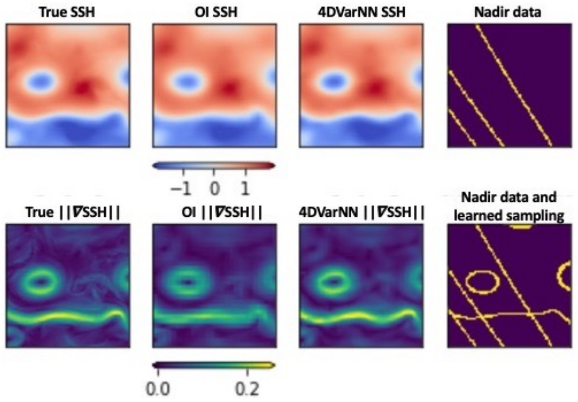


4DVarNN #2: Key messages

- **Learning jointly variational priors, observation models and solvers**
- **Optimal sampling as a learning issue under sparsity constraint**
- **Multimodal DA as a learning issue with a trainable feature extraction operator**
- **Generic framework beyond the considered testbed on SSH mapping**







Preprint: https://arxiv.org/abs/2006.03653
Code: https://github.com/CIA-Oceanix/DinAE_4DVarNN_torch

Synthesis: current status for 4DVarNN framework

Trainable Variational DA formulation

$$\|H * y - G * x\|_{\Omega}^{2} + \lambda \|x - \Phi(x)\|^{2}$$

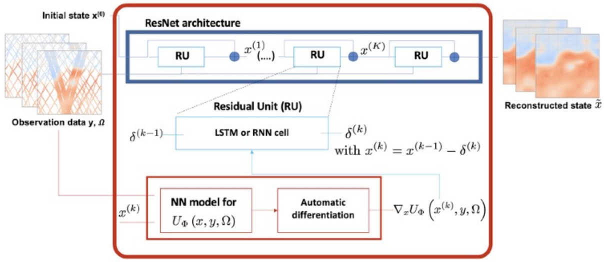
(Trainable) obs. model

Identity model
Sampling operator
Linear operator

Trainable prior

ODE-based
U-Net

Trainable solver



Fixed-point
gradient-based LSTM

Learning scheme

Variational cost (non-supervised)
Reconstruction error (supervised)

Synthesis: ongoing/future developments

New applications / case-studies

Uncertainty/stochasticity in 4DVarNN

Dealing with extremes (PhD N. Lafon)

Application to (unobserved) states (eg, vertical velocities)

Conditional forecasting

Trainable Variational DA formulation

$$\|H(z,y) - G * x\|_{\Omega}^{\alpha} + \lambda \|x - \Phi(x)\|^{\beta}$$

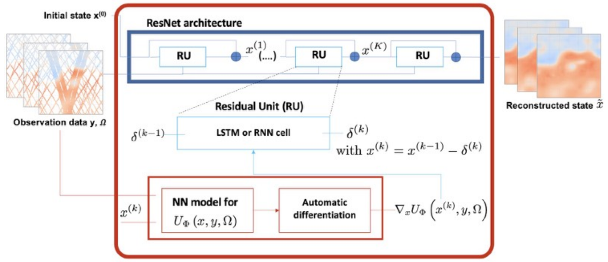
(Trainable) obs. model

Non-linear model without identity term ?

Trainable prior

Stochastic priors ?
"Functional" priors ?

Trainable solver



Multigrid/multiscale solver ?
Stochastic/Ensemble solver ?

Learning scheme

Beyond MSE losses ?
Adversarial learning ?

Synthesis: SSH mapping case-study

Current status

Benchmarking of 4DVarNN frameworks vs. AnDA/DinEOF on a Gulf Stream region

Promising results of 4DVarNN models vs. OI

New version of benchmarking experiments (To be validated/Melody WP4) (cf. Quentin's slides)

Data challenge framework available on git (cf. Quentin's slides)

Planned/targeted developments

Proposal for a SSH mapping data challenge for SWOT ST DA working group

Scaling up to the ocean basin scale

From OSSEs to real observations: which (transfer) learning strategies ?

Embedding uncertainties (cf. Said's talk)

Some references

Generic 4DVarNN framework

Arxiv preprint on 4DVarNN with applications on L63/L96: https://arxiv.org/abs/2007.12941

Short version in Proc. ICASSP'2021, https://hal-imt-atlantique.archives-ouvertes.fr/hal-03139133

Applications/case-studies

Benchmarking experiments for SSH mapping (fixed-point solver), Rem. Sens., https://www.mdpi.com/2072-4292/12/22/3806

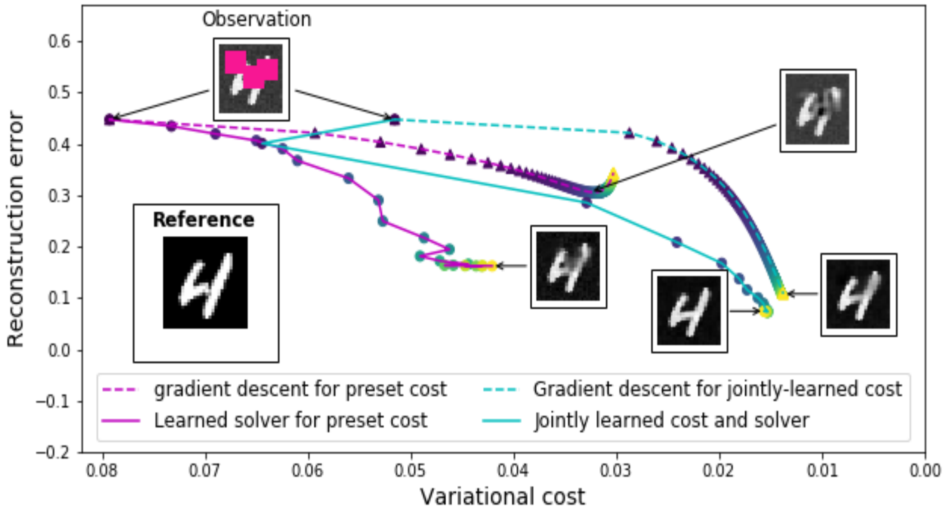
ISPRS'2021 paper (first illustration of forecasting/optimal sampling for SSH mapping): https://www.researchgate.net/publication/350592046_END-TO-END_PHYSICS-INFORMED_REPRESENTATION_LEARNING_FOR_SATELLITE_OCEAN_REMOTE_SENSING_DATA_APPLICATIONS_TO_SATELLITE_ALTIMETRY_AND_SEA_SURFACE_CURRENTS

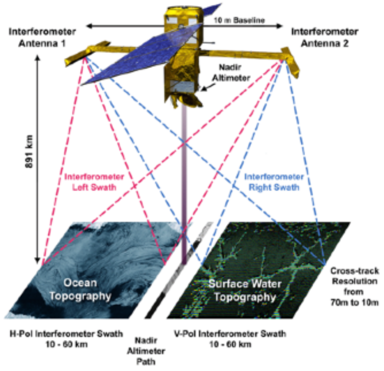
Application of satellite-derived sea surface turbidity, https://www.researchgate.net/publication/350739763_DATA-DRIVEN_SPATIO-TEMPORAL_INTERPOLATION_OF_SEA_SURFACE_SEDIMENT_CONCENTRATION_FROM_SATELLITE-DERIVED_DATA_AN_OSSE_CASE-STUDY_IN_THE_BAY_OF_BISCAY

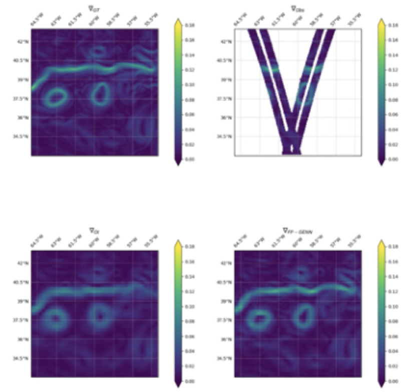
4DVarNN #1: end-to-end-learning of 4DVar models

Key messages

- We can bridge DNN and variational models to solve inverse problems
- **Learning both variational priors and solvers**
- **Learning “optimal” parameterisations w.r.t. a predefined performance metrics (e.g., reconstruction score)**







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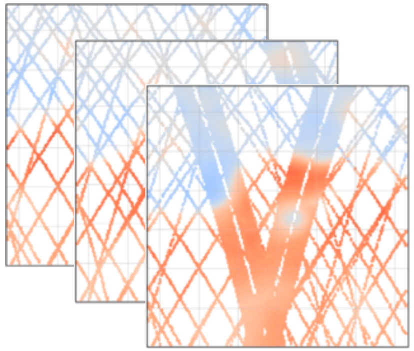
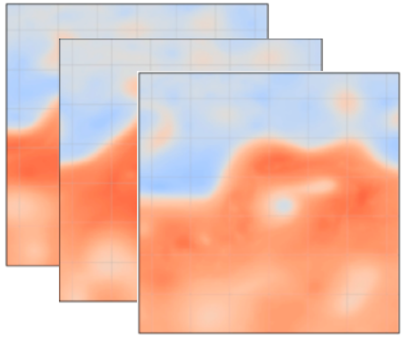
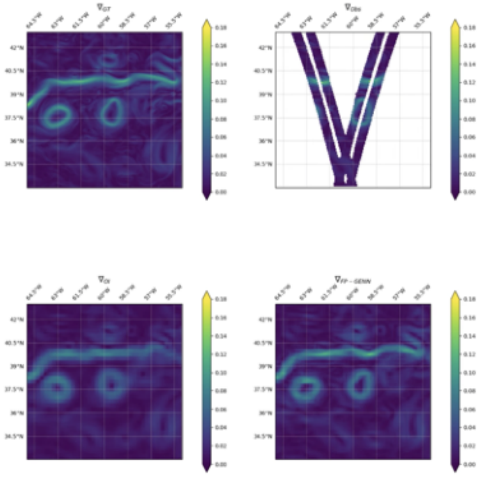
4DVarNN: Application to satellite-derived SSH mapping



Partial observations y



True states x



OSSE:

- NATL60 data
- Noise-free SWOT+4-nadir/4-nadir observation dataset
- Gap-free/noise-free SST
- Test period on 20 days (remaining data used for training)

Results

Models	4DVarNN-L2-LSTM	4DVarNN-L2-LSTM+SST
relative MSE gain vs. OI for SSH	53 %	64 %
Relative MSE gain vs. OI for gSSH	45 %	58 %

SWOT+4-nadir

Models	4DVarNN-L1-LSTM	4DVarNN-L2-LSTM+SST
relative MSE gain vs. OI for SSH	12 %	52 %
Relative MSE gain vs. OI for gSSH	18 %	52 %

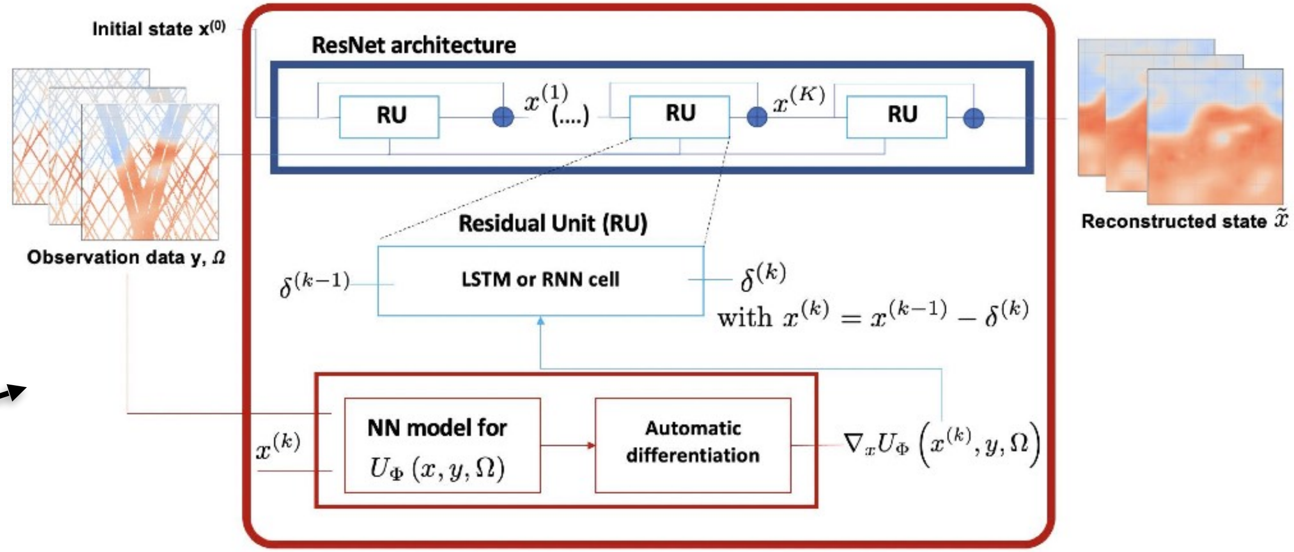
4-nadir

4DVarNN: end-to-end-learning of 4DVar models

From a Variational DA formulation

$$\widehat{x} = \arg\min_{x} \|x - y\|^2_{\Omega} + \lambda \|x - \Phi(x)\|^2$$

To a End-to-end architecture



Trainable prior operator

Trainable gradient-based solver using AD