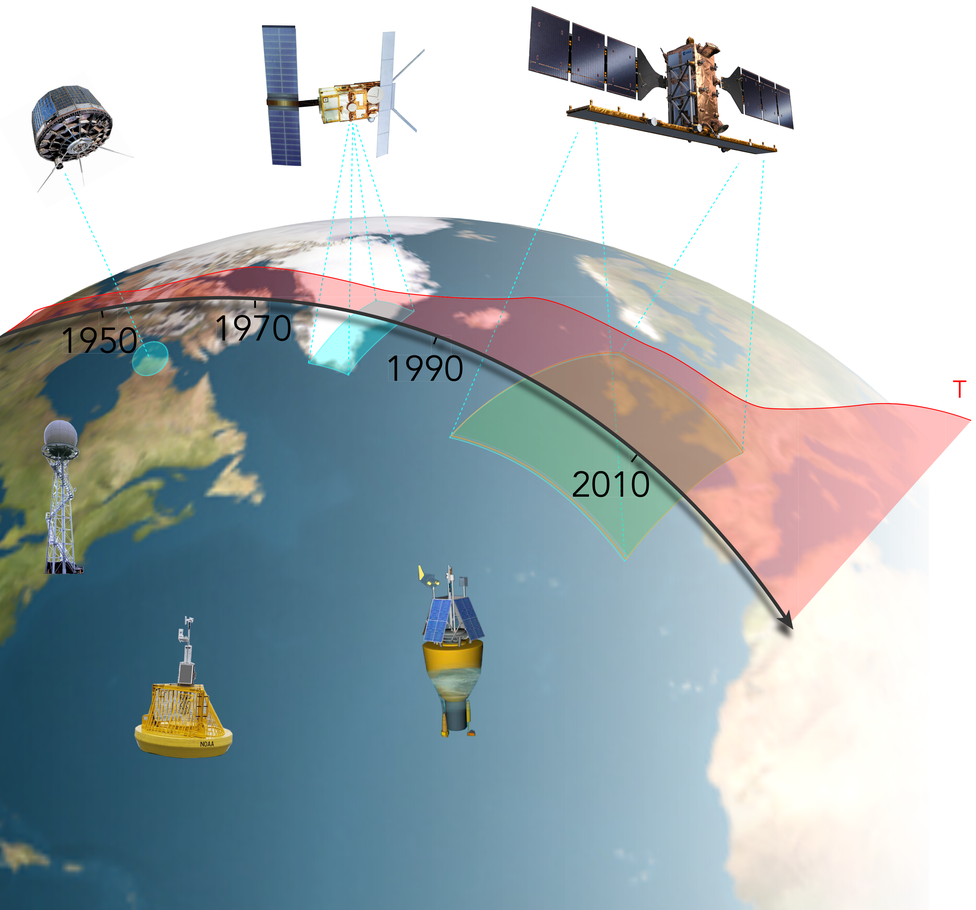
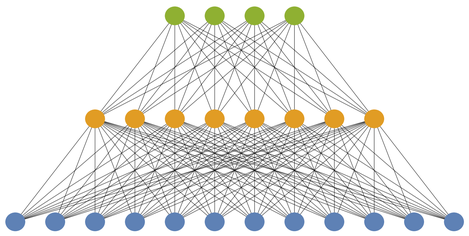


AtmoRep

Large scale representation learning of atmospheric dynamics

Christian Lessig, Ilaria Luise, Martin Schultz, et al.



applications

large scale representation learning

scientific insight

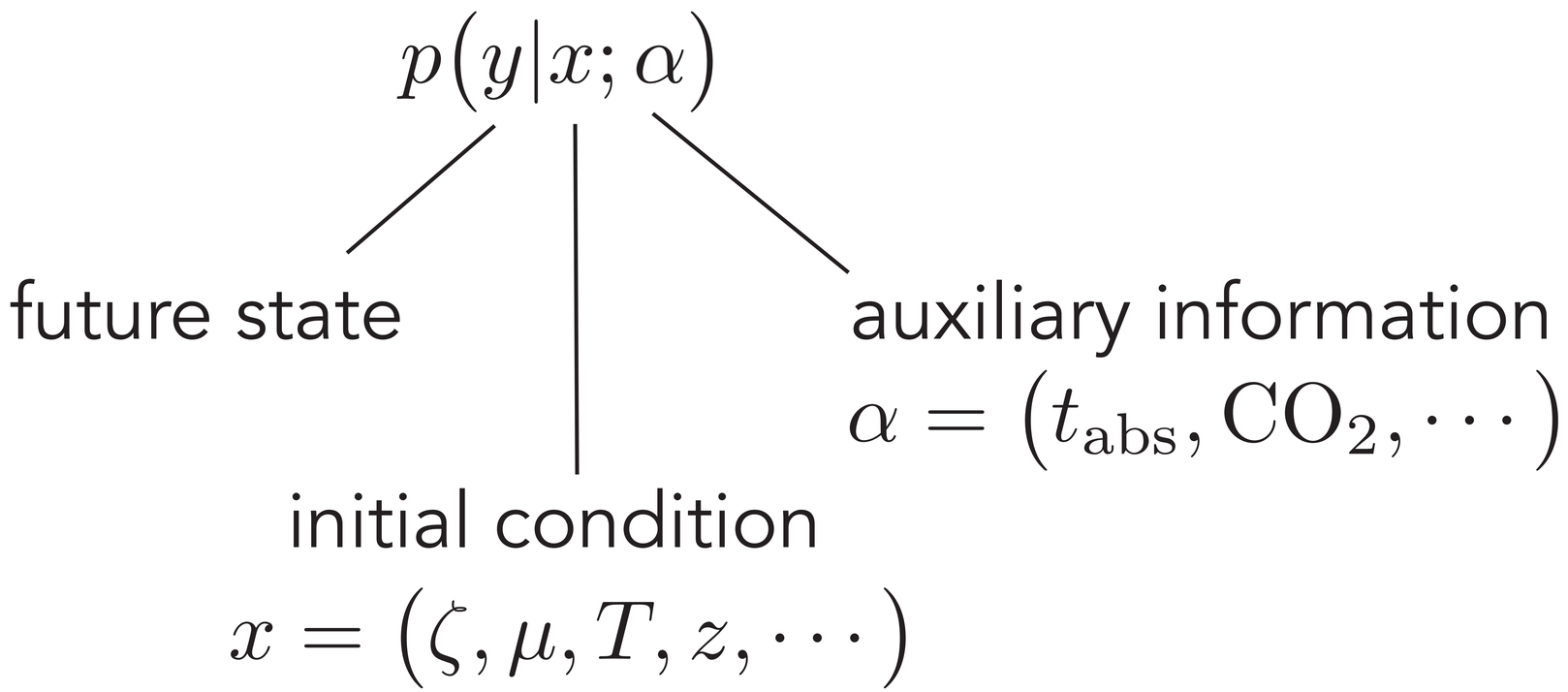
Theoretical formulation

- Atmosphere as stochastic dynamical system:

$$p\big(y|x;\alpha\big)$$

Theoretical formulation

- Atmosphere as stochastic dynamical system:



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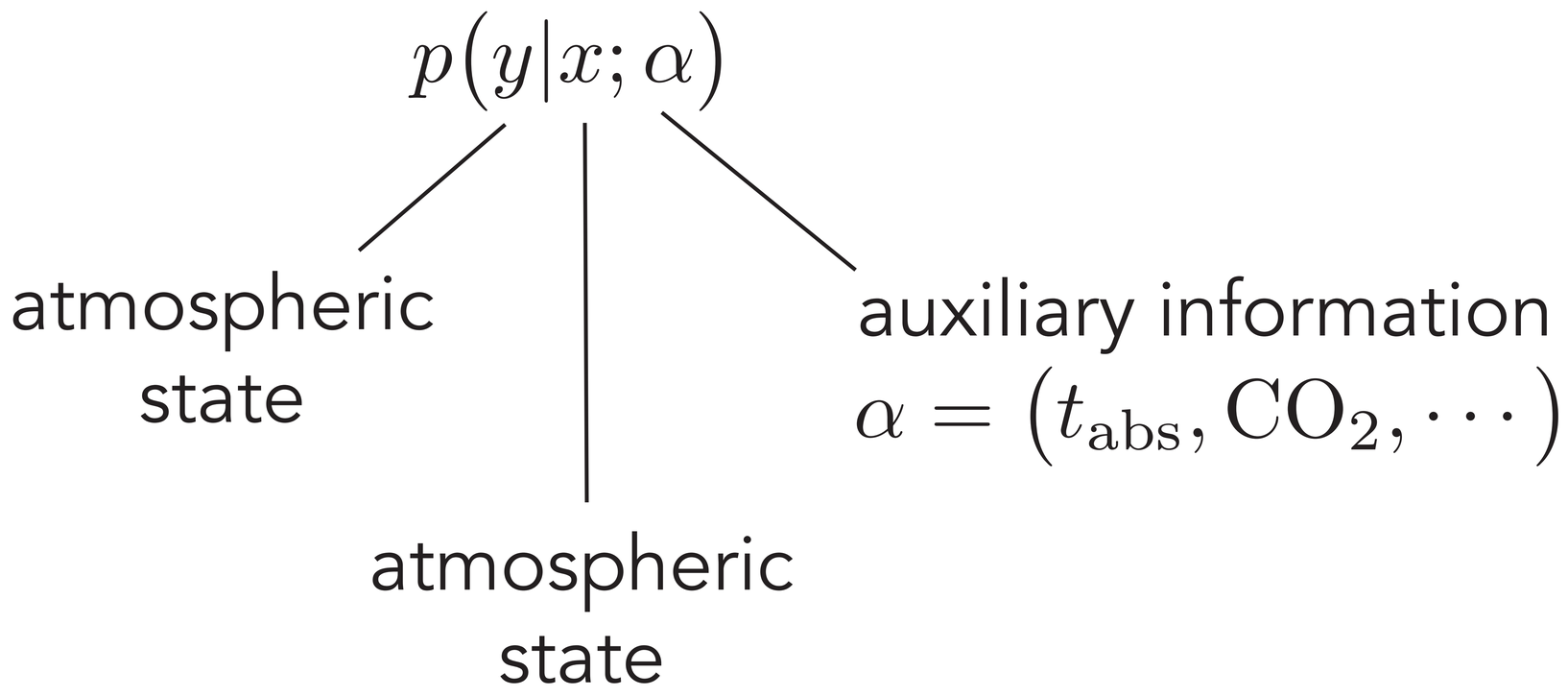

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  - Forecasting, downscaling, interpolation: $p\big(y|x;\alpha\big)$

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  - Climate: $p_\alpha(y) = \int p\big(y|x;\alpha\big)\, p(x)\, \mathrm{d}x$

Theoretical formulation

- Atmosphere as stochastic dynamical system:

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  - Medium/extended range forecasting:

$$p(x_T|x_0;\alpha) = \prod_{i=1}^{T} p_\theta(x_{i+1}|x_i;\alpha)$$

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highly complex, in-stationary distribution

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approx. future state approx. initial condition

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highly complex, instationary distribution

Theoretical formulation

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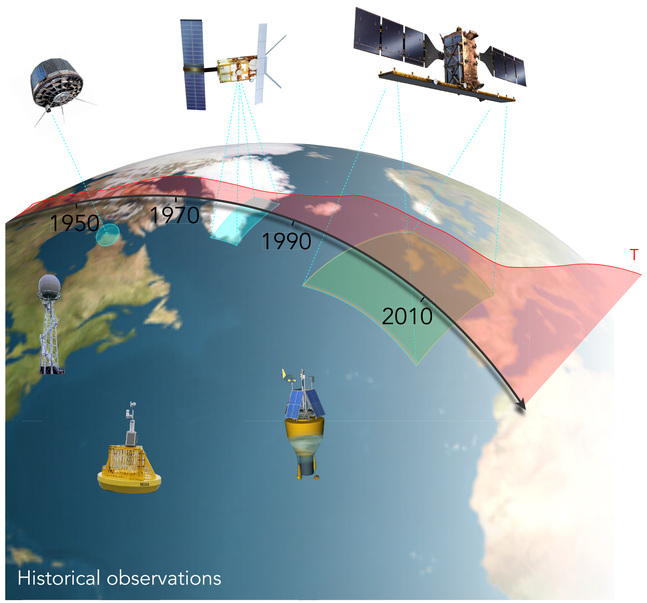
very large neural network

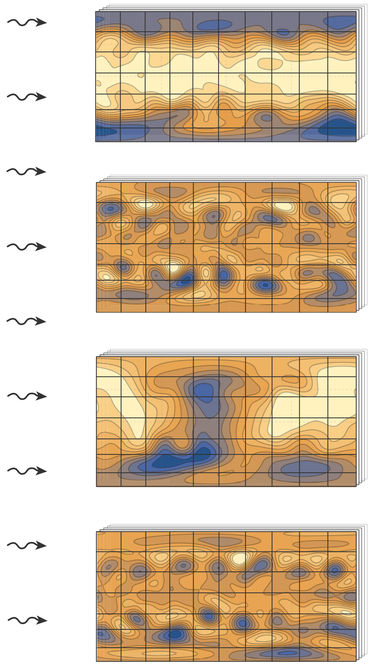
$$\tilde{p}_\theta\big(\tilde{y}|\tilde{x};\tilde{\alpha}\big) \approx p\big(y|x;\alpha\big)$$

highly complex, instationary distribution

AtmoRep



ERA5 reanalysis



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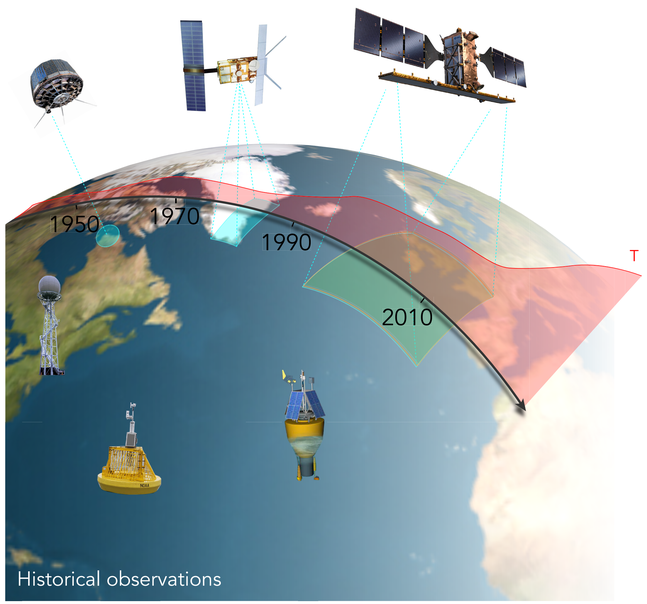

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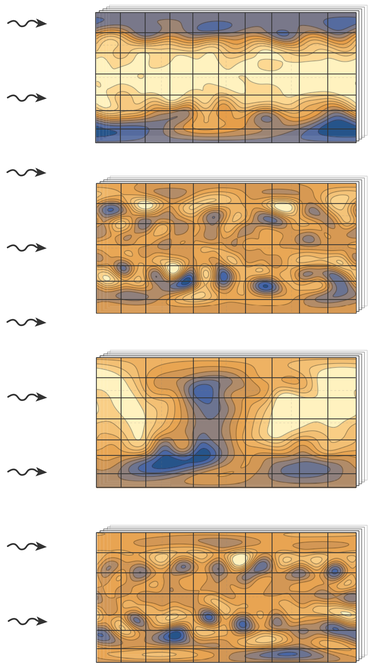
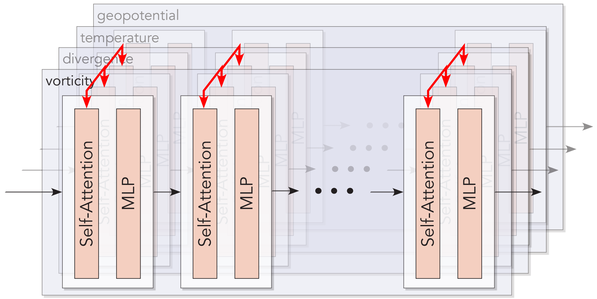


$$p_\theta(y|x)$$



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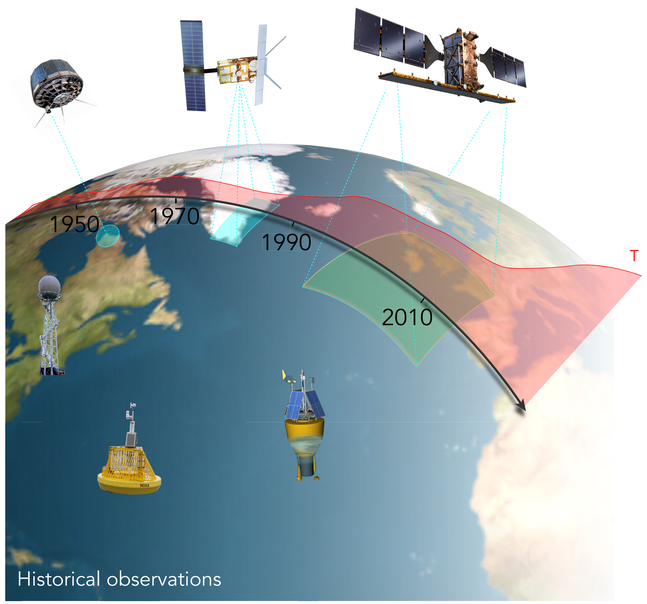
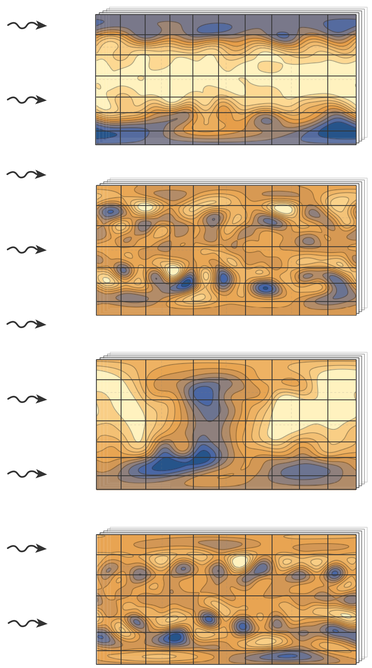
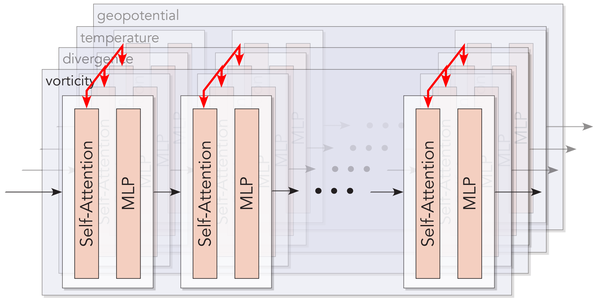


ERA5 reanalysis

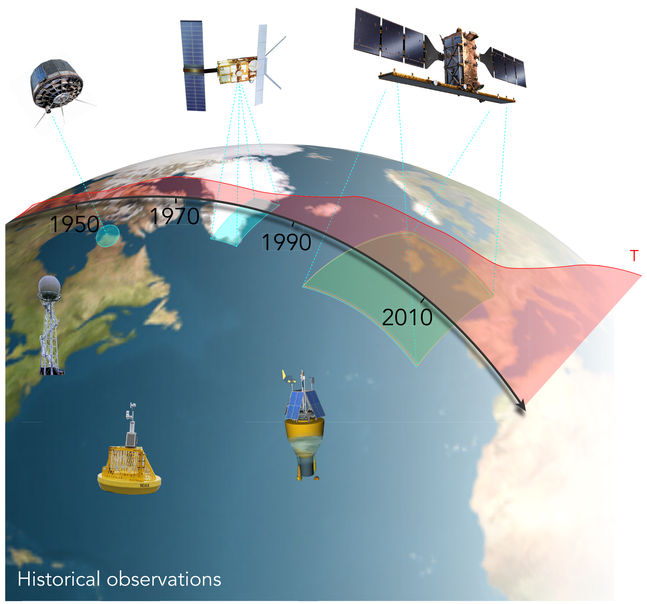


$$p_\theta(y|x)$$



large transformer
with 3.5 x 10^9 parameters

AtmoRep



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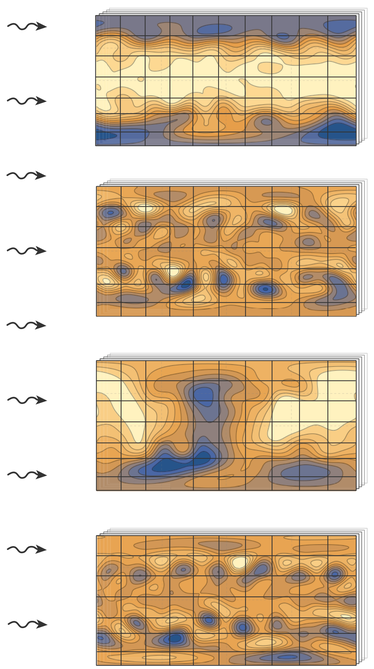

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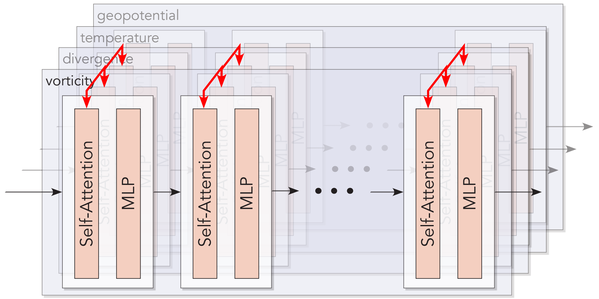

large transformer
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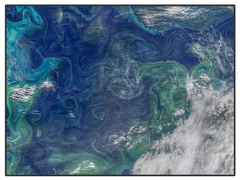
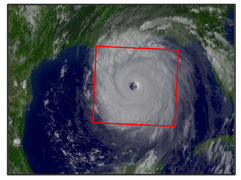
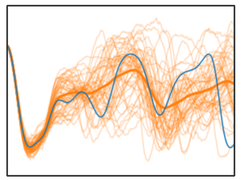
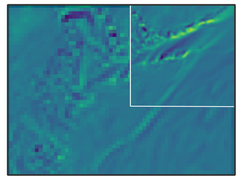
applications

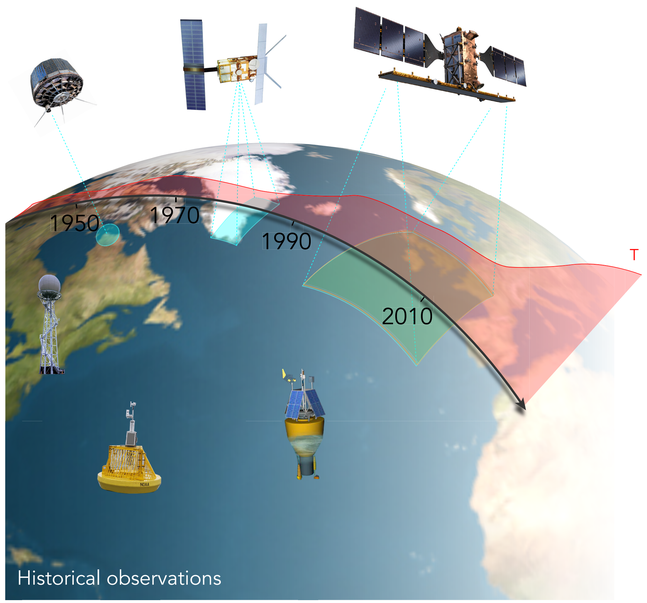

Forecasting


Impact analysis

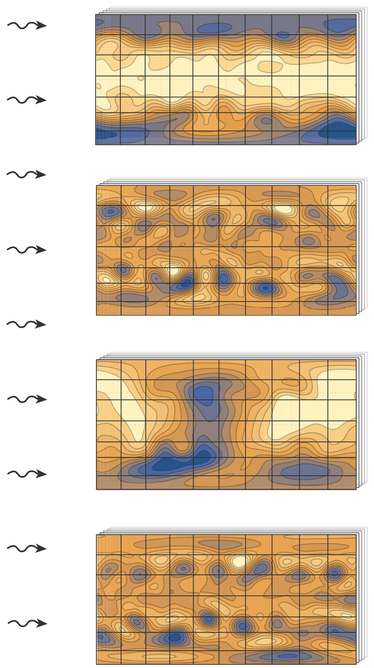

Statistical analysis


Downscaling

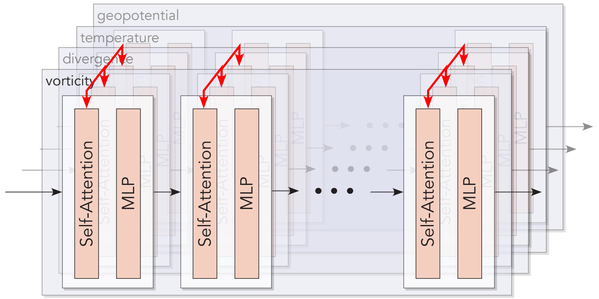
AtmoRep



ERA5 reanalysis



$p_\theta(y|x)$



large transformer
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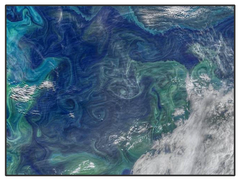
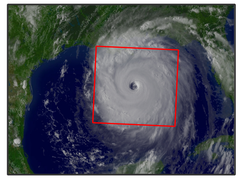
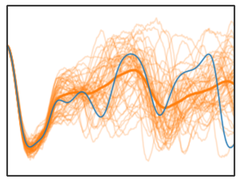
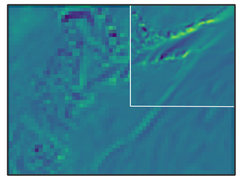
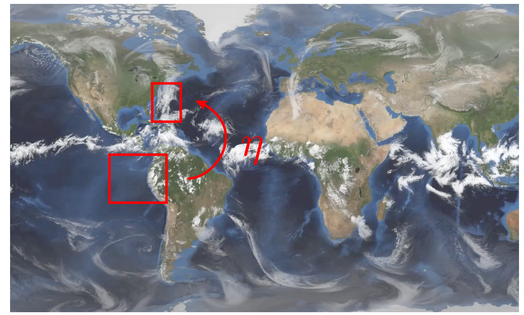

Forecasting


Impact analysis


Statistical analysis

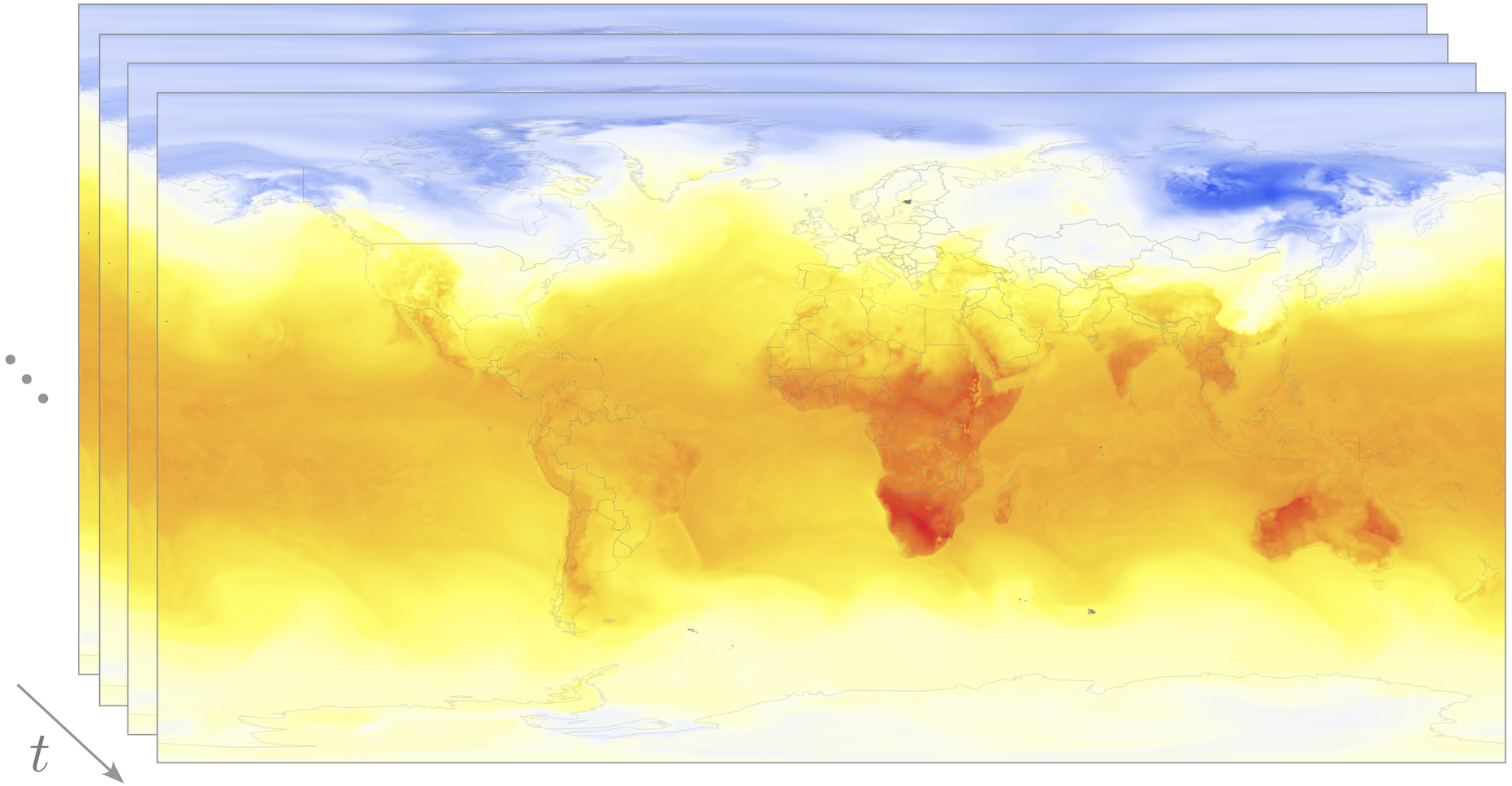

Downscaling



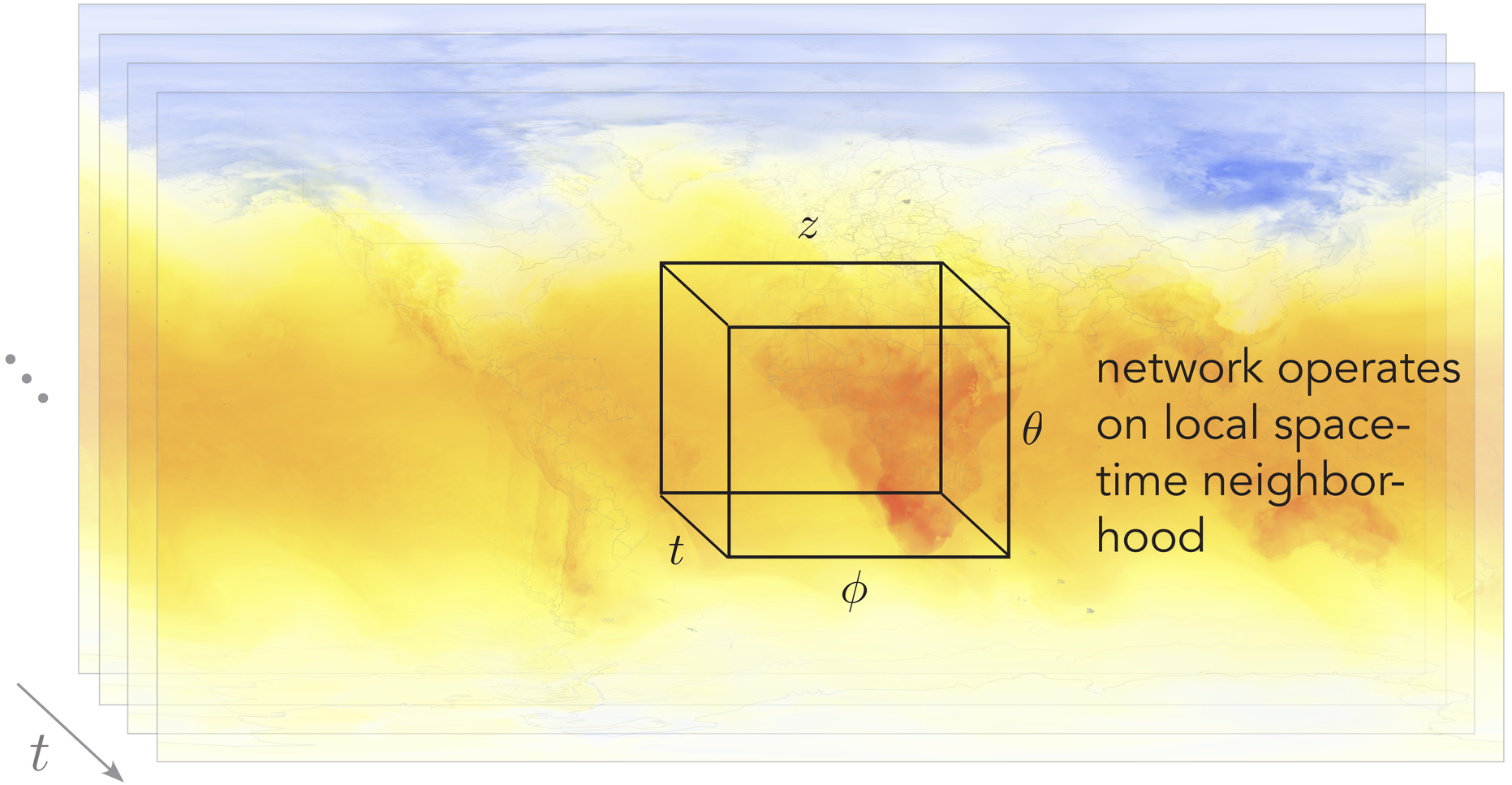
scientific insight

Network architecture

AtmoRep network architecture



AtmoRep network architecture



network operates on local space-time neighbor-hood

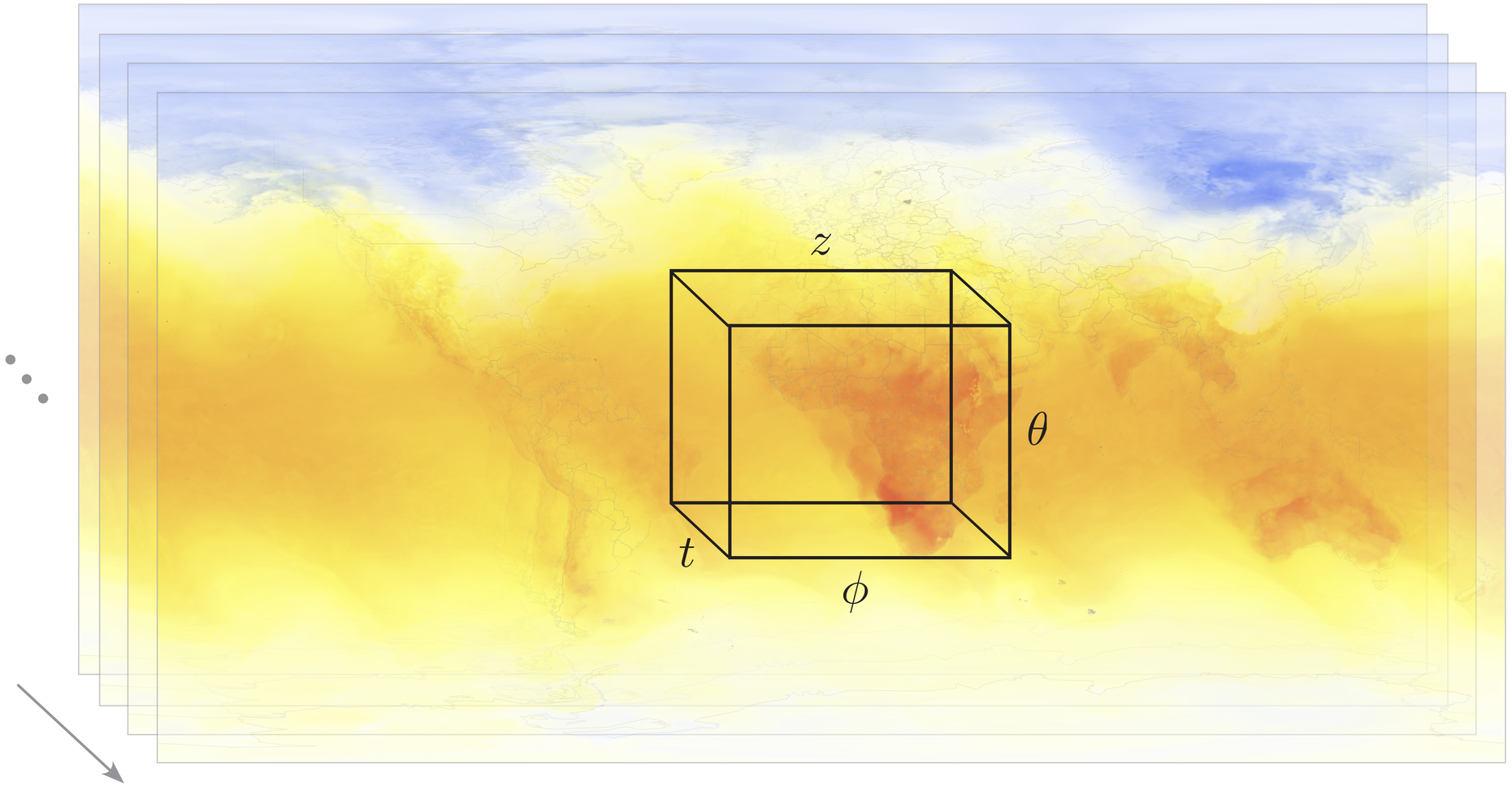
AtmoRep network architecture

- Network is local in space-time
  - Physics are universally valid
  - Machine learning model can be leaner and learn faster
  - Local particularities can be learned by providing time + space position as network input

AtmoRep network architecture

- Network is local in space-time
  - Physics are universally valid
  - Machine learning model can be leaner and learn faster
  - Local particularities can be learned by providing time + space position as network input
- Network is an extended transformer architecture

What is a token?



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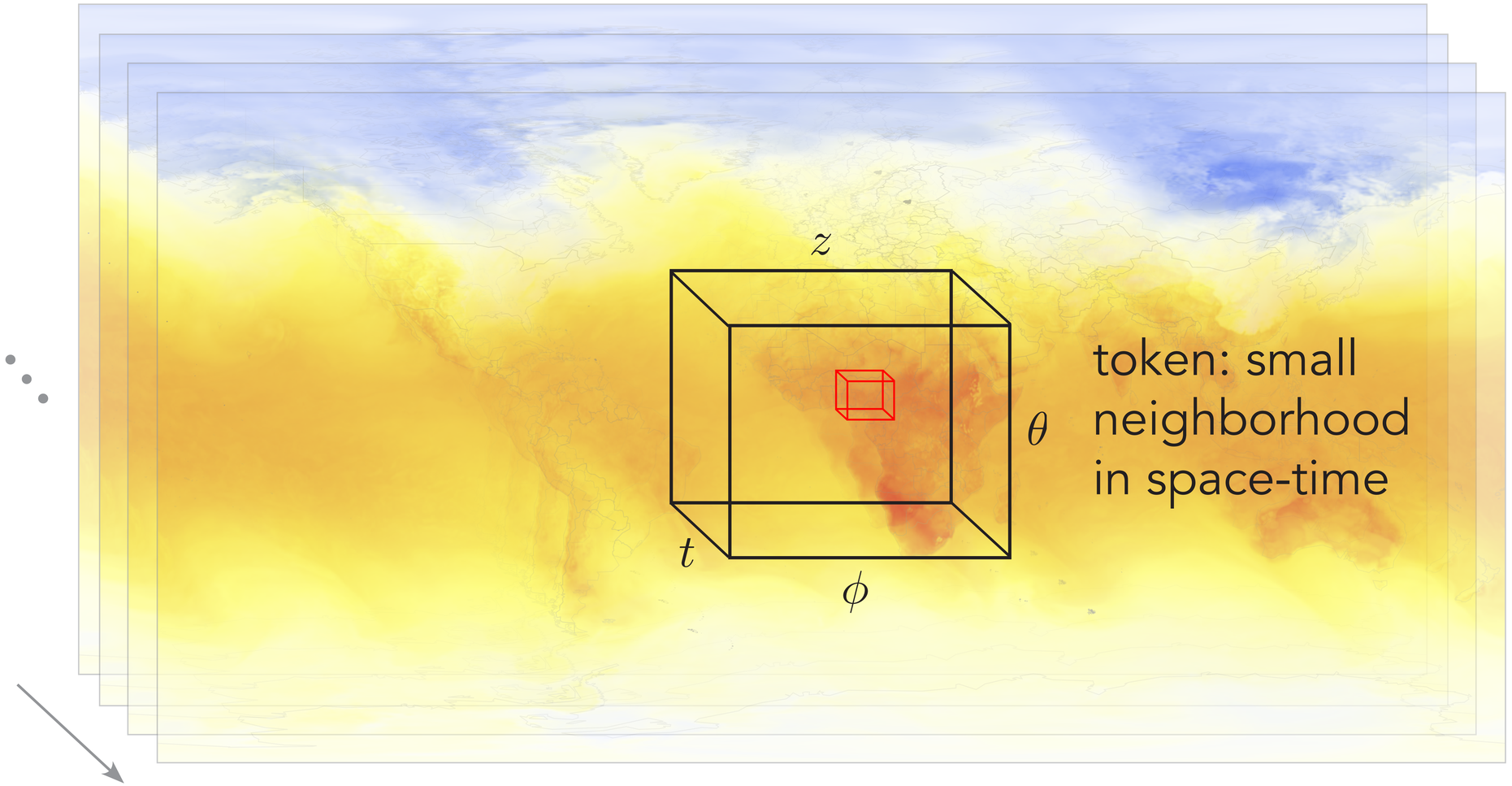

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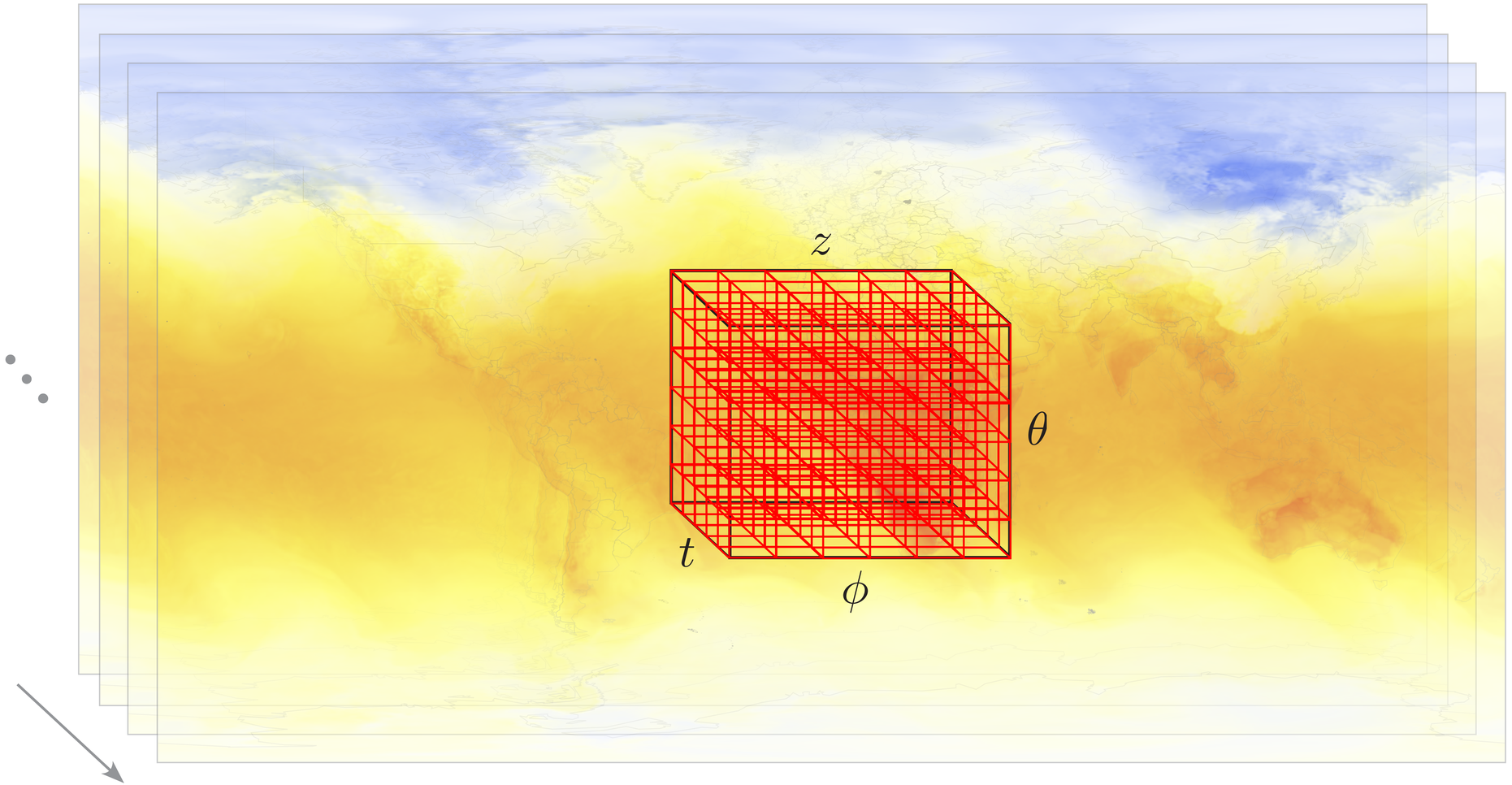
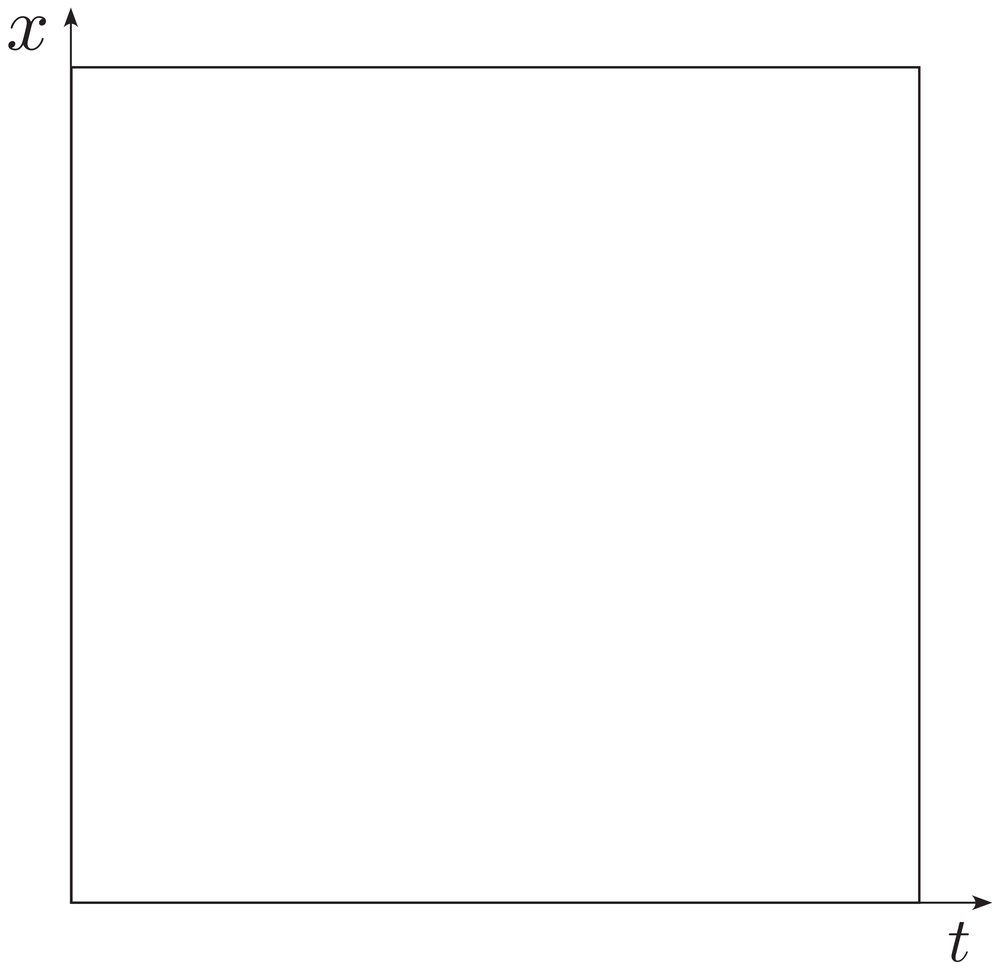


What is a token?

- Flatland view:



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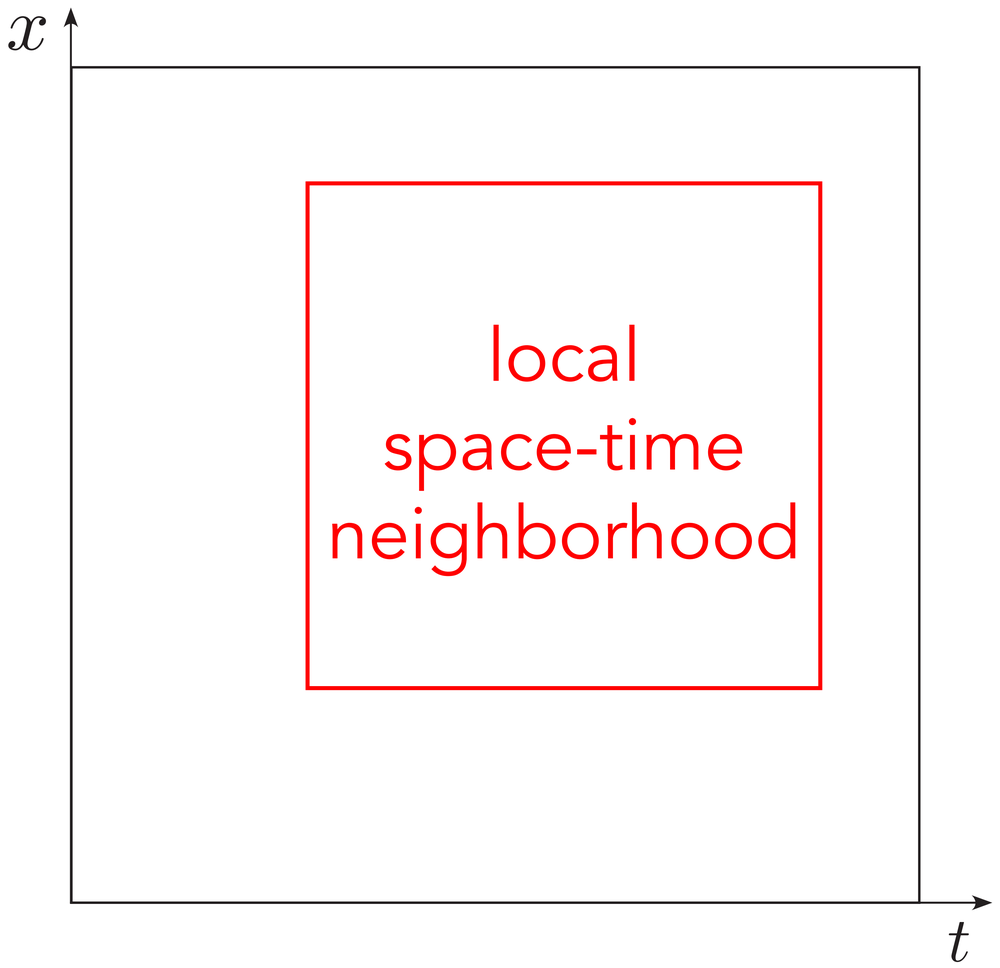

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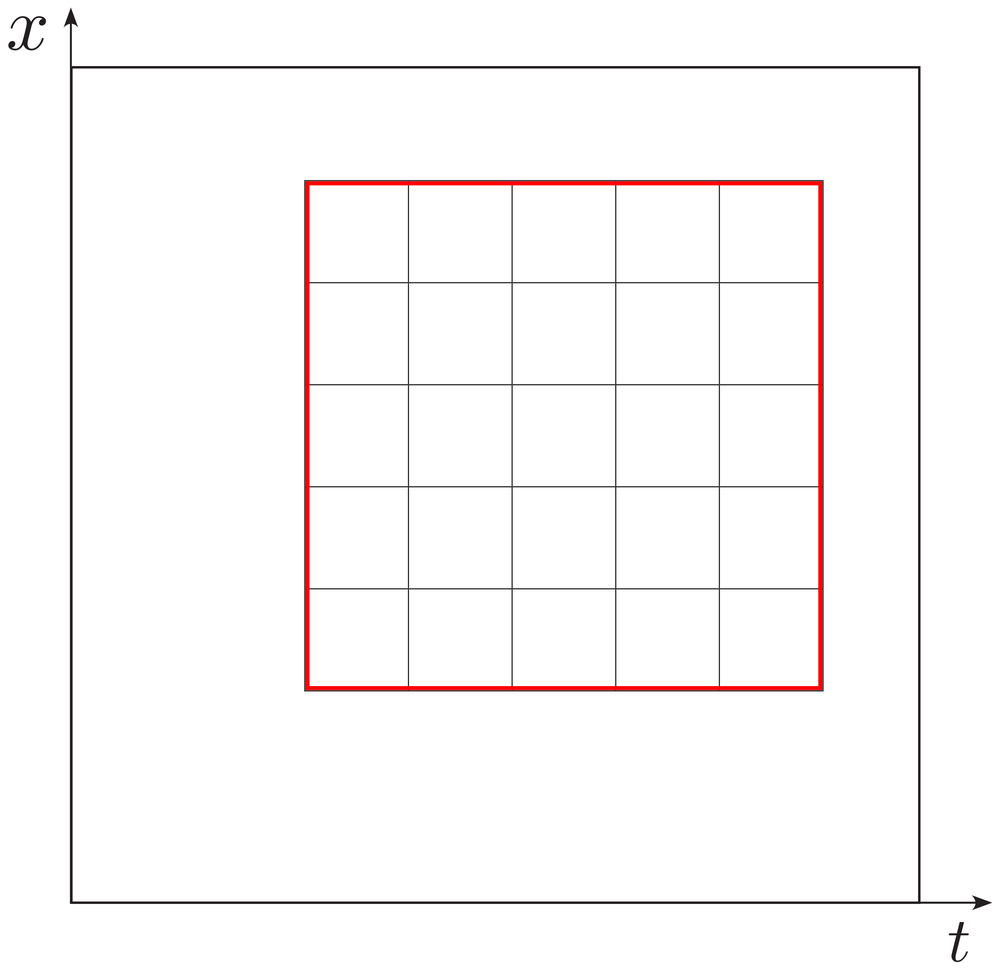
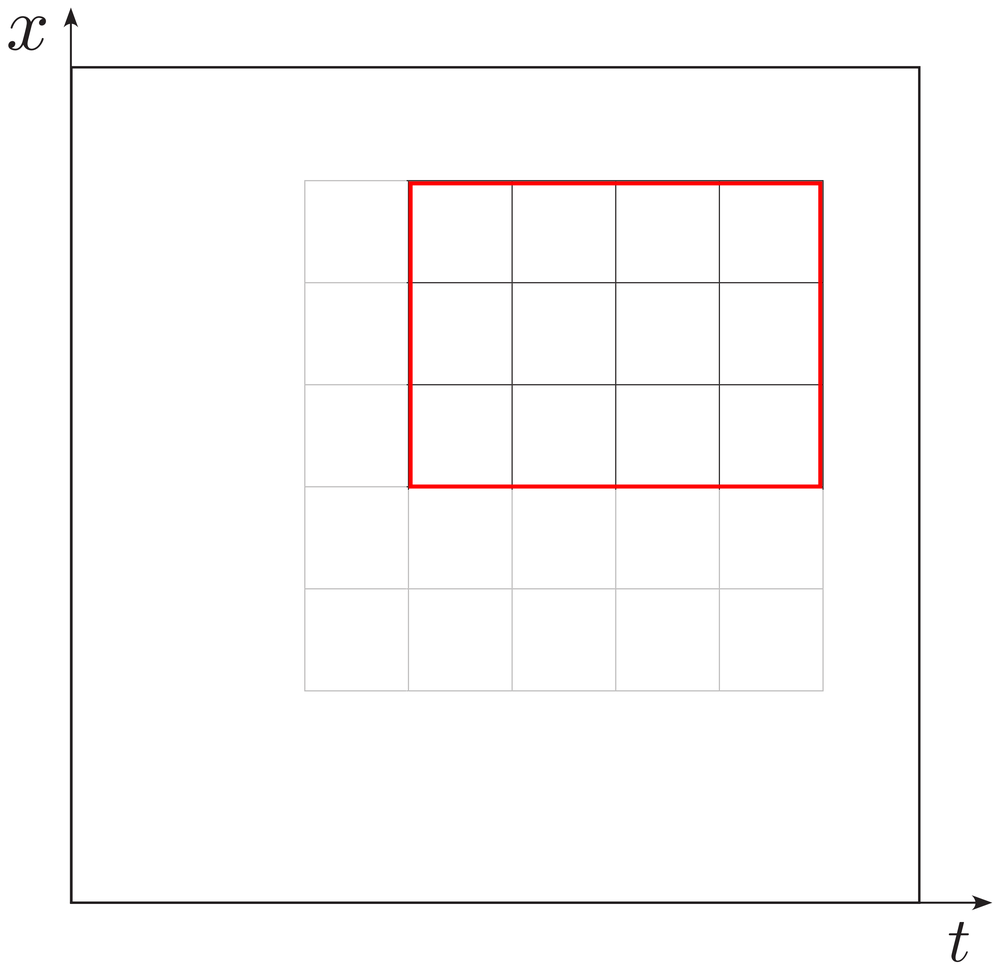


What is a token?

- Flatland view:

local window
size is flexible



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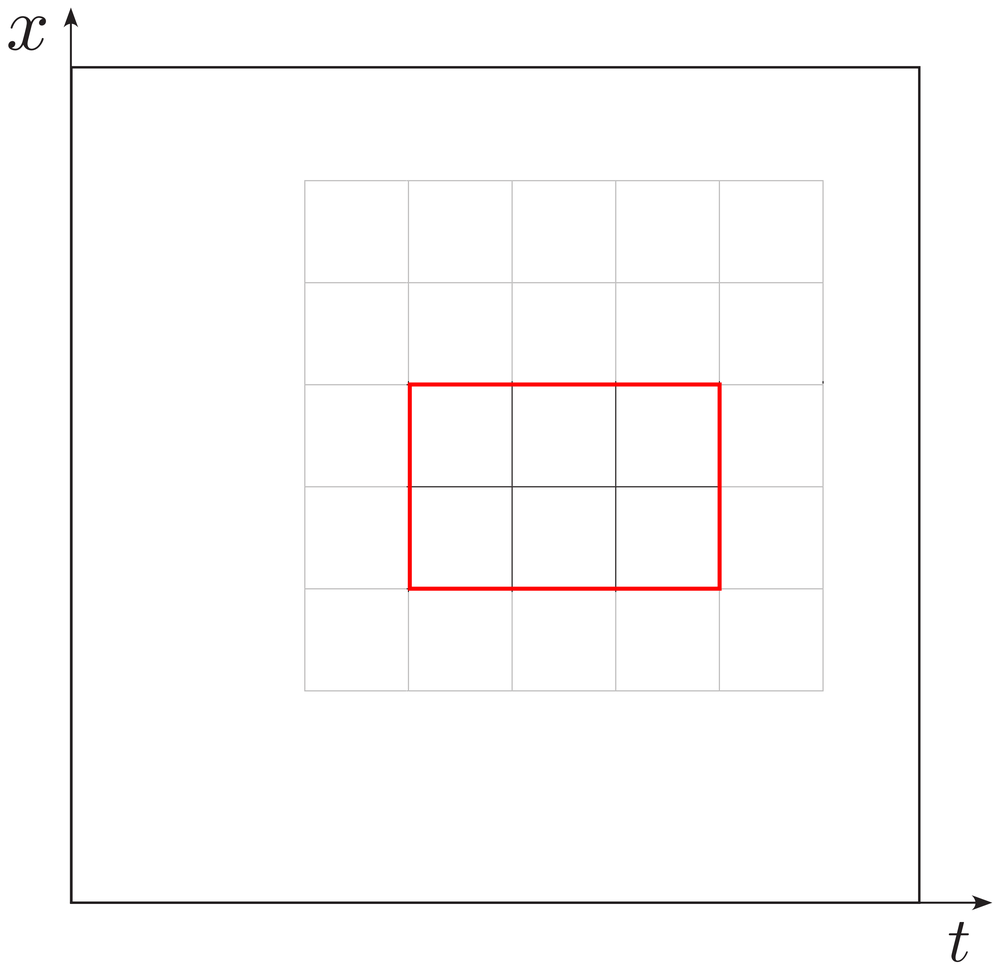
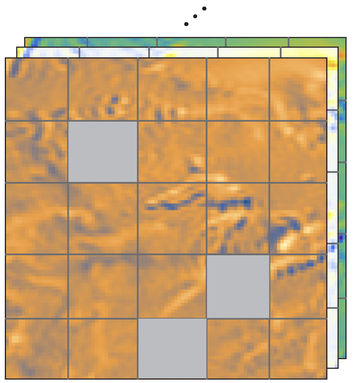
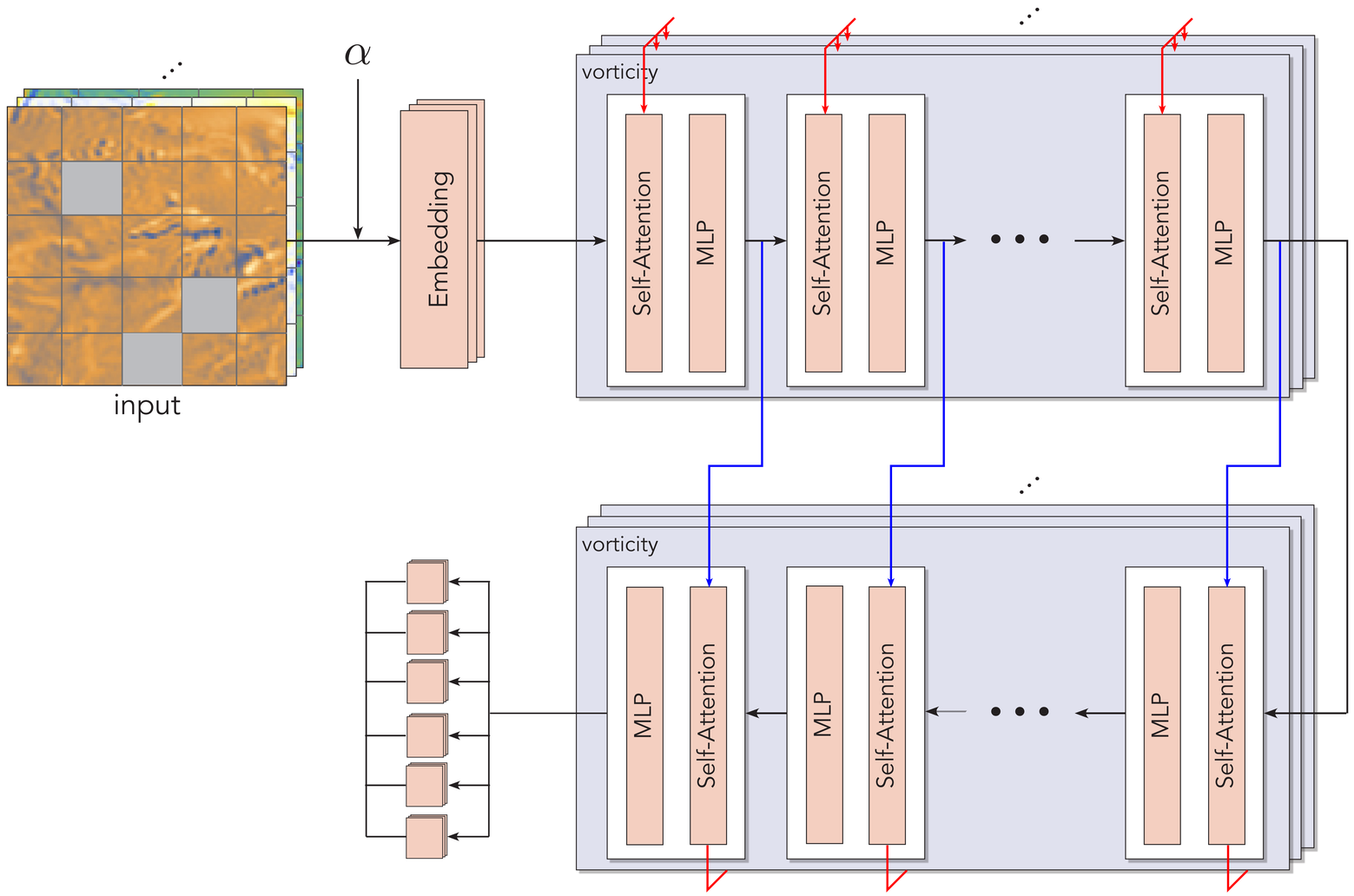


Multiformer



input

Multiformer



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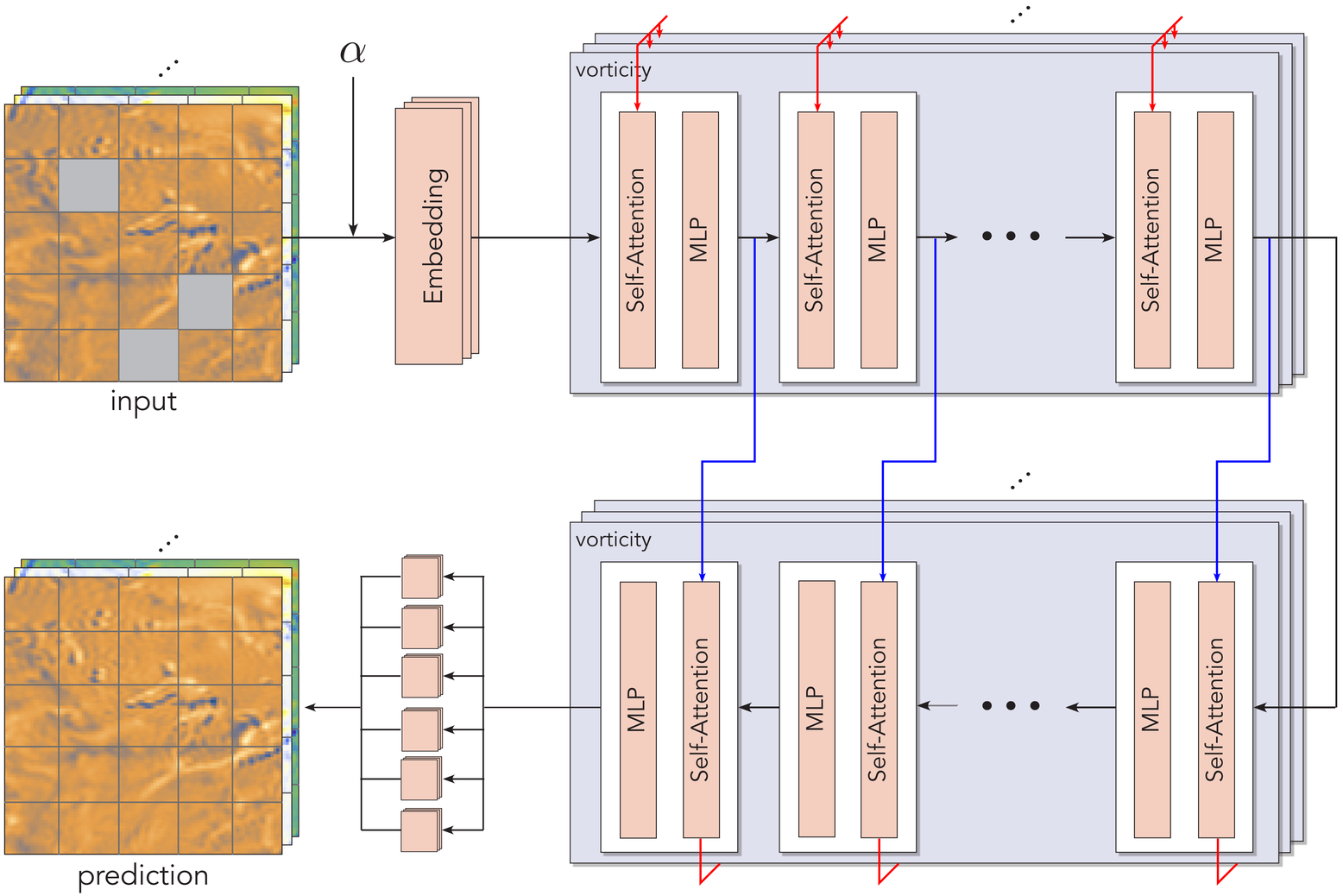

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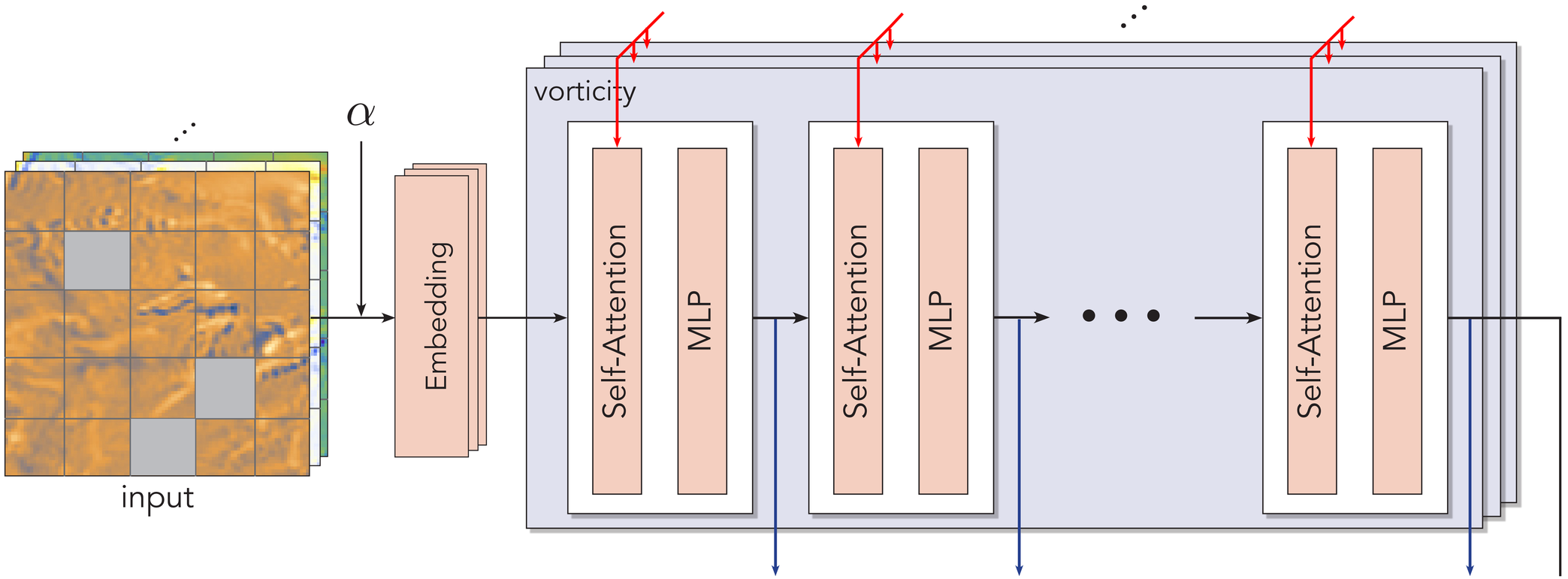

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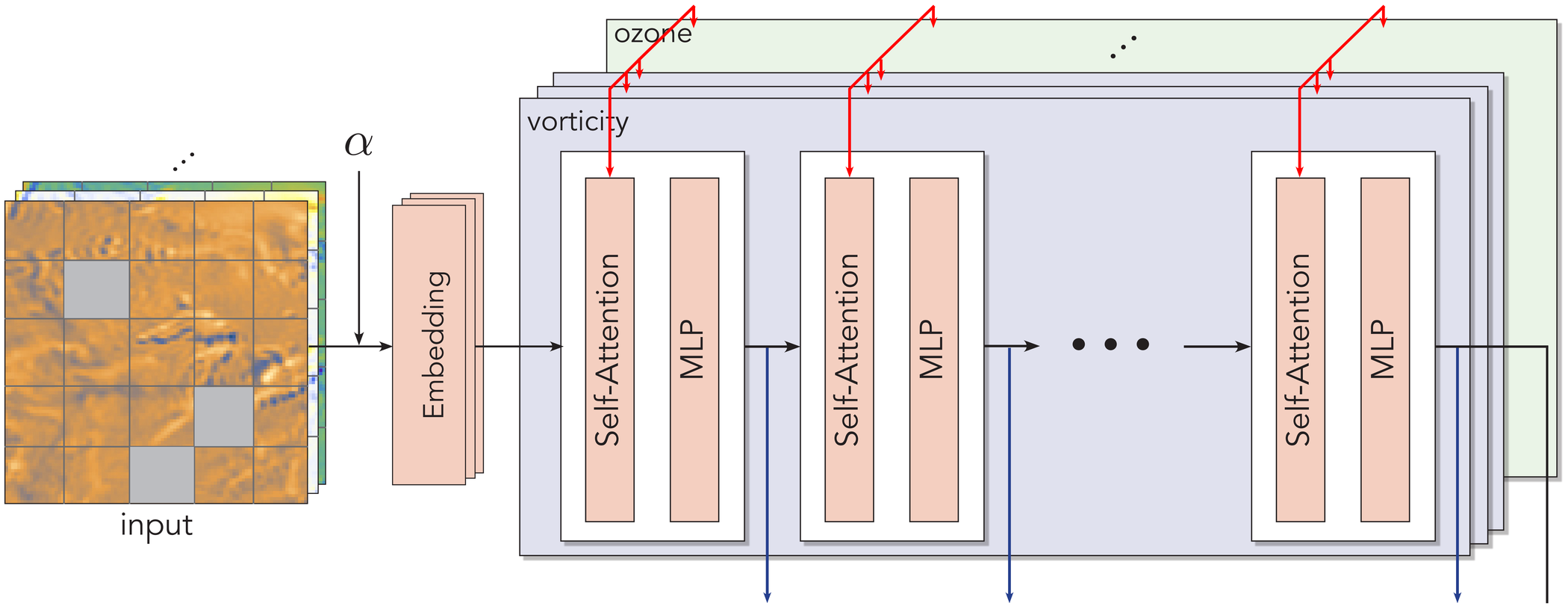

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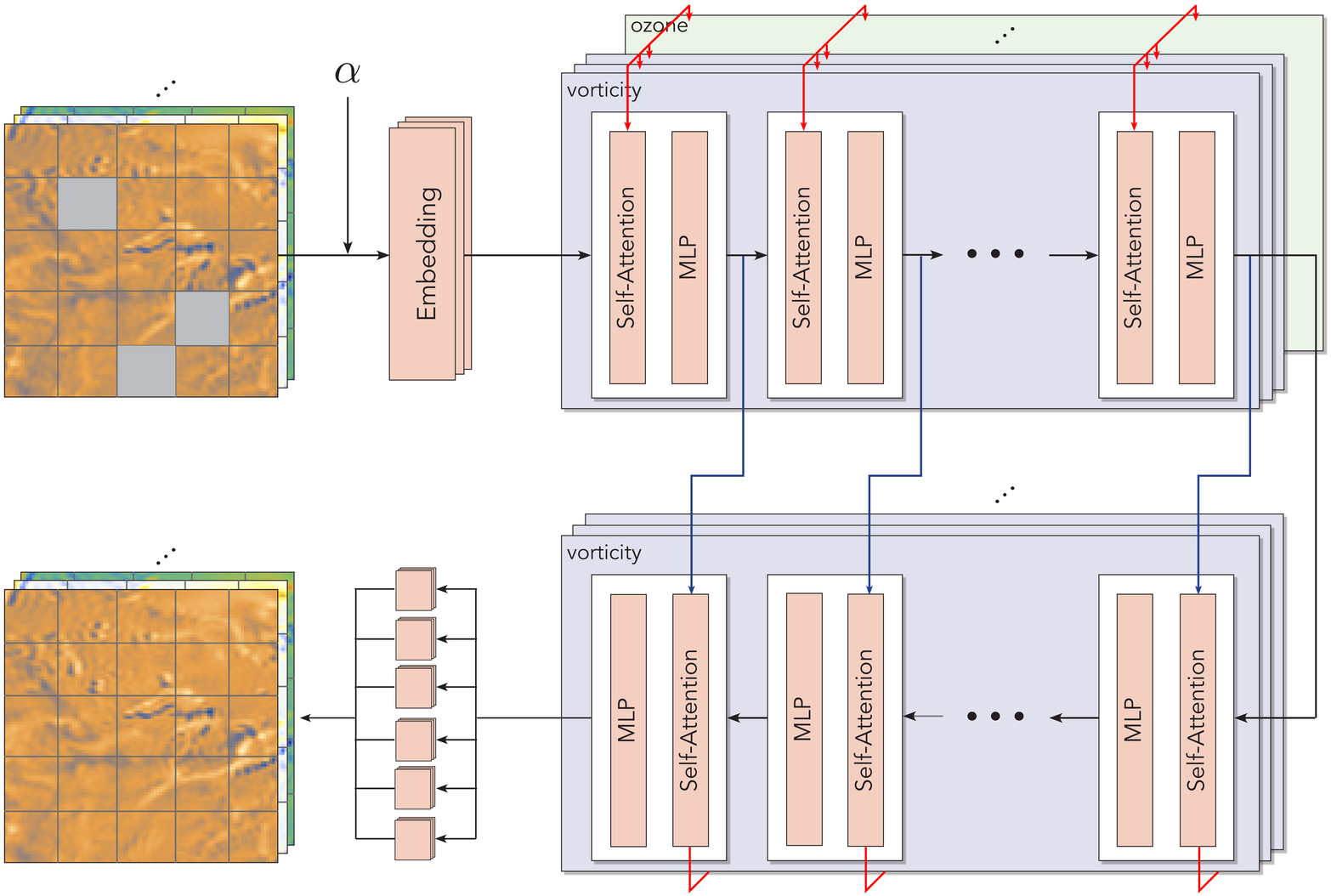


Loss and Pre-training

Training objective

- Numerical statistical atmospheric model

$$p_\theta\left(y|x,\alpha\right)$$

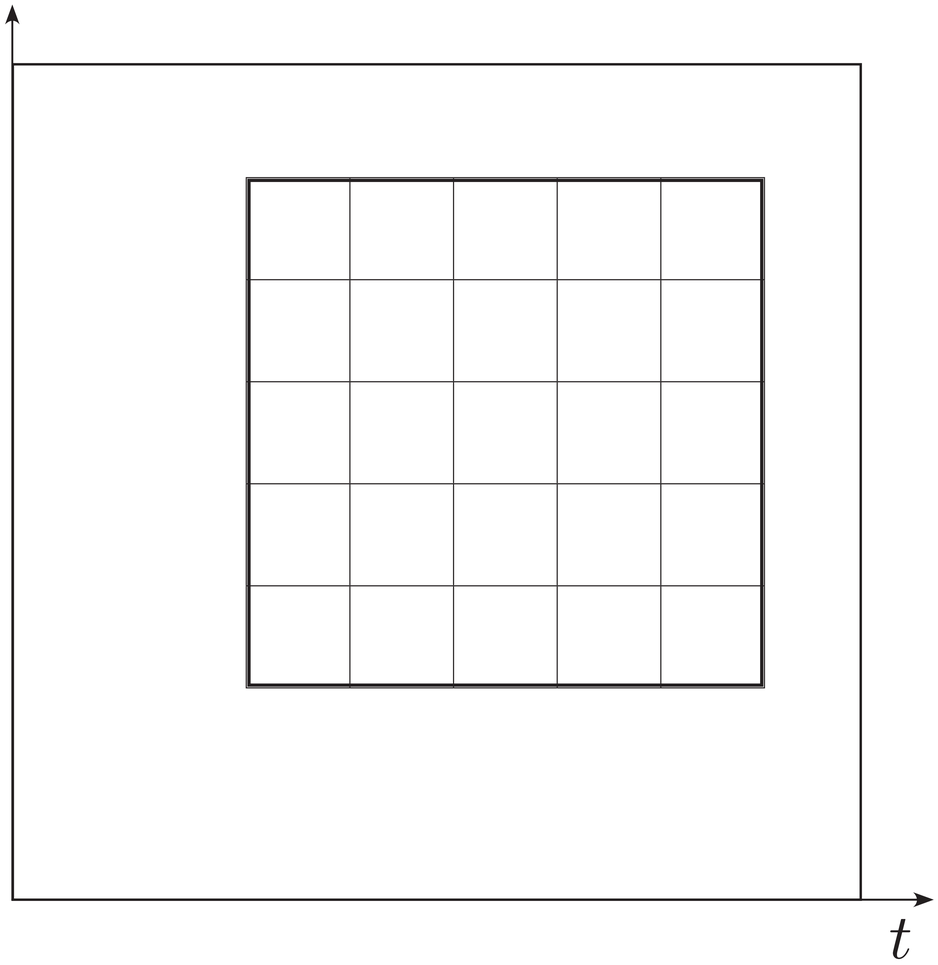
Training objective

- Numerical statistical atmospheric model

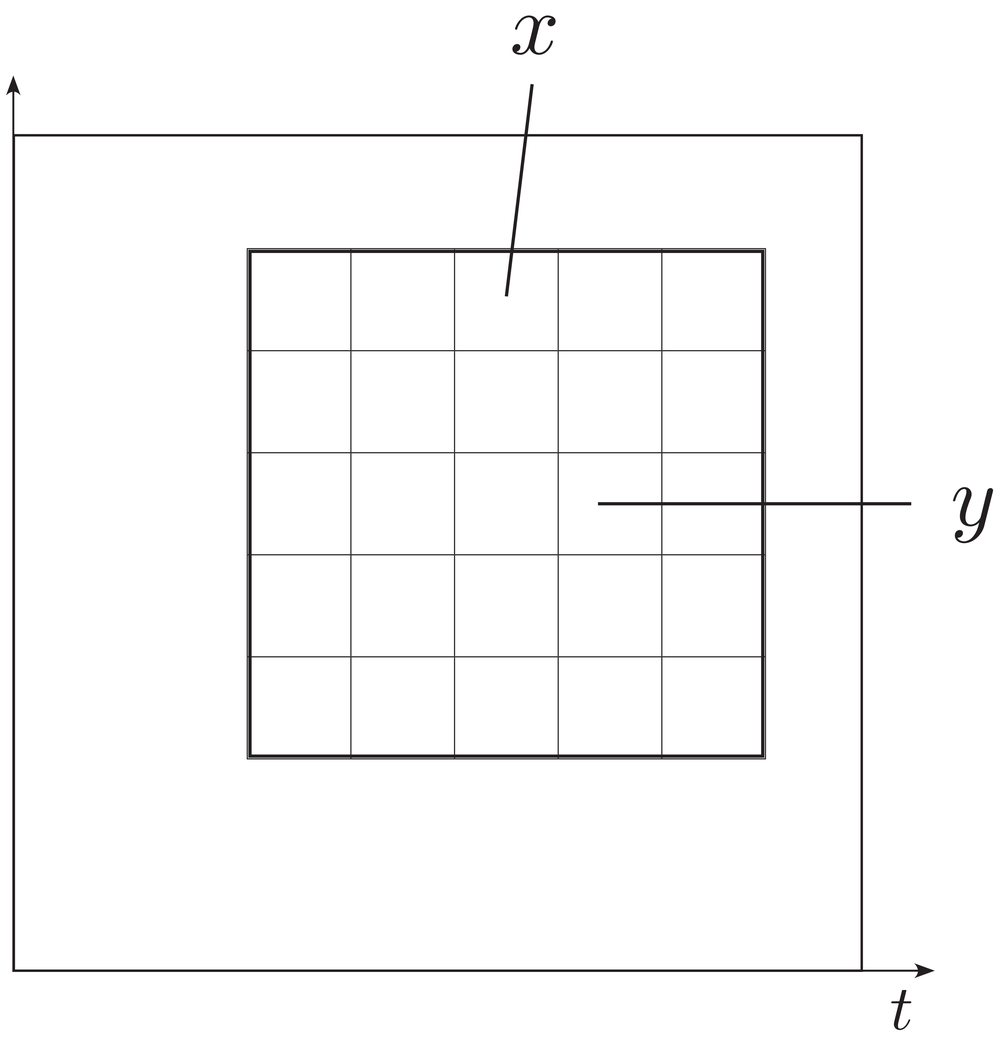
$$p_\theta\left(y|x,\alpha\right)$$

  - Training should model spatio-temporal relationship between arbitrary state x and y

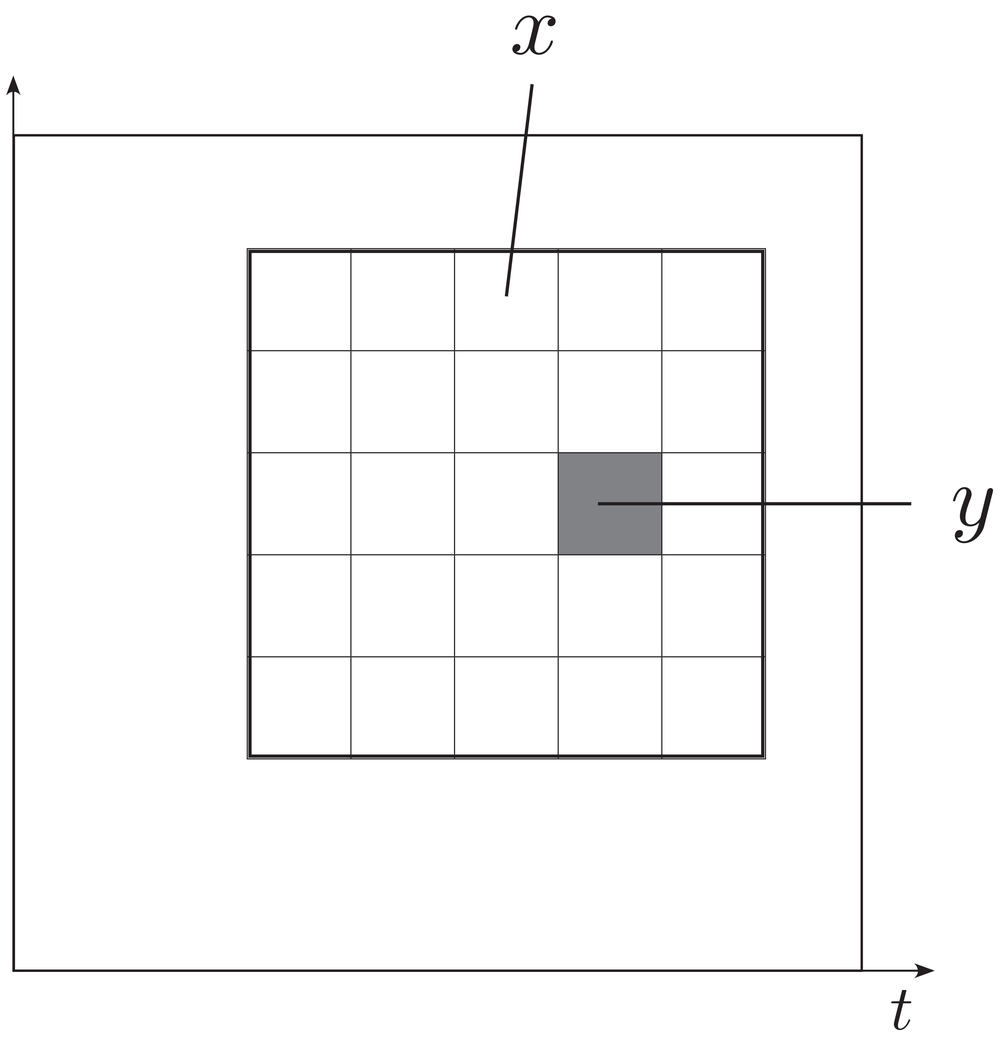
Training objective



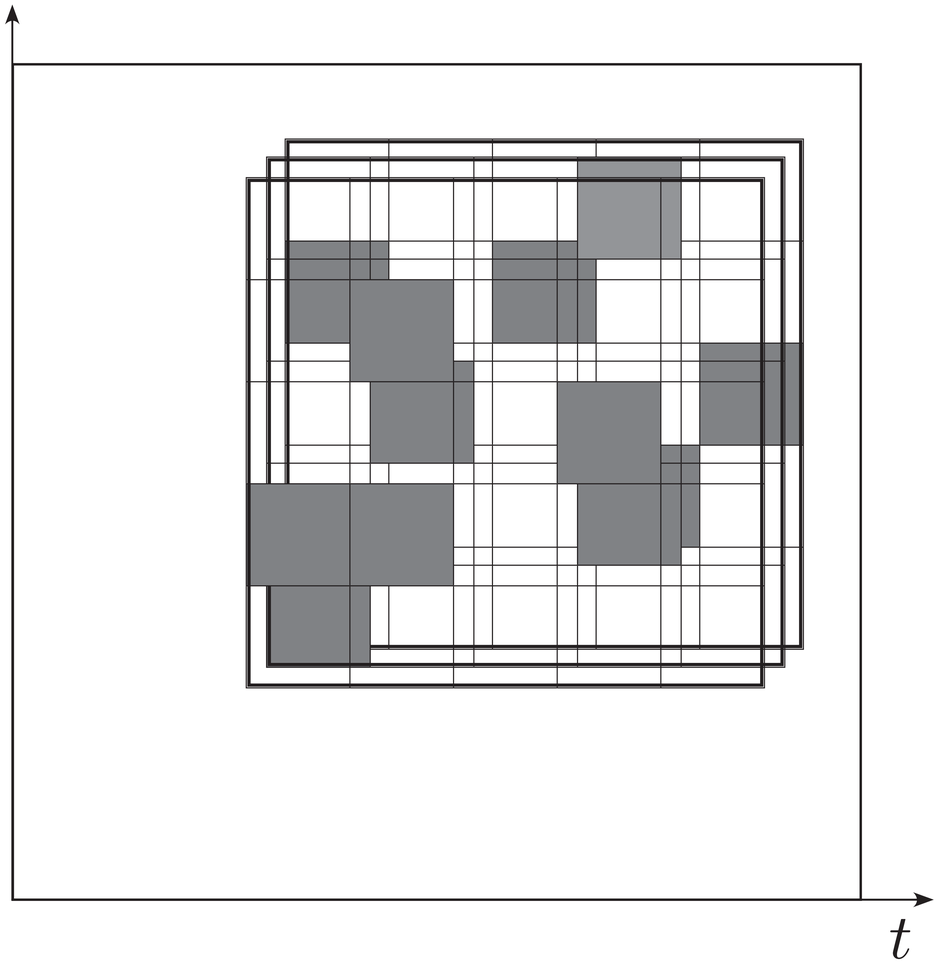
Training objective



Training objective



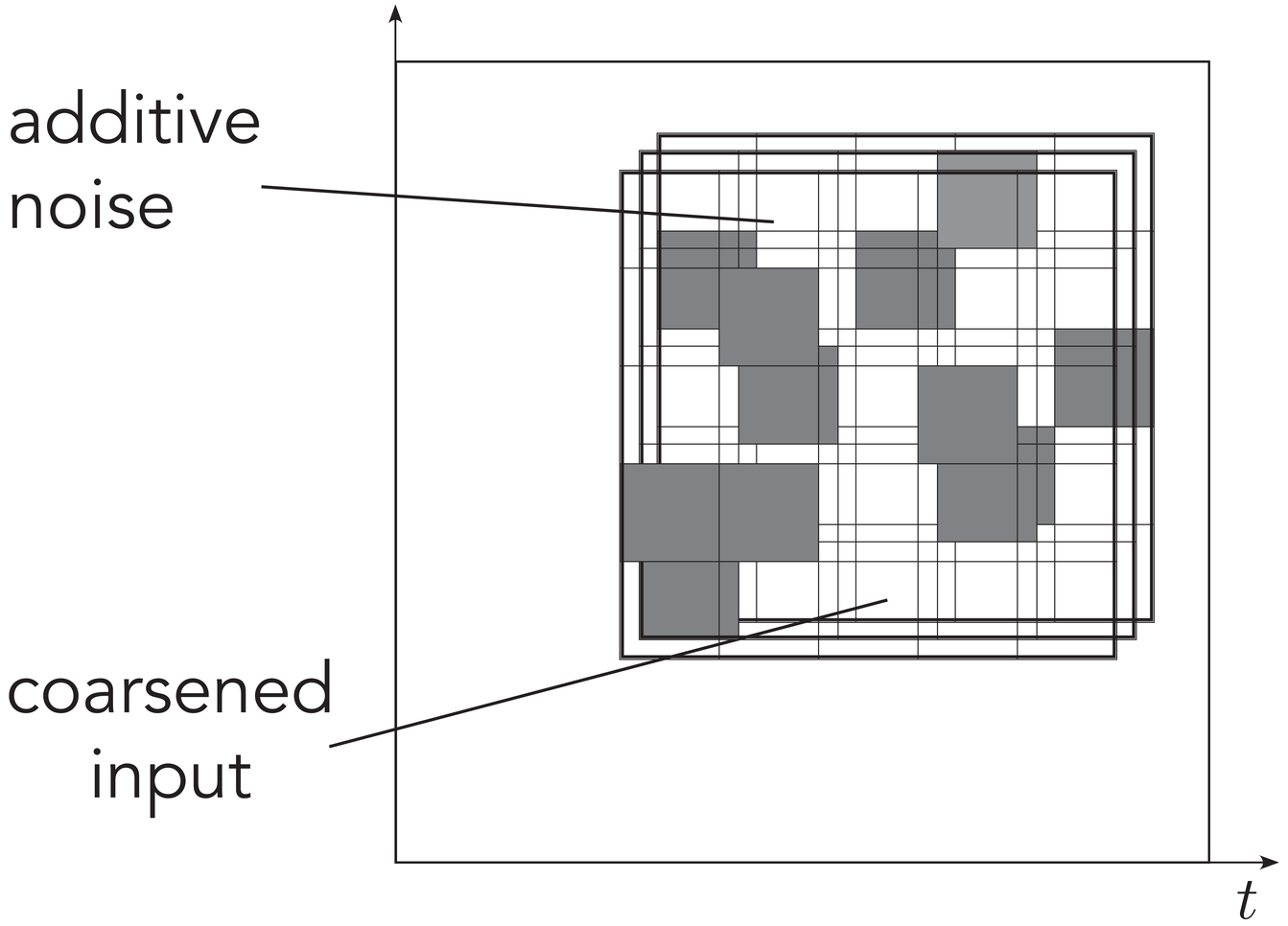
Training objective



masked
token model:

training to predict
randomly masked
information

Training objective



masked
token model:

training to predict
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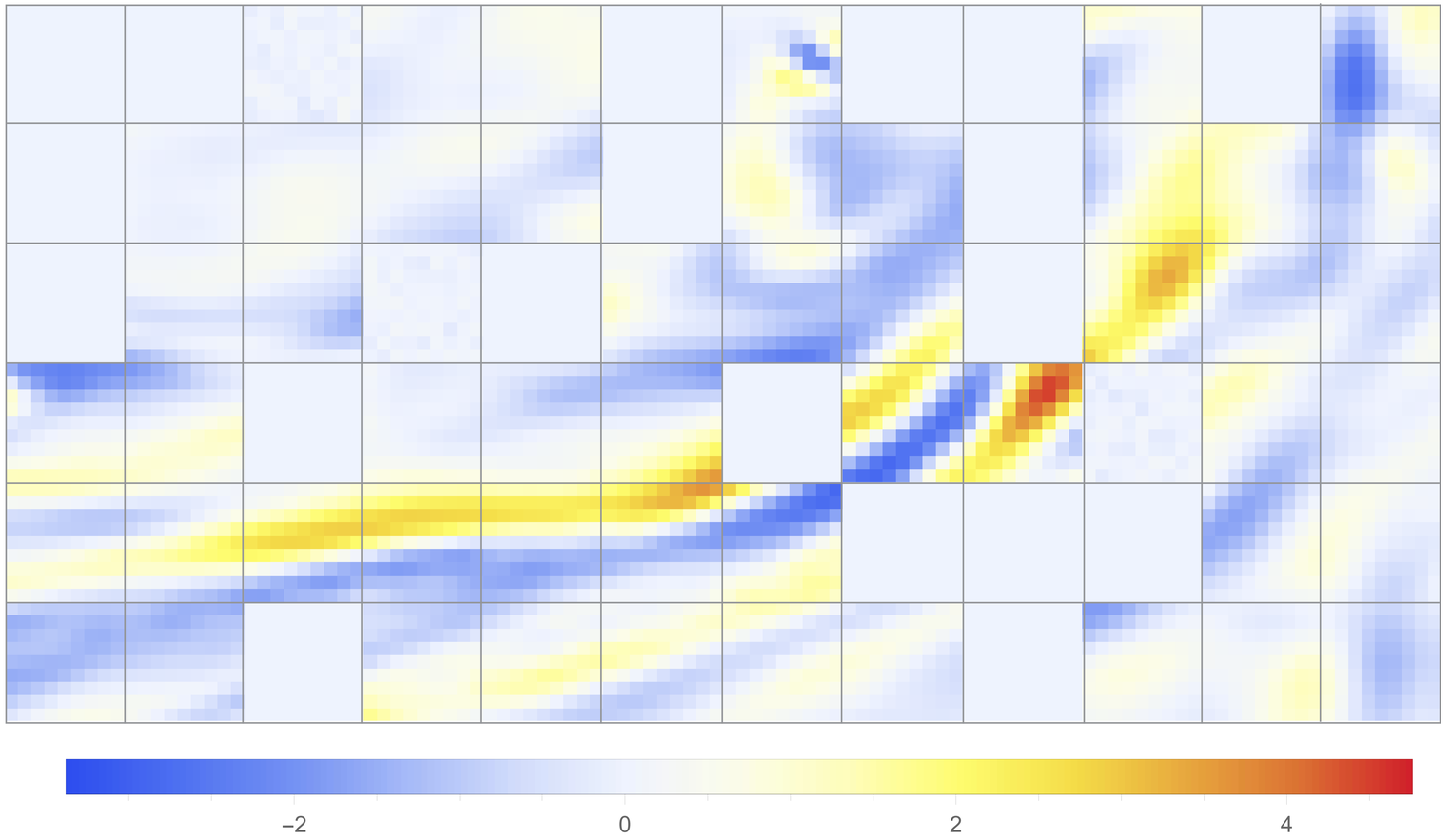
information

Training objective

divergence, ml=96



Loss

- MSE measures only very approximately what is of interest in applications
- To train a statistical model, deterministic training and loss is insufficient

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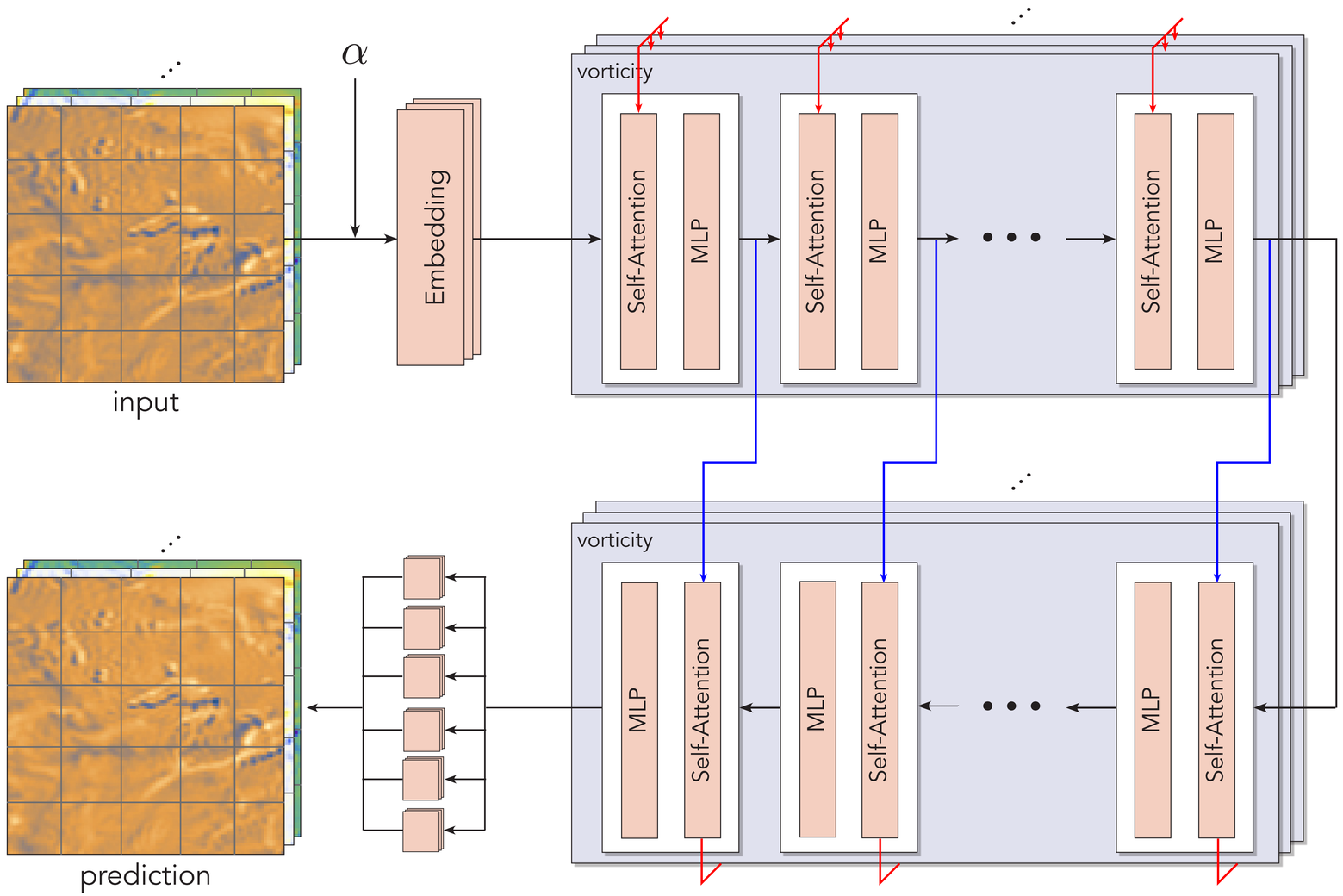
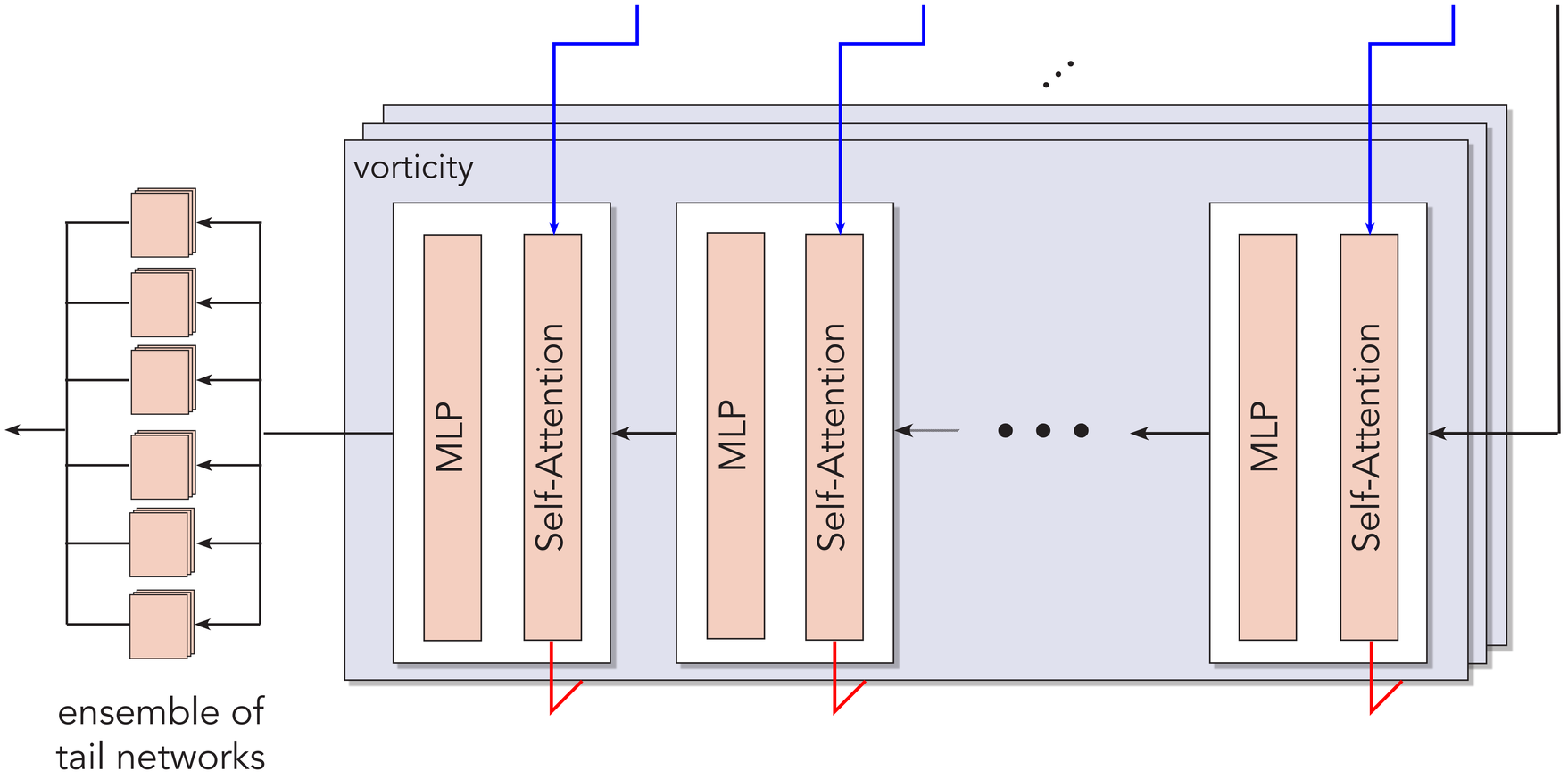
- MSE measures only very approximately what is of interest in applications
- To train a statistical model, deterministic training and loss is insufficient

=> Analog of cross-entropy loss for regression problems?

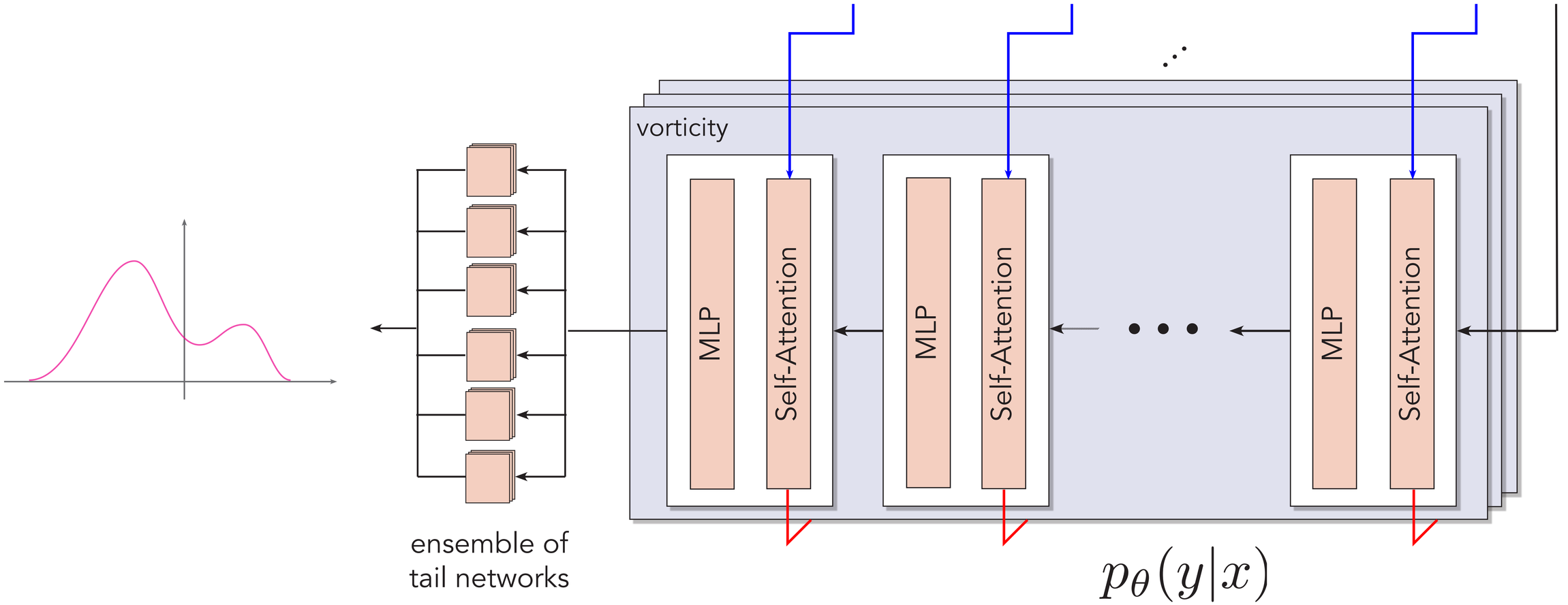
Statistical loss



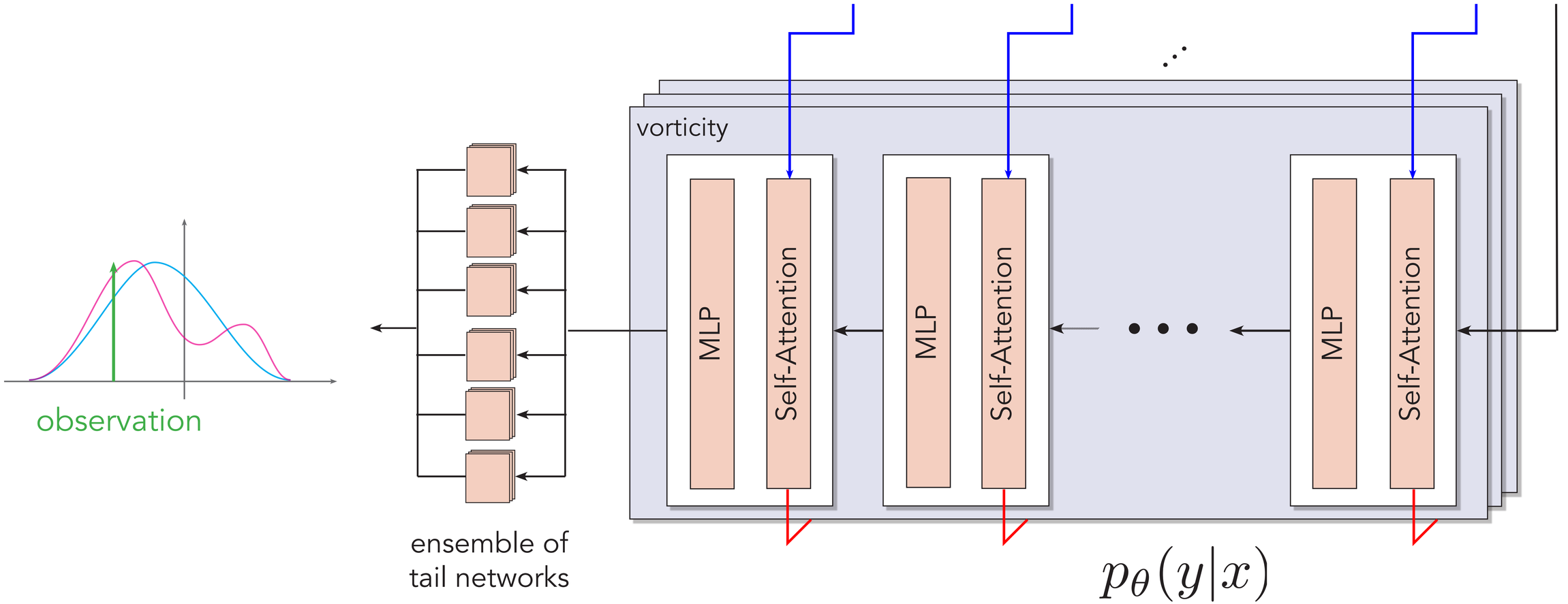
Statistical loss



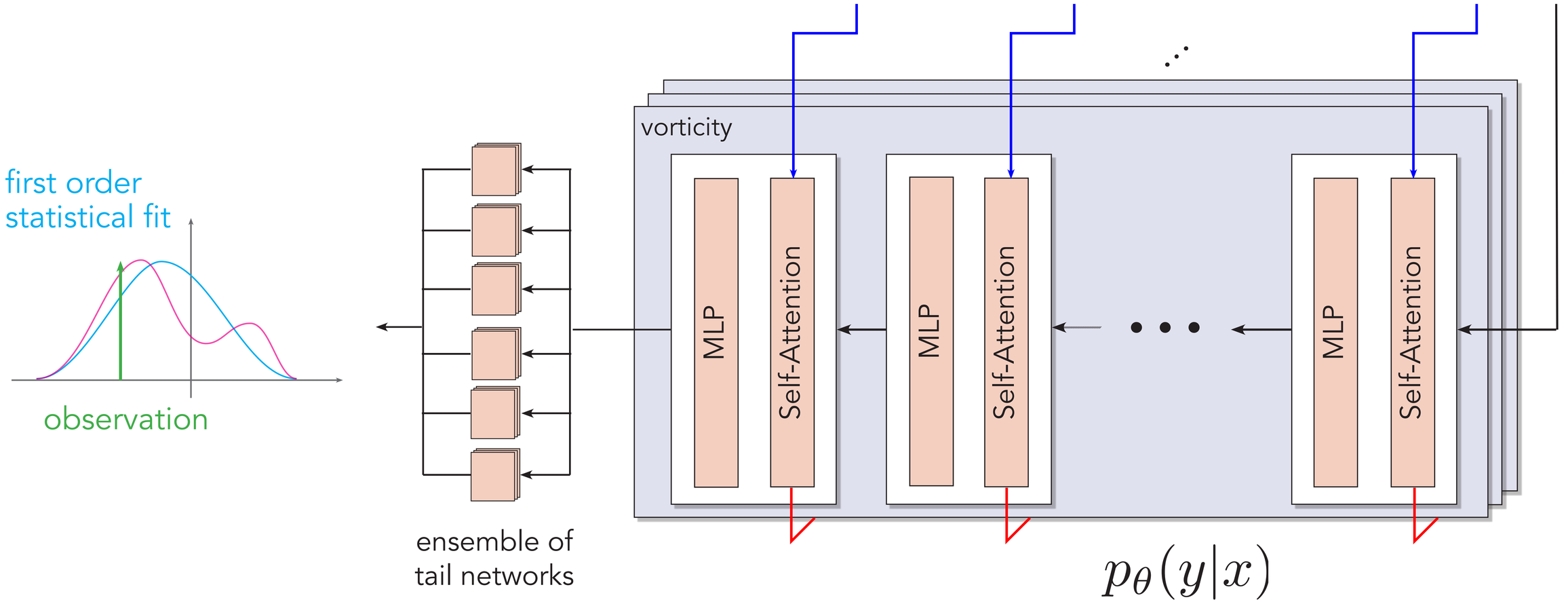
Statistical loss



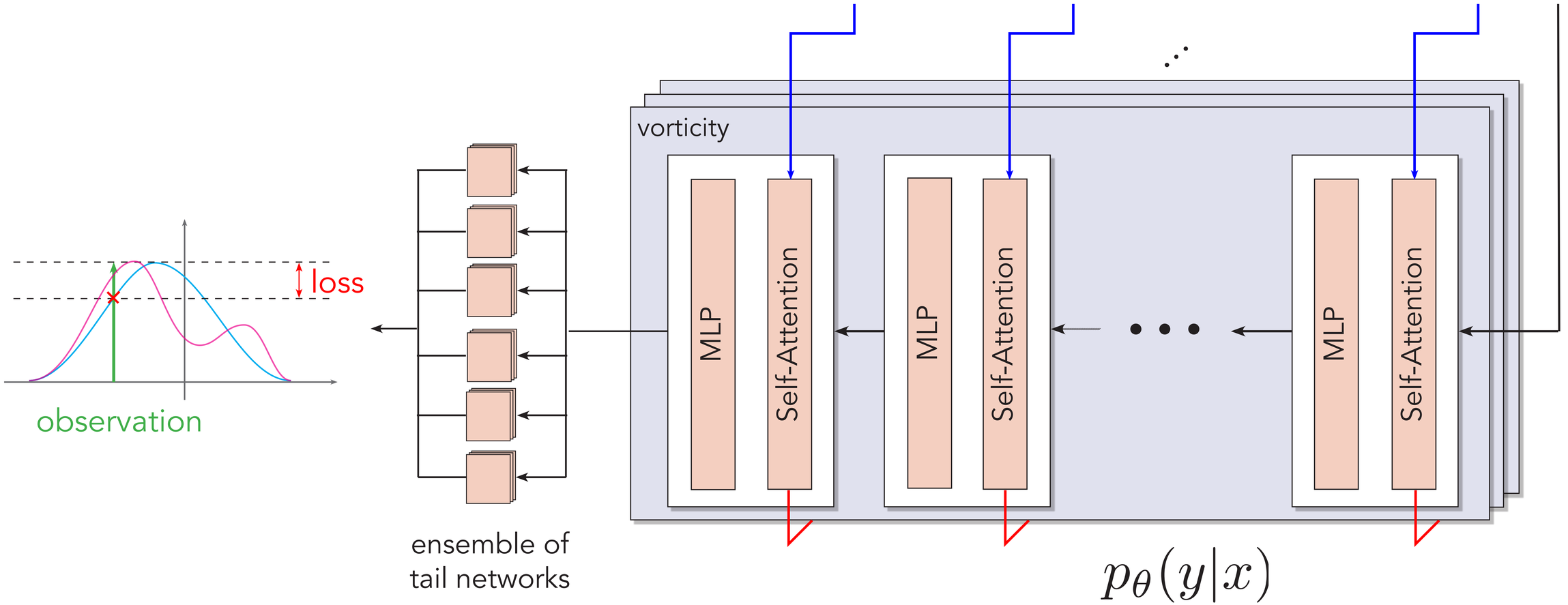
Statistical loss



Statistical loss

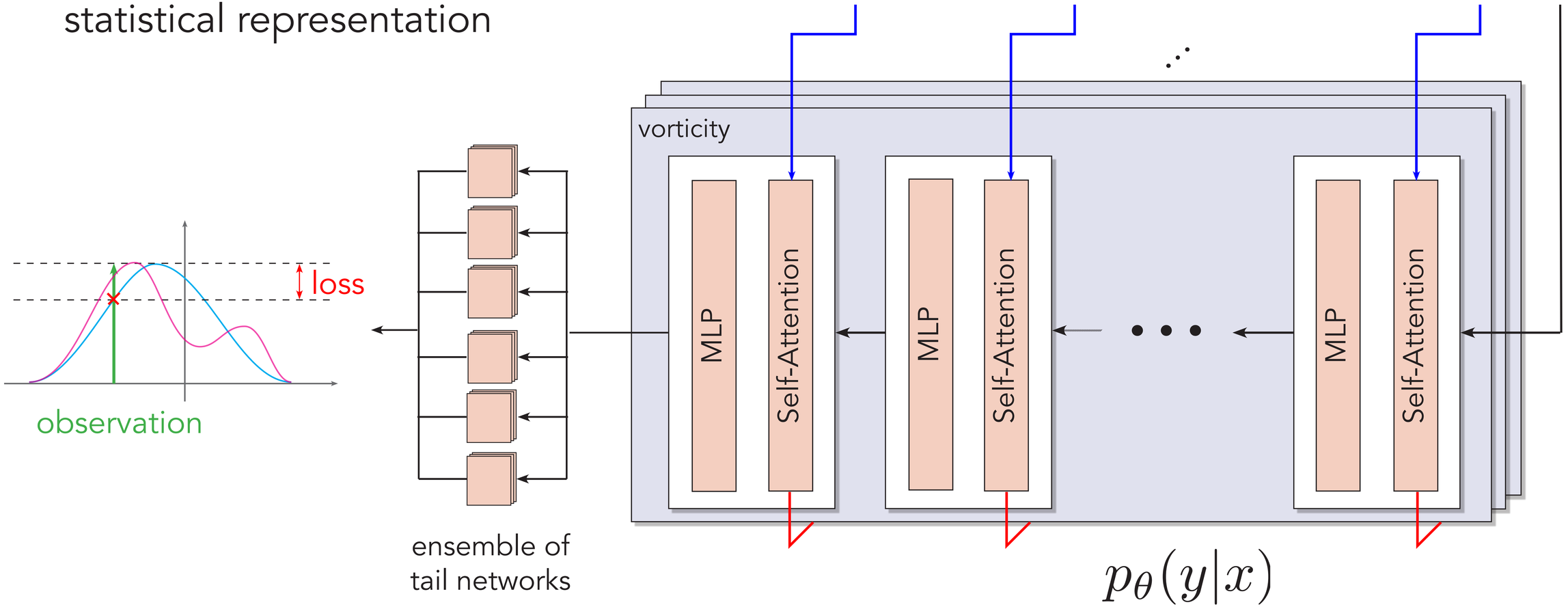


Statistical loss

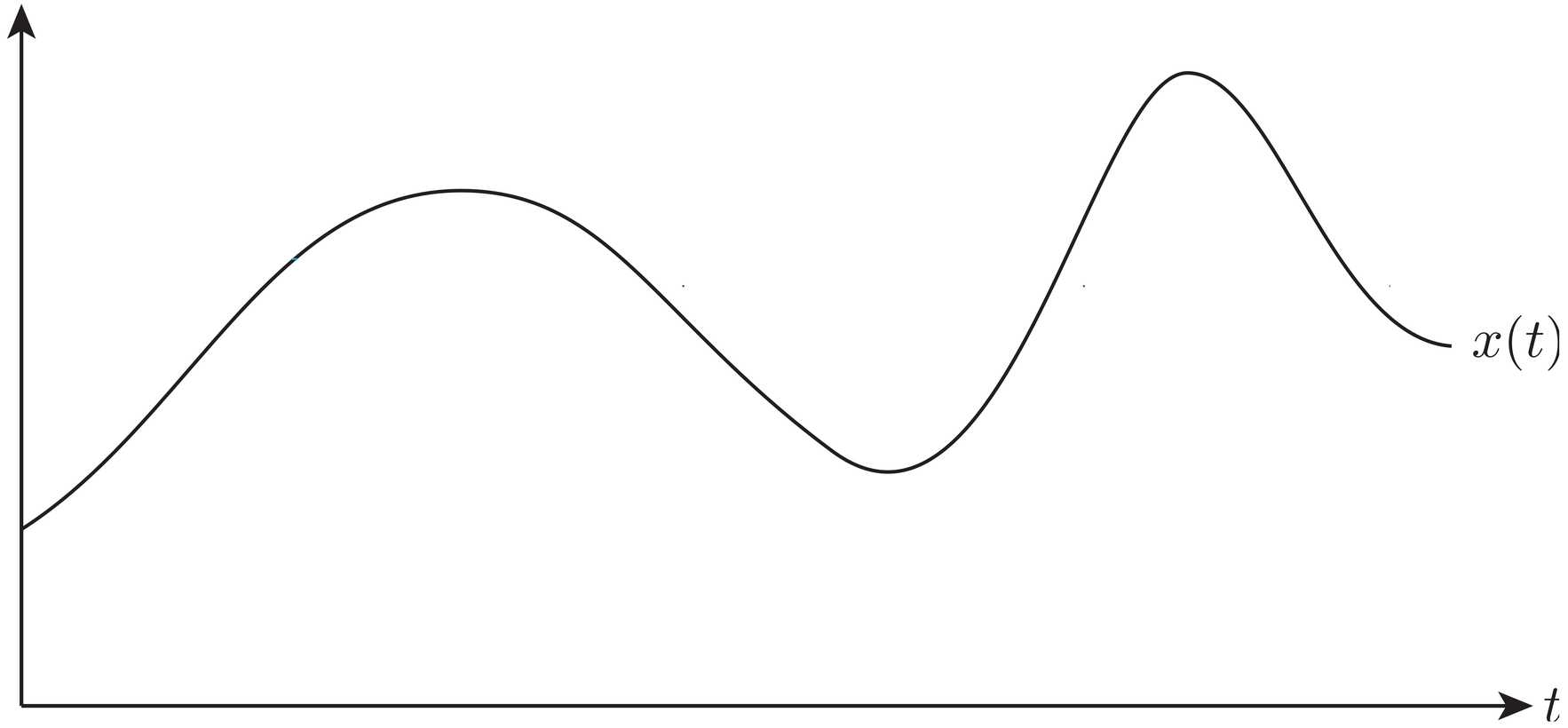


Statistical loss

end-to-end training encourages
statistical representation



Statistical loss



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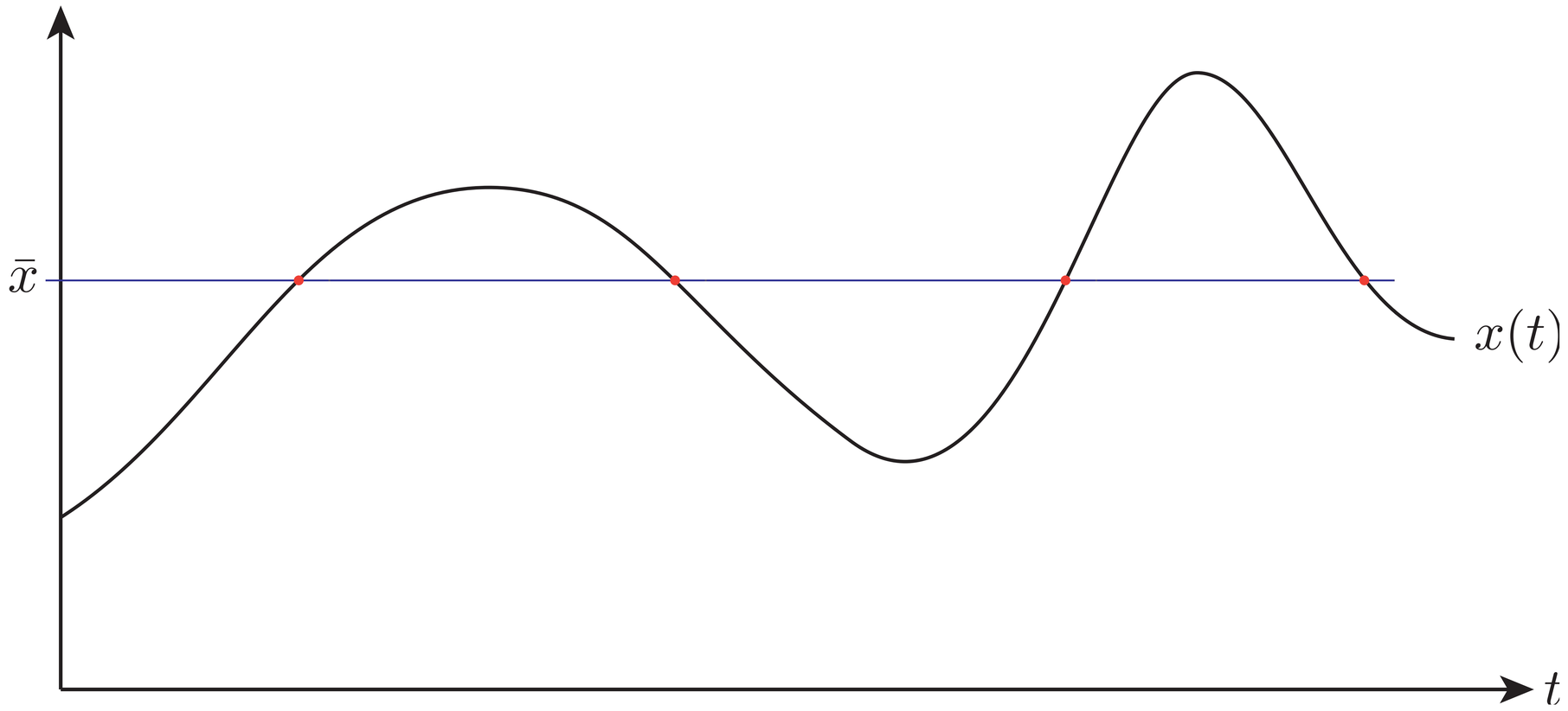
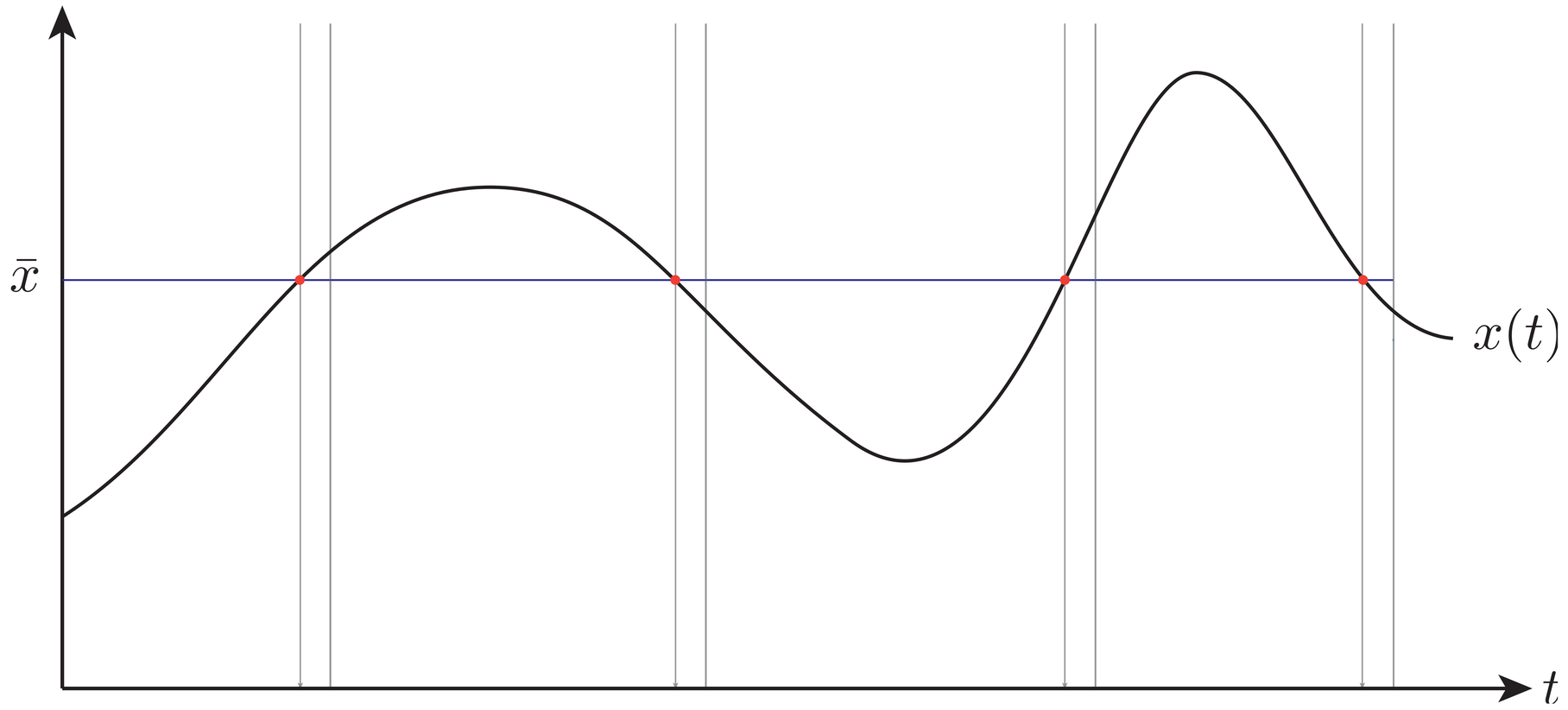
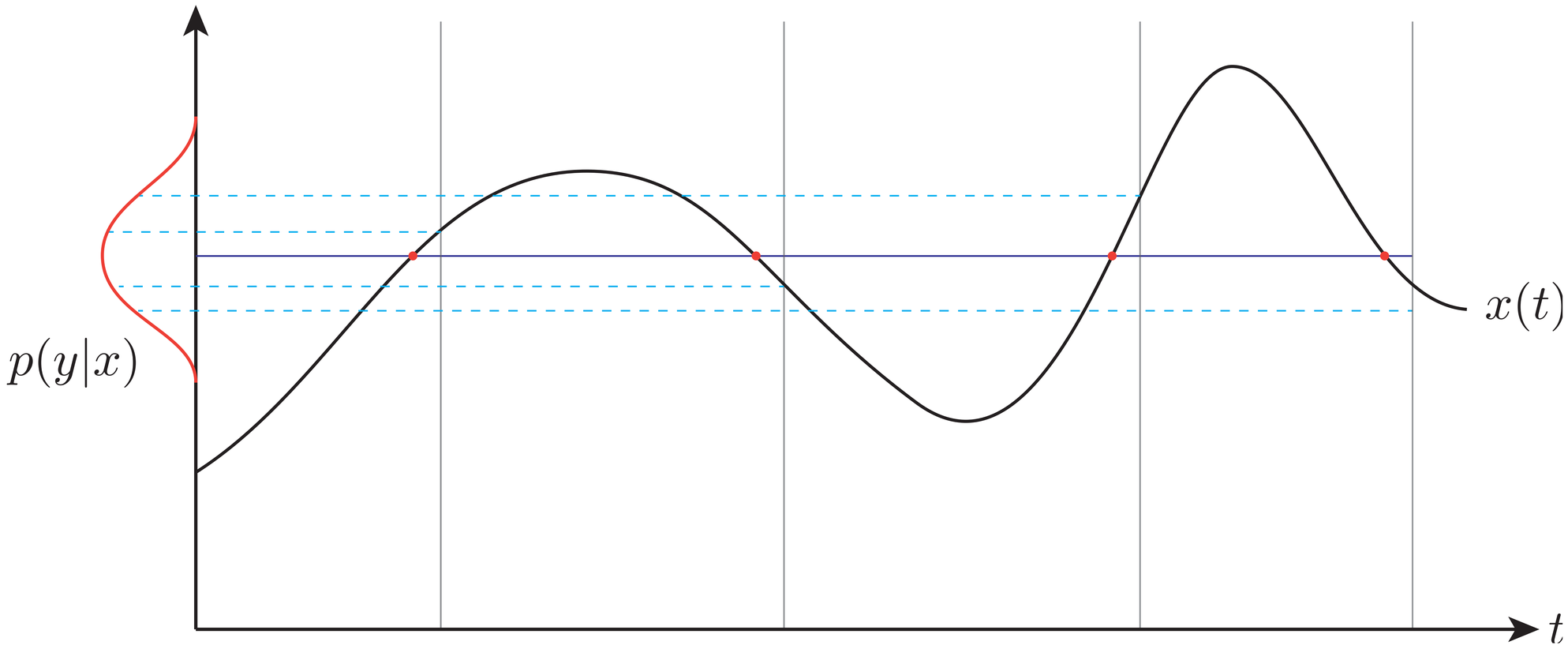


Statistical loss

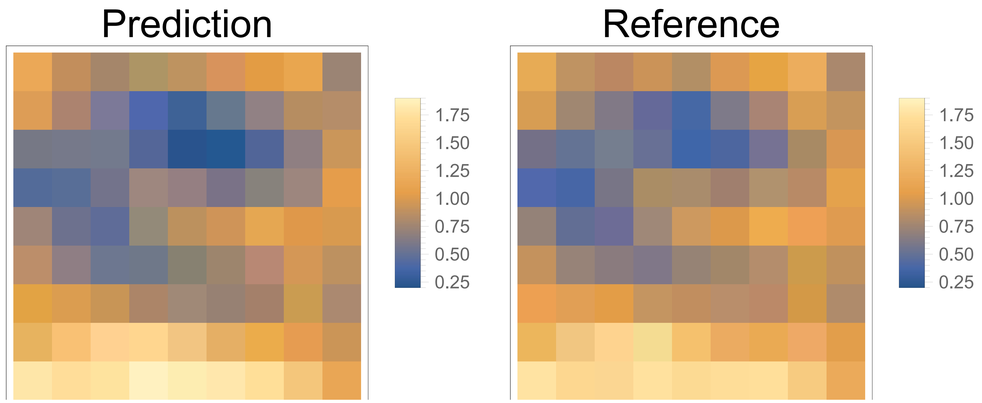


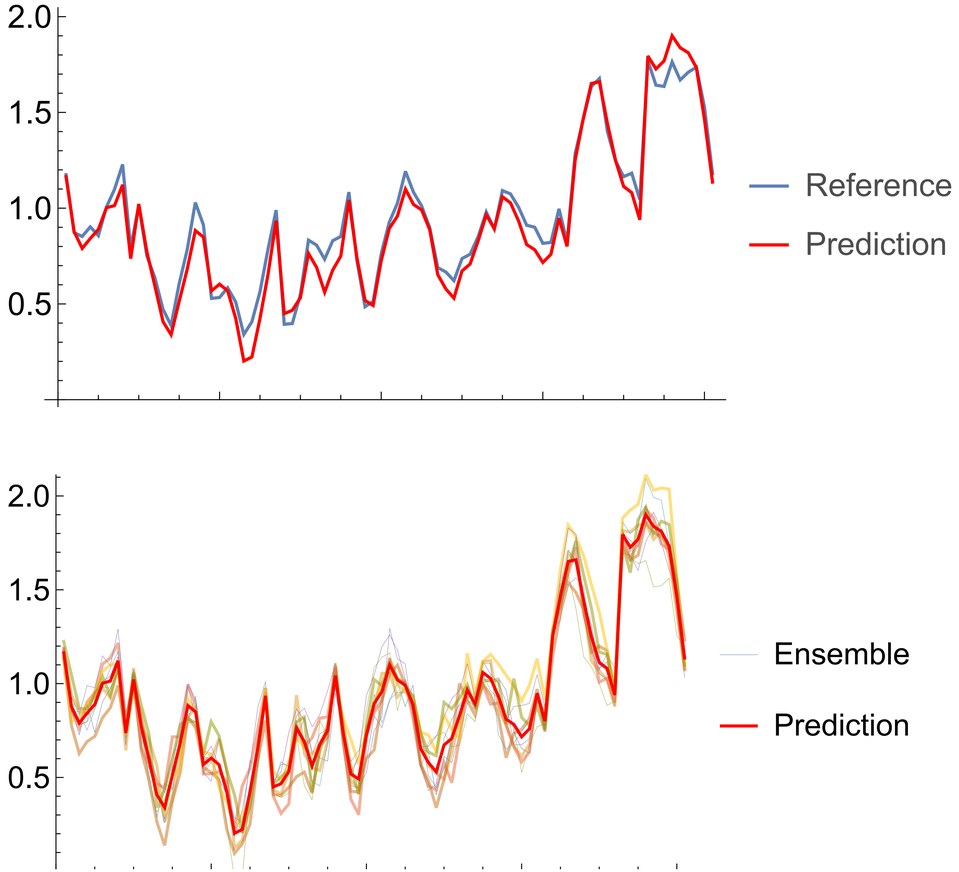
Statistical loss



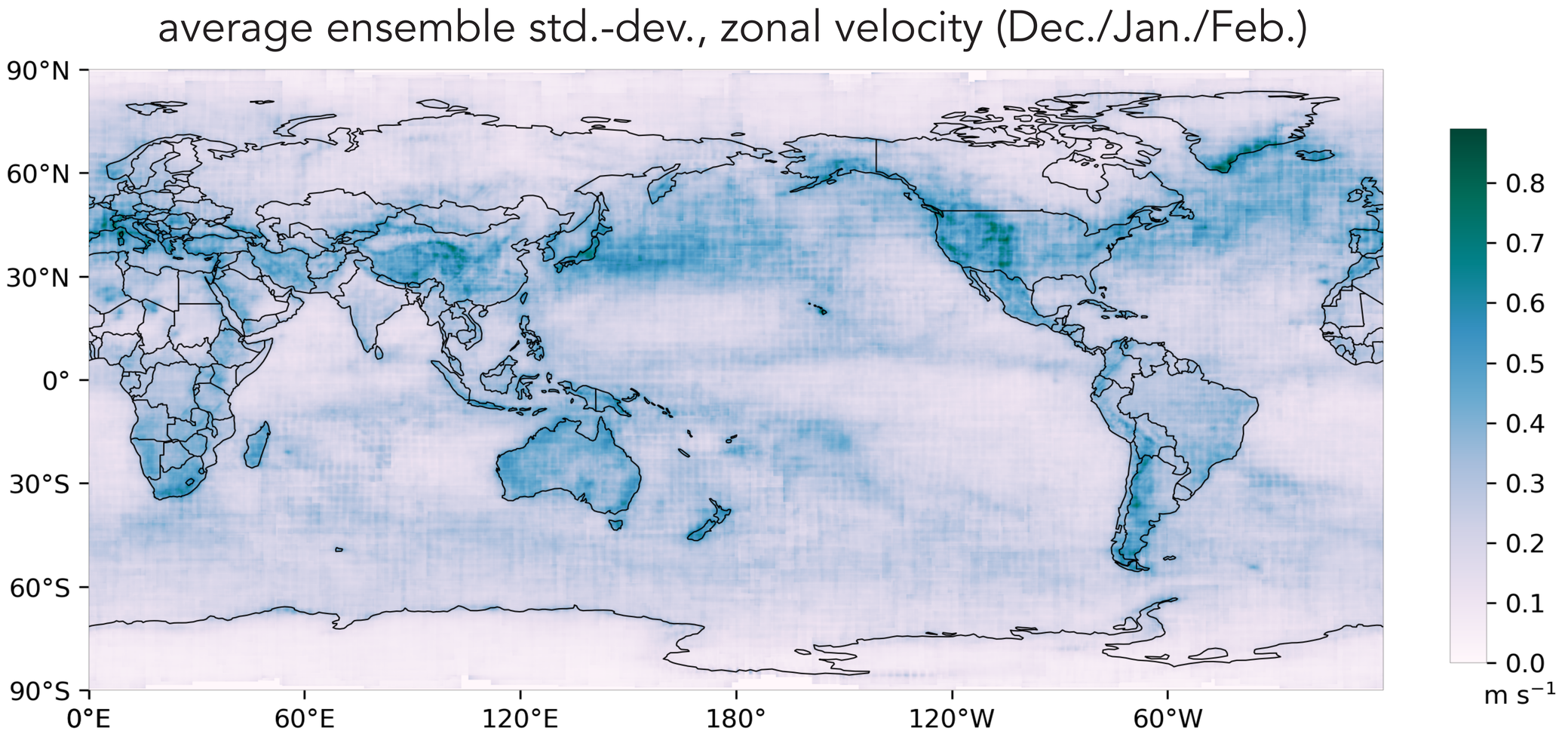
Statistical loss

- Predictions:

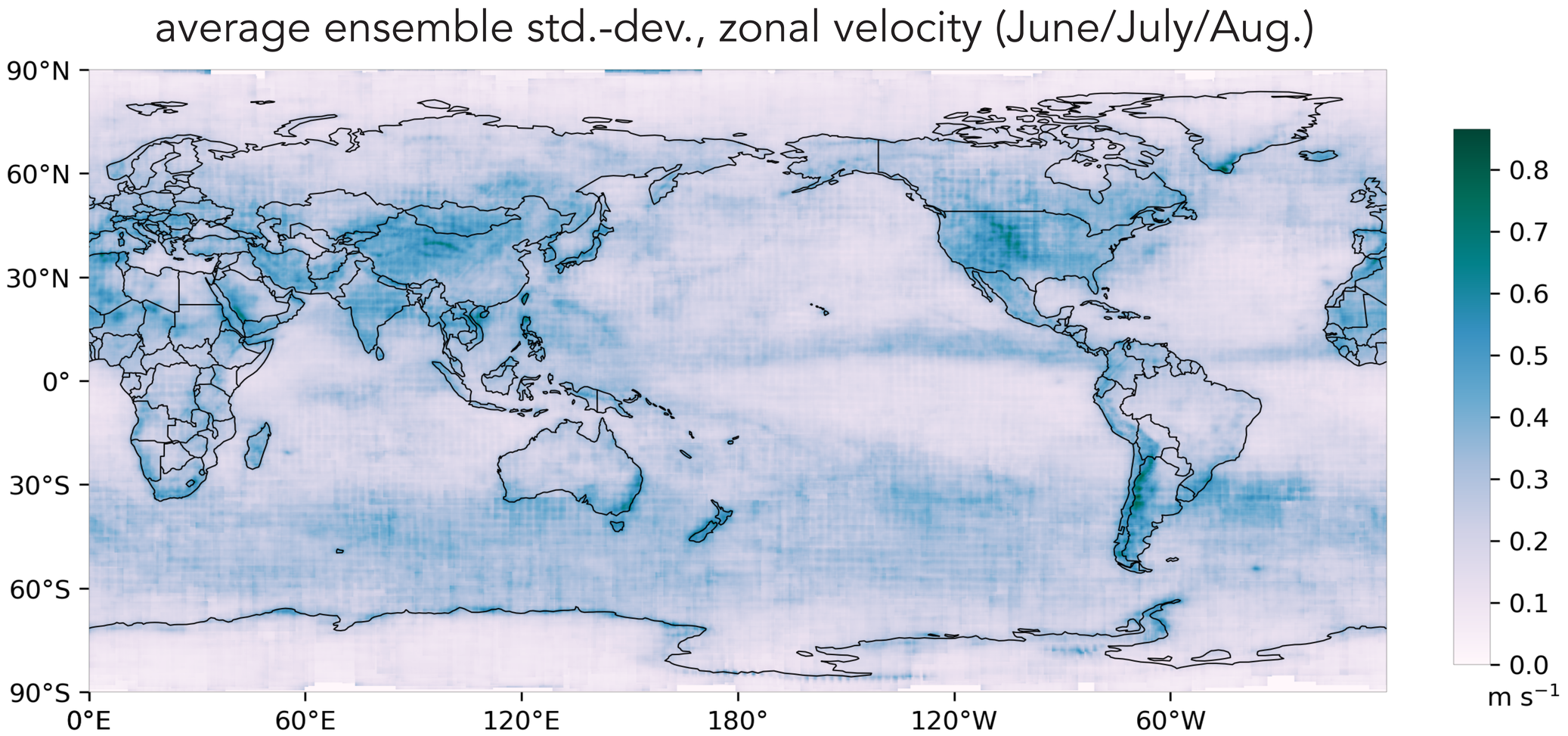




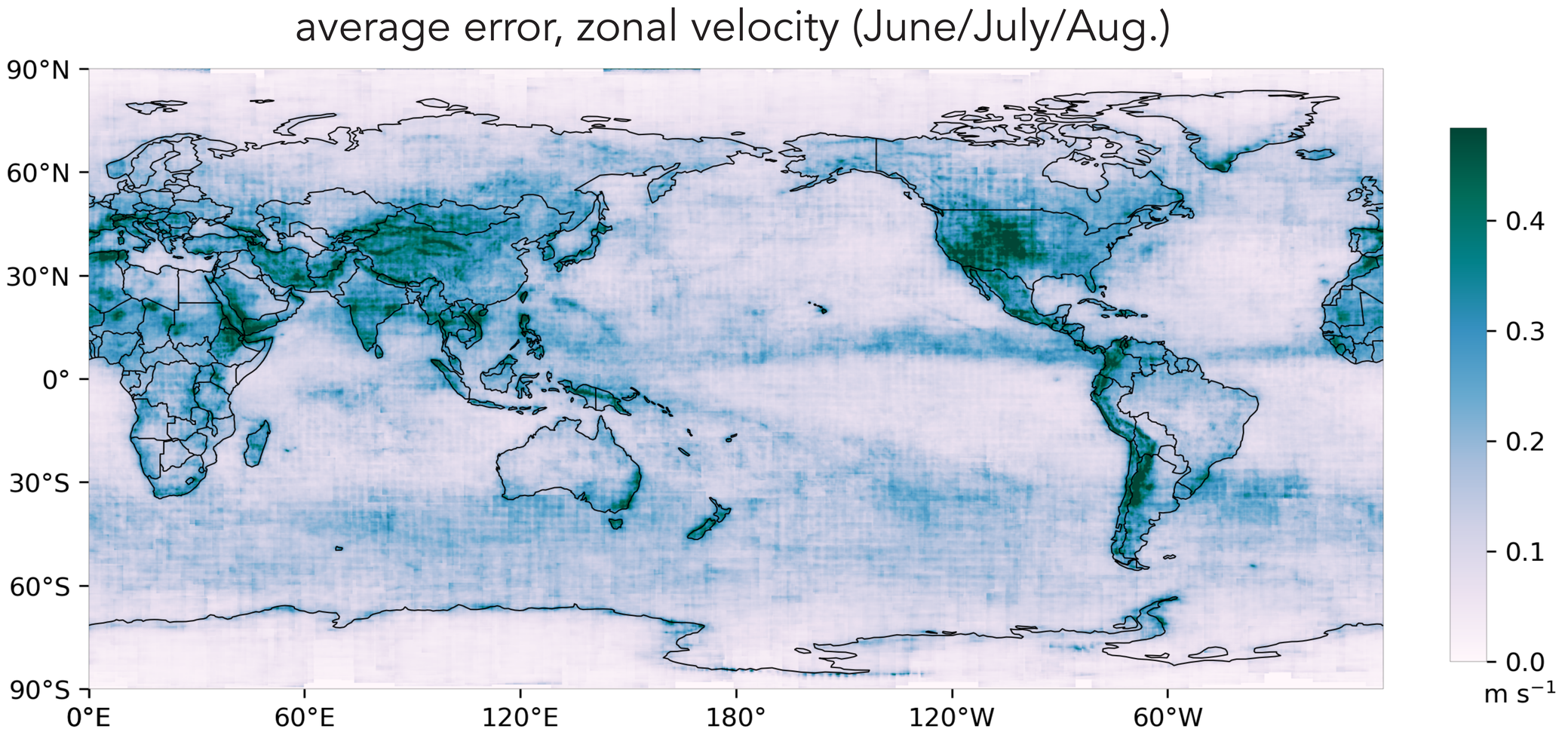
Statistical loss



Statistical loss



Statistical loss



Intrinsic Capabilities

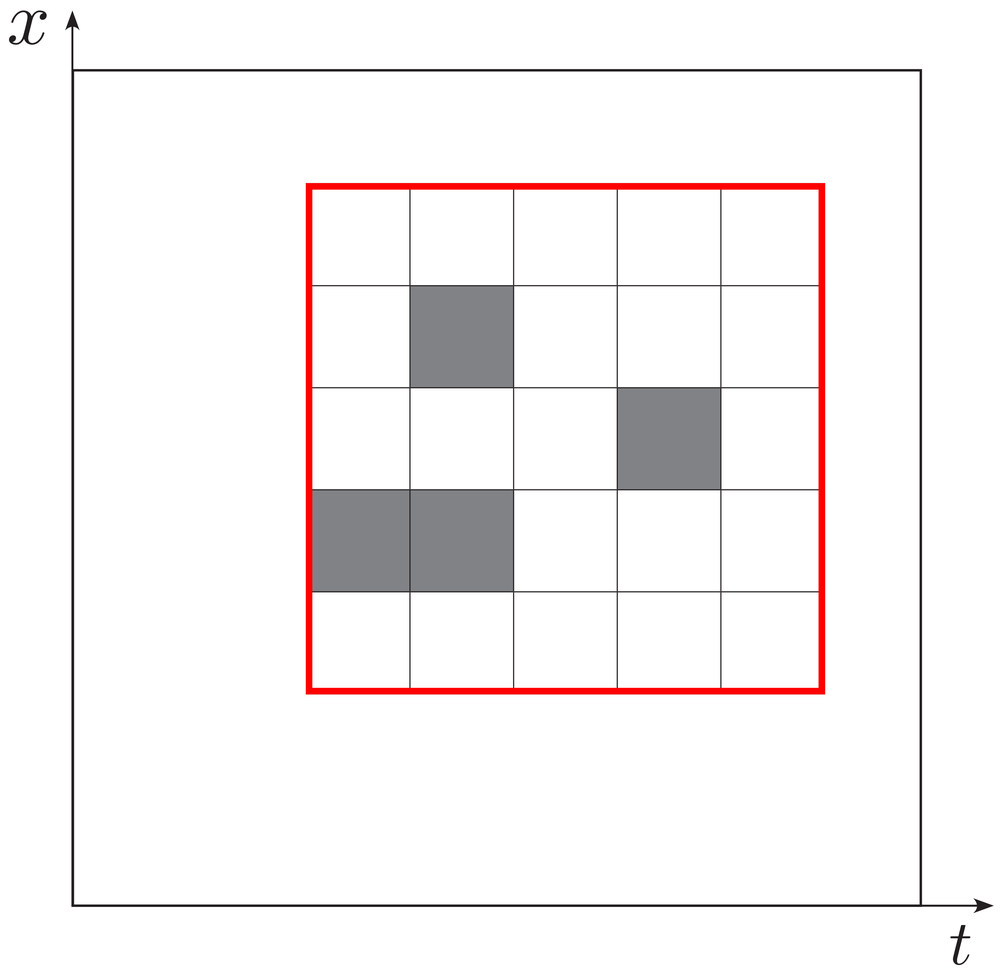
Zero-shot capabilities

- Numerical statistical atmospheric model:

$$p_\theta\left(y|x,\alpha\right)$$

- Model directly includes important applications: forecasting, downscaling, temporal interpolation, ...

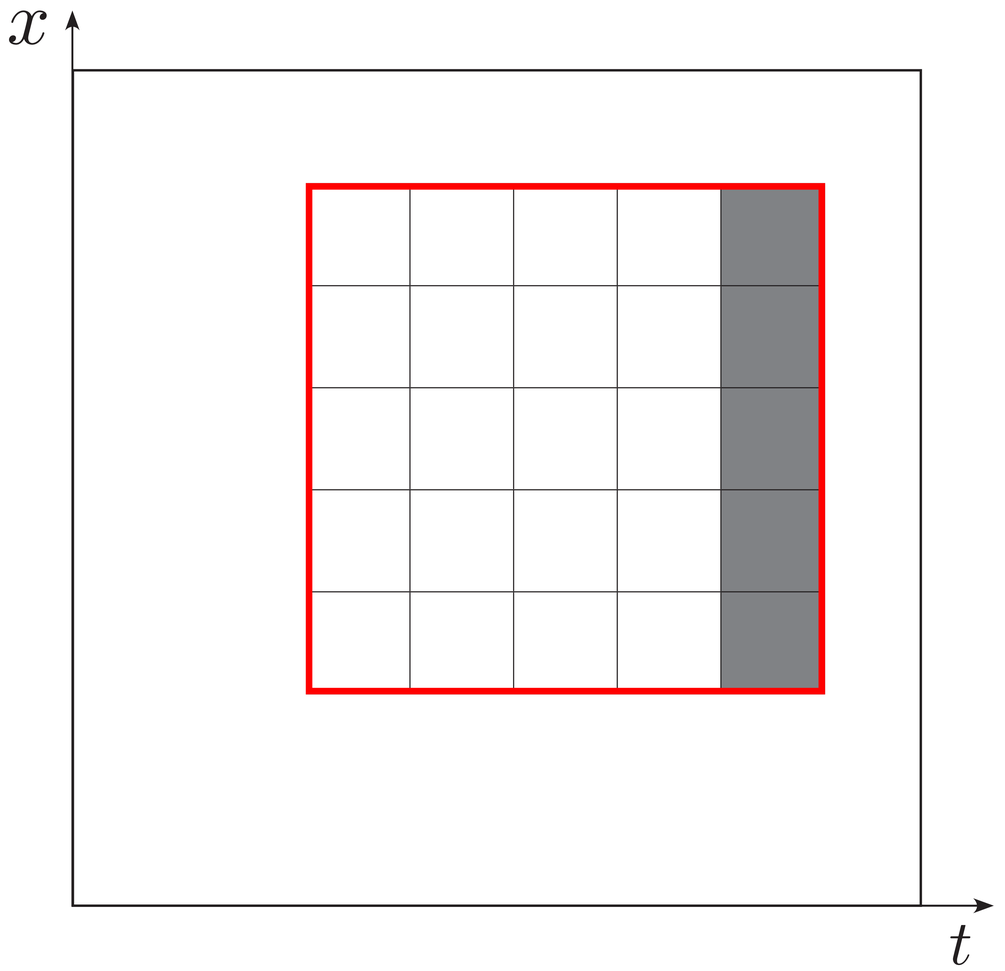
Zero-shot capabilities



Training task:

predict randomly masked neighbor-hoods in space-time

Zero-shot capabilities

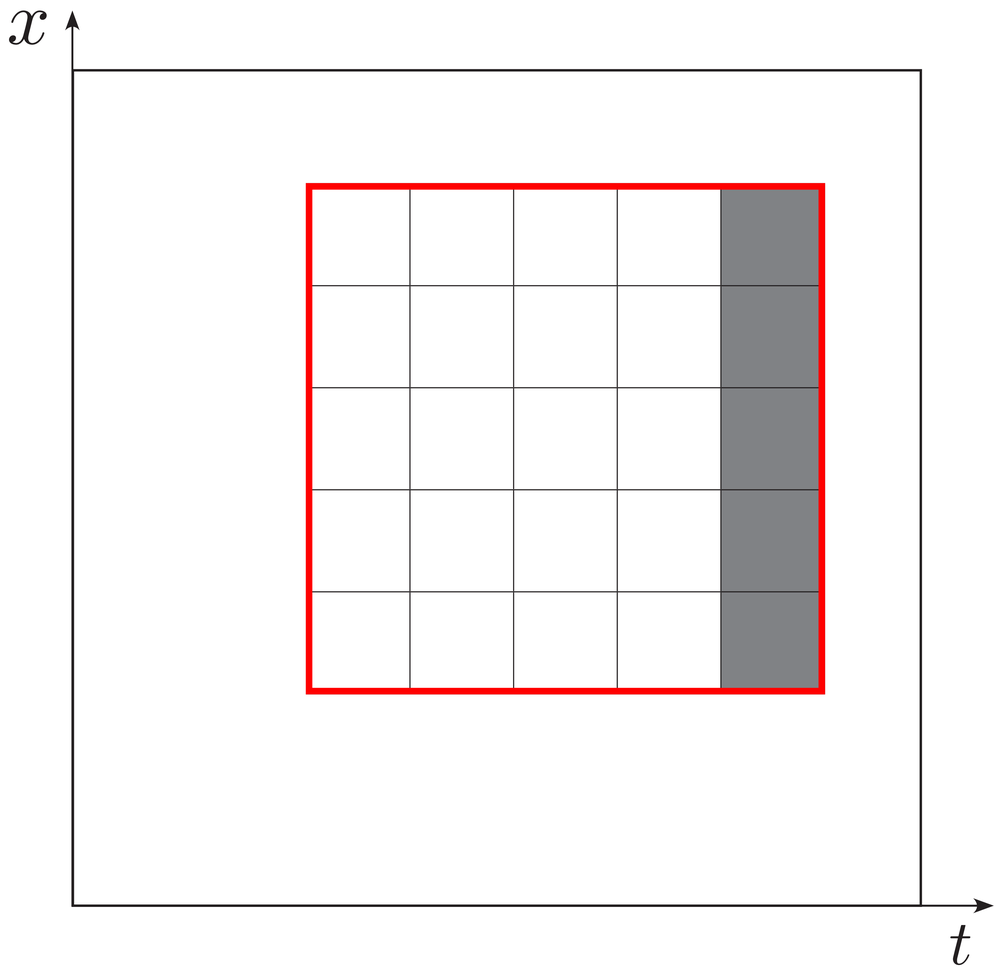


Training task:

predict randomly masked neighbor-hoods in space-time

Zero-shot capabilities

Forecasting

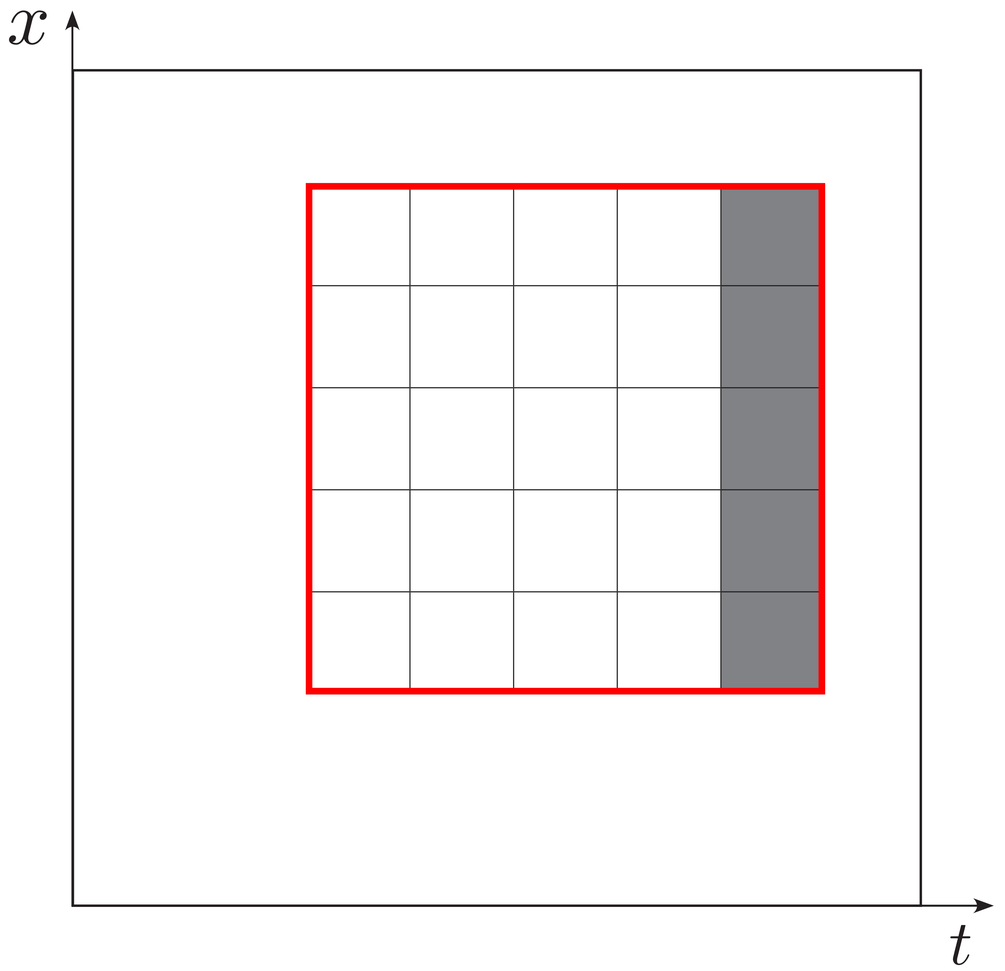


Training task:

predict randomly masked neighbor-hoods in space-time

Zero-shot capabilities

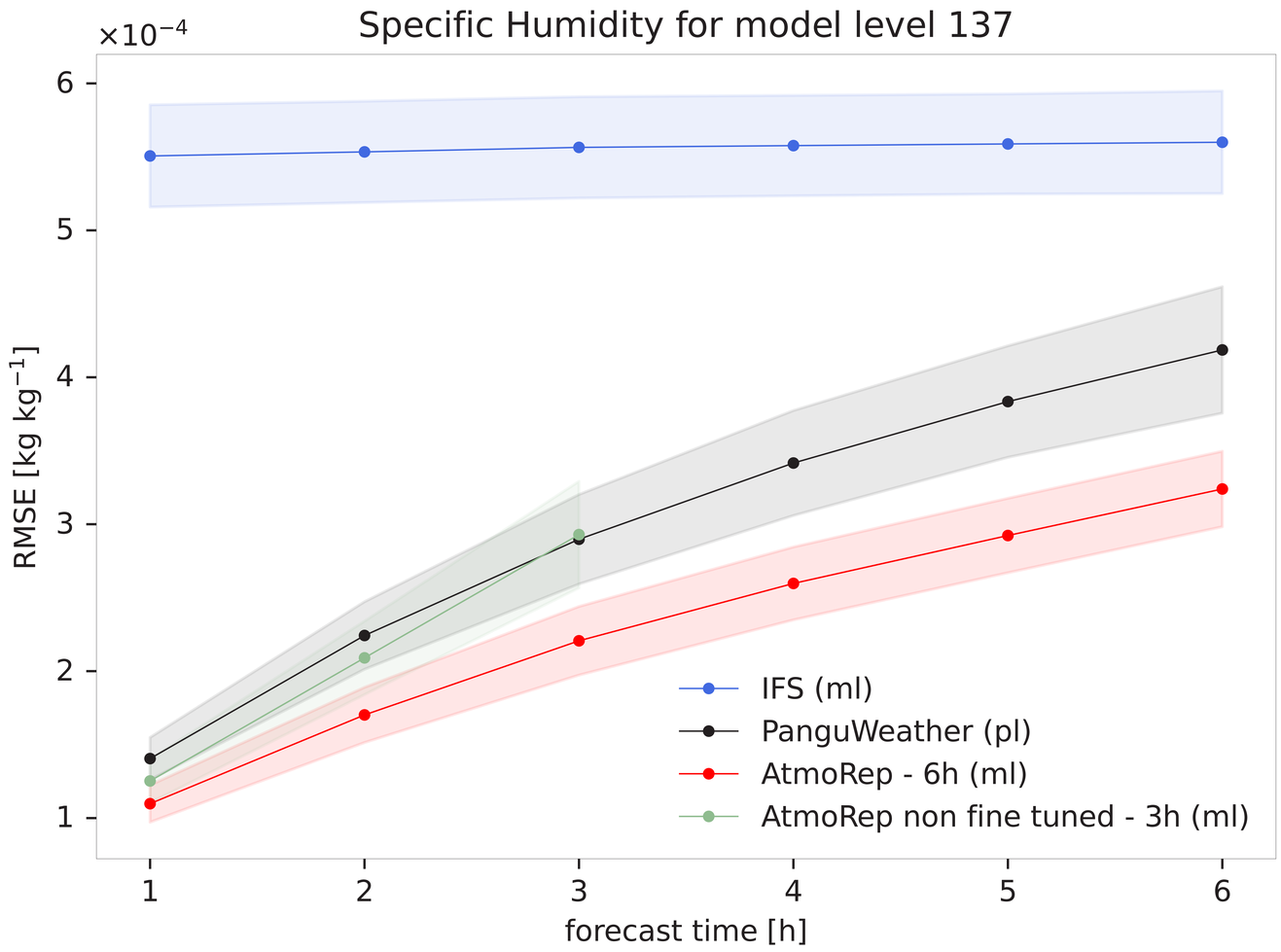
Forecasting



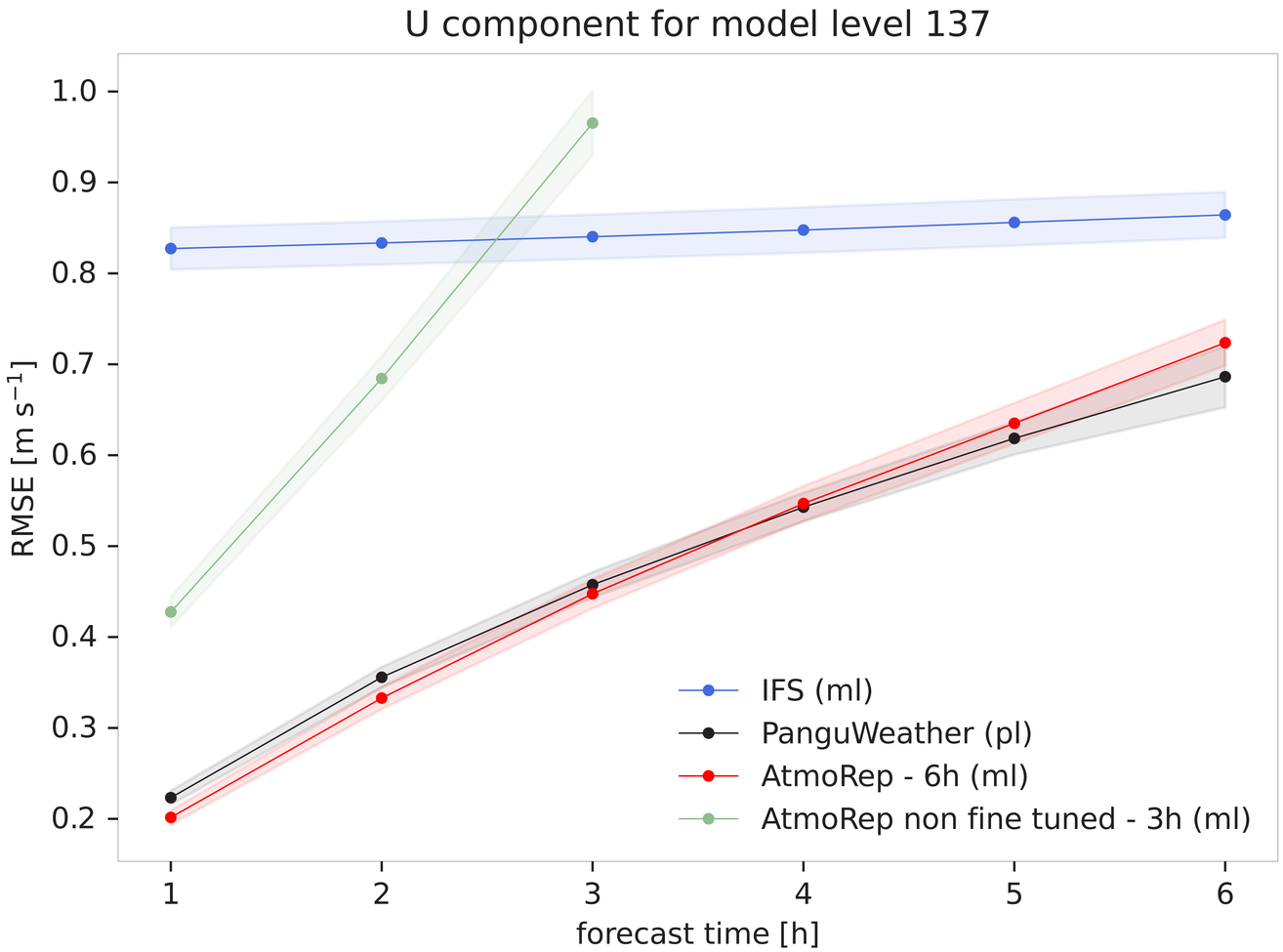
Training task:

predict randomly masked neighbor-hoods in space-time

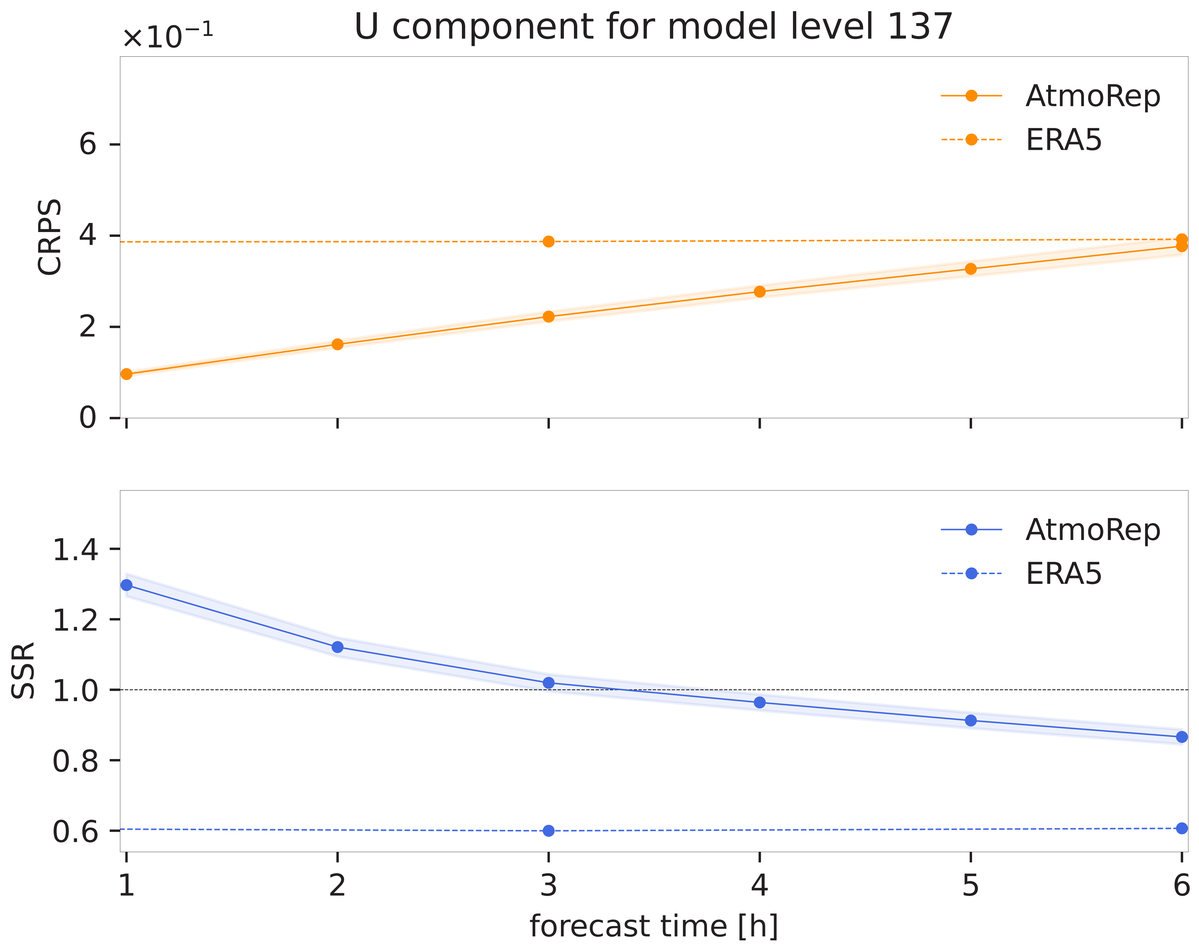
Zero-shot capabilities



Zero-shot capabilities

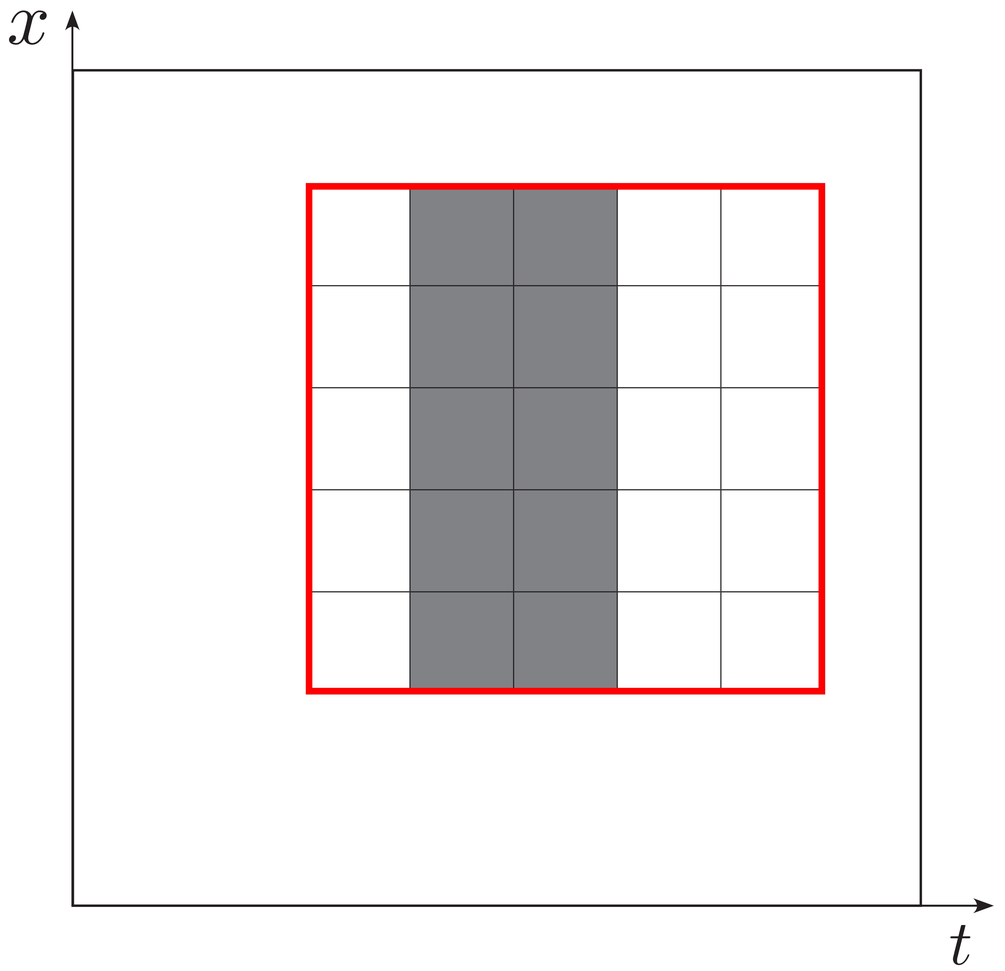


Zero-shot capabilities



Zero-shot capabilities

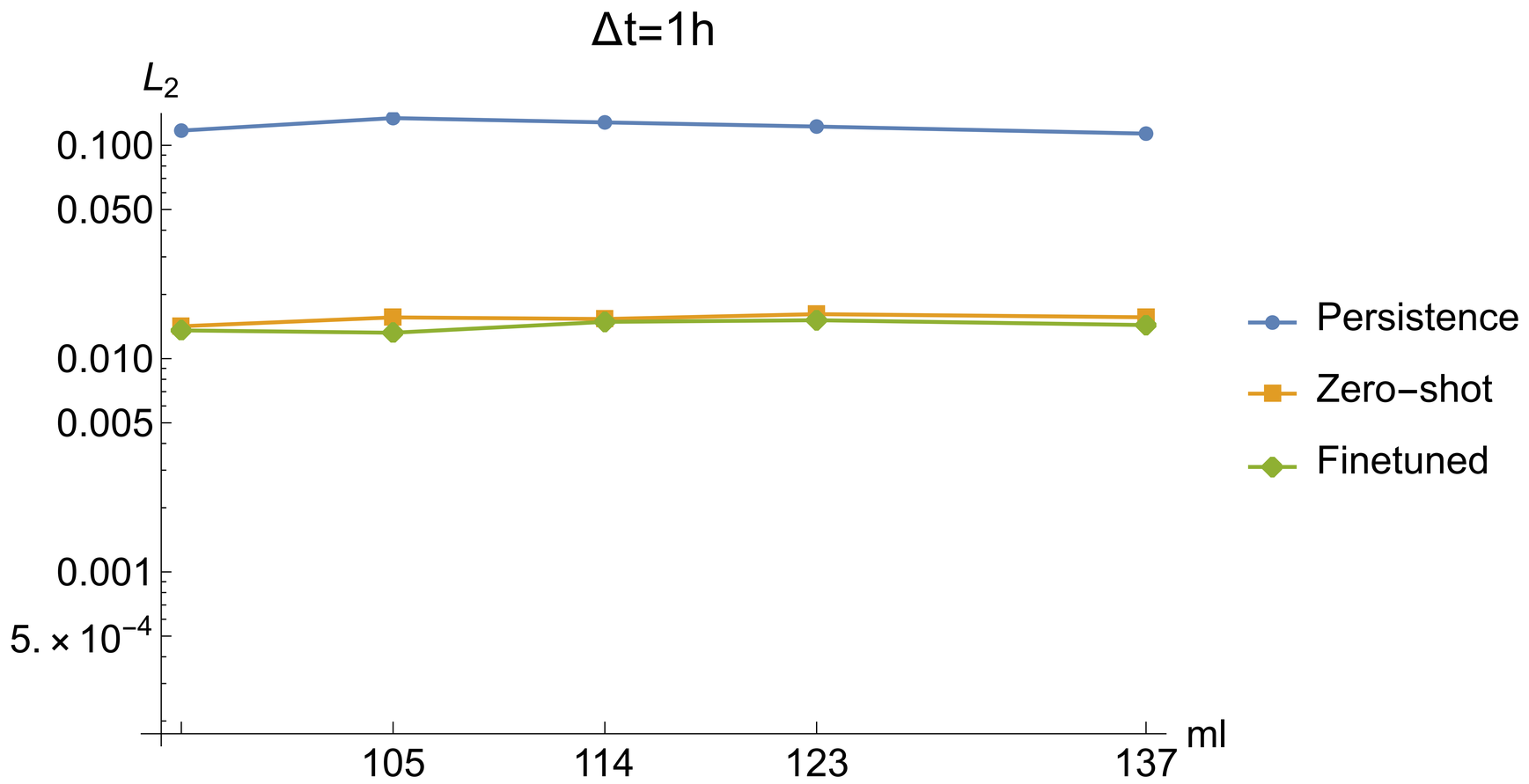
Temporal interpolation



Training task:

predict randomly masked neighbor-hoods in space-time

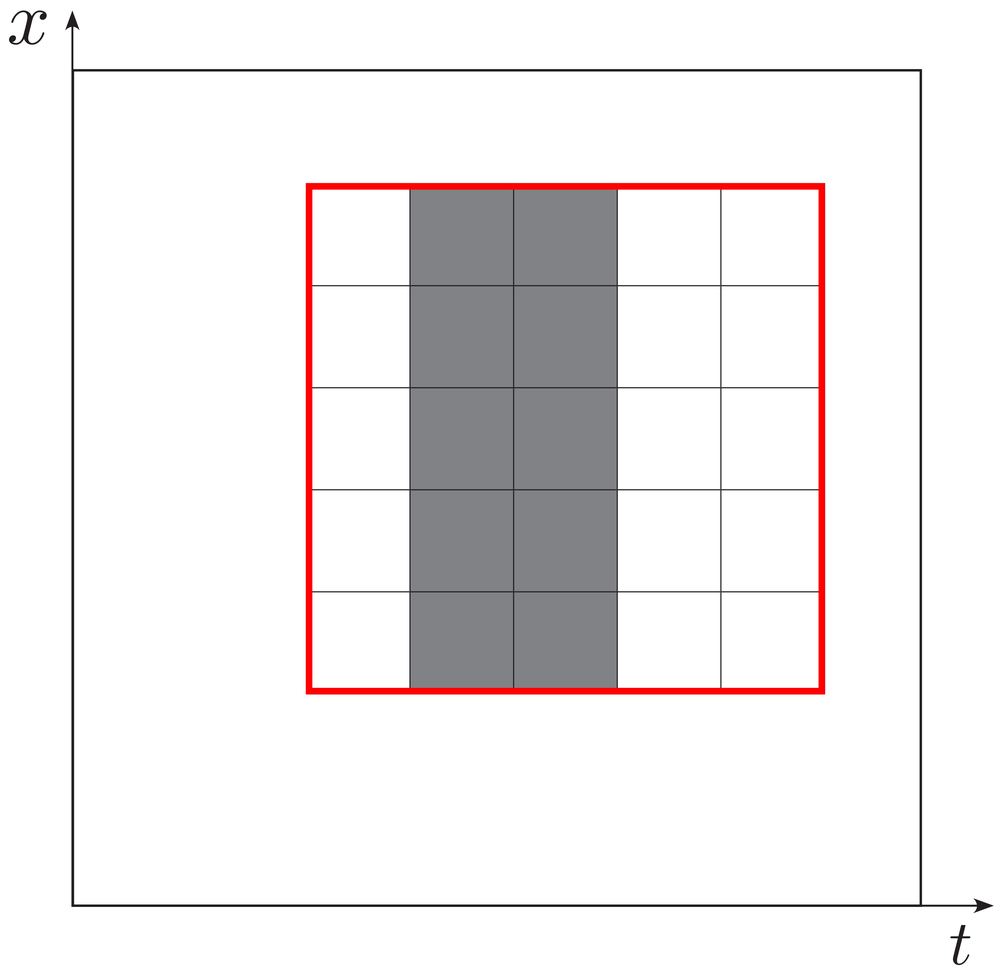
Zero-shot capabilities



Zero-shot capabilities

Also:

- spatial interpolation (missing data)
- downscaling
- ...



Training task:

predict randomly masked neighborhoods in space-time

Model correction

- Numerical statistical atmospheric model:

$$p_\theta\left(y|x,\alpha\right)$$

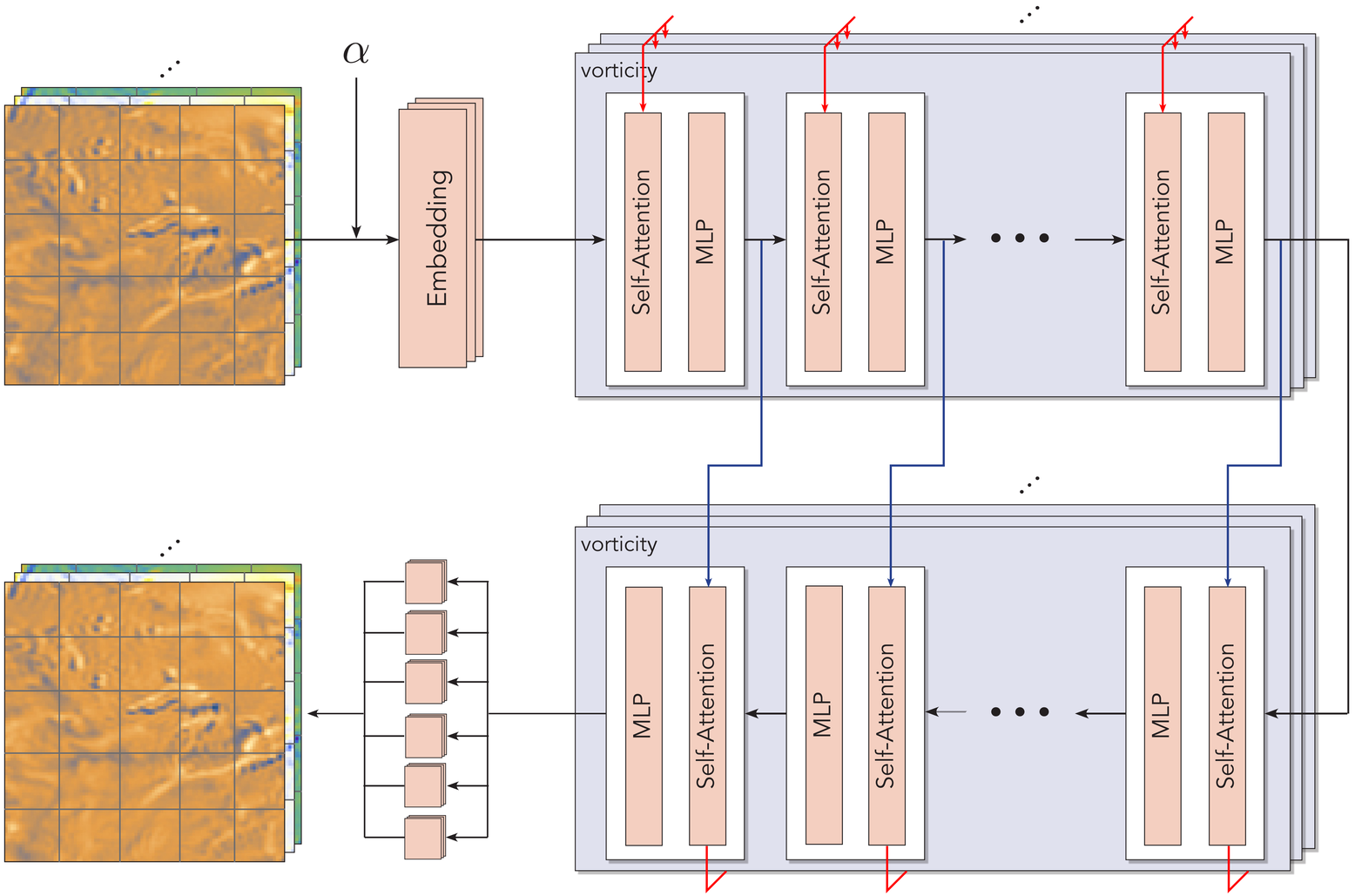
Model correction

- Numerical statistical atmospheric model:

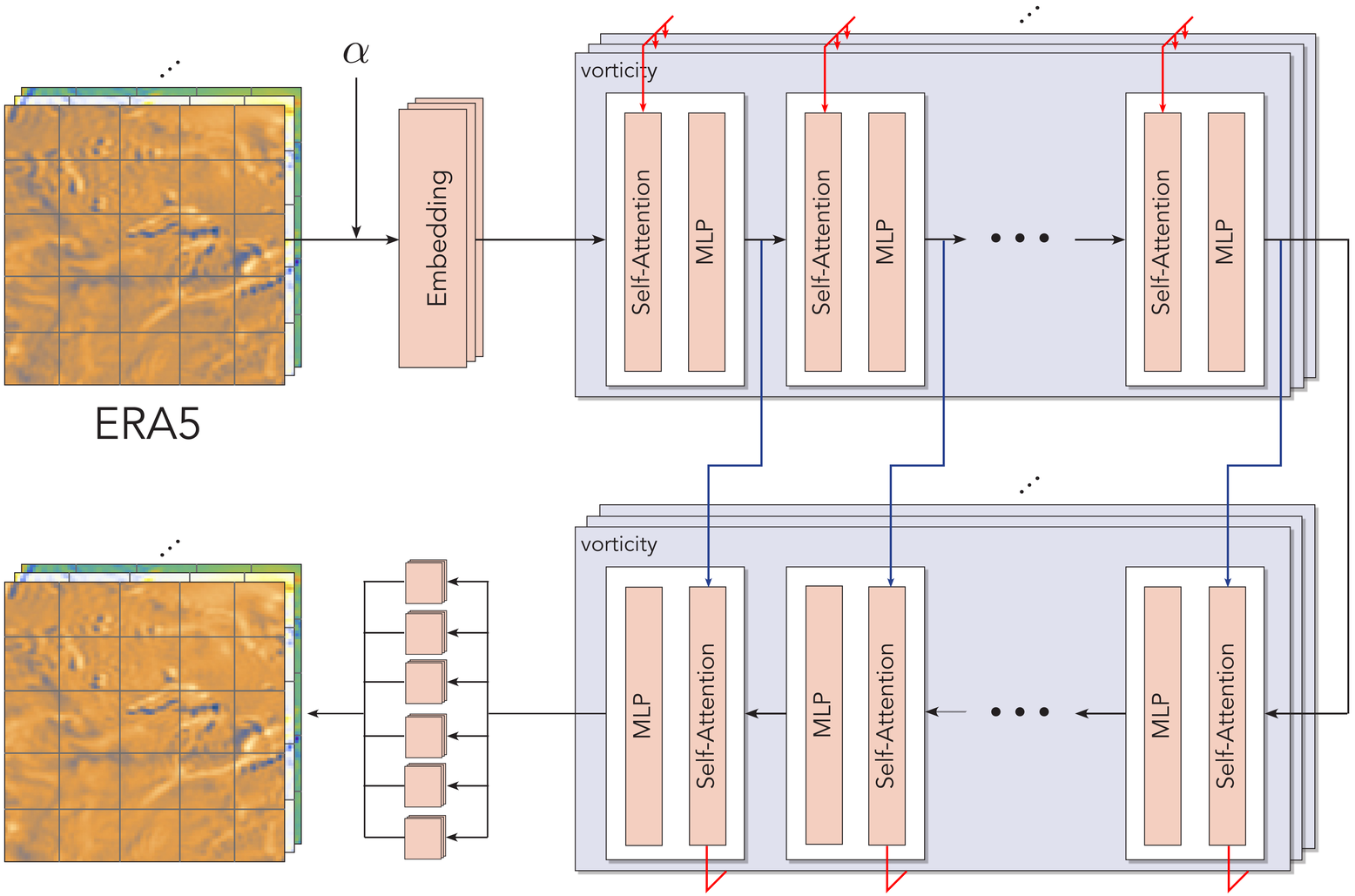
$$p_\theta\left(y|x,\alpha\right)$$

approximate initial state

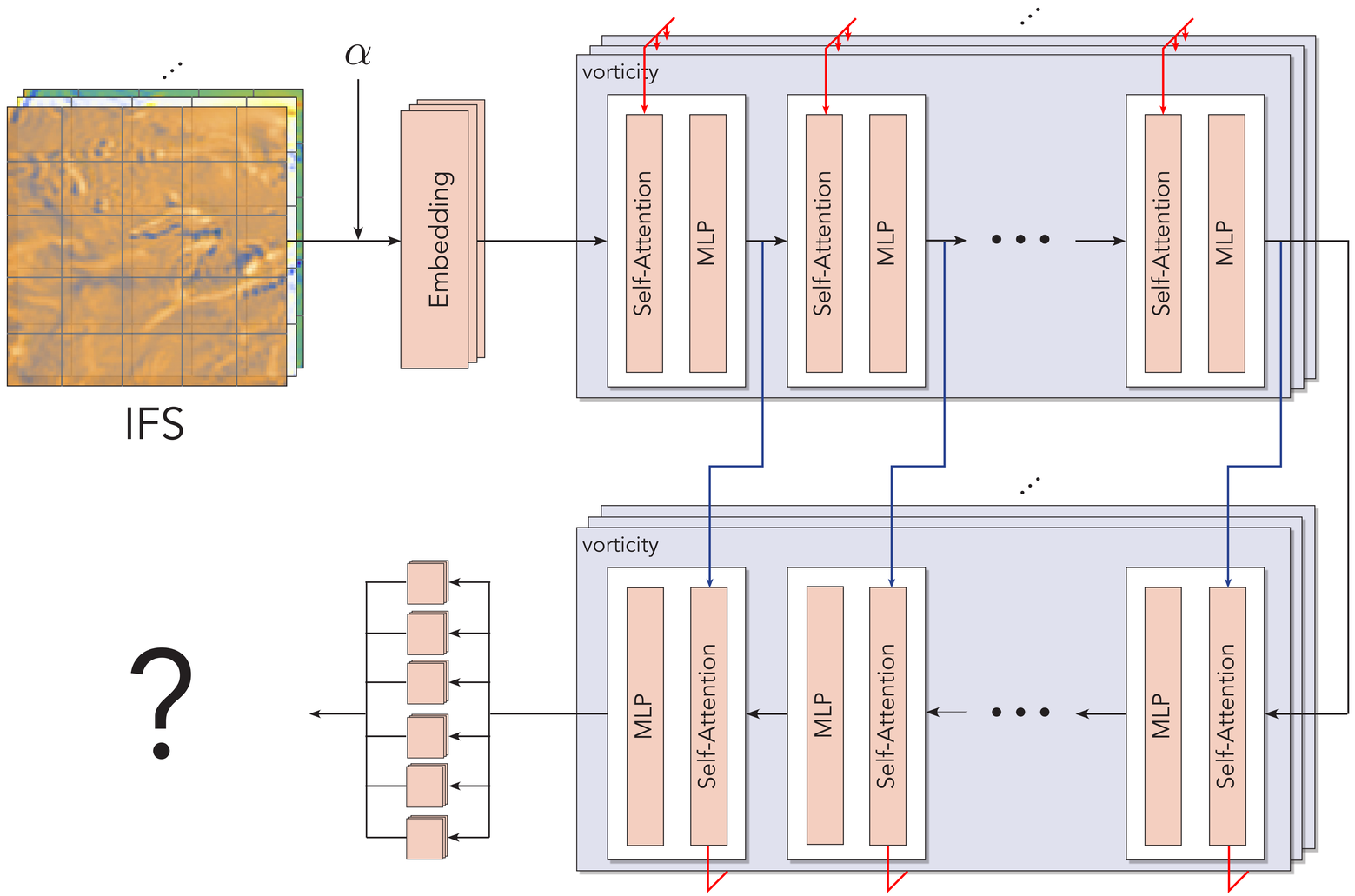
Model correction



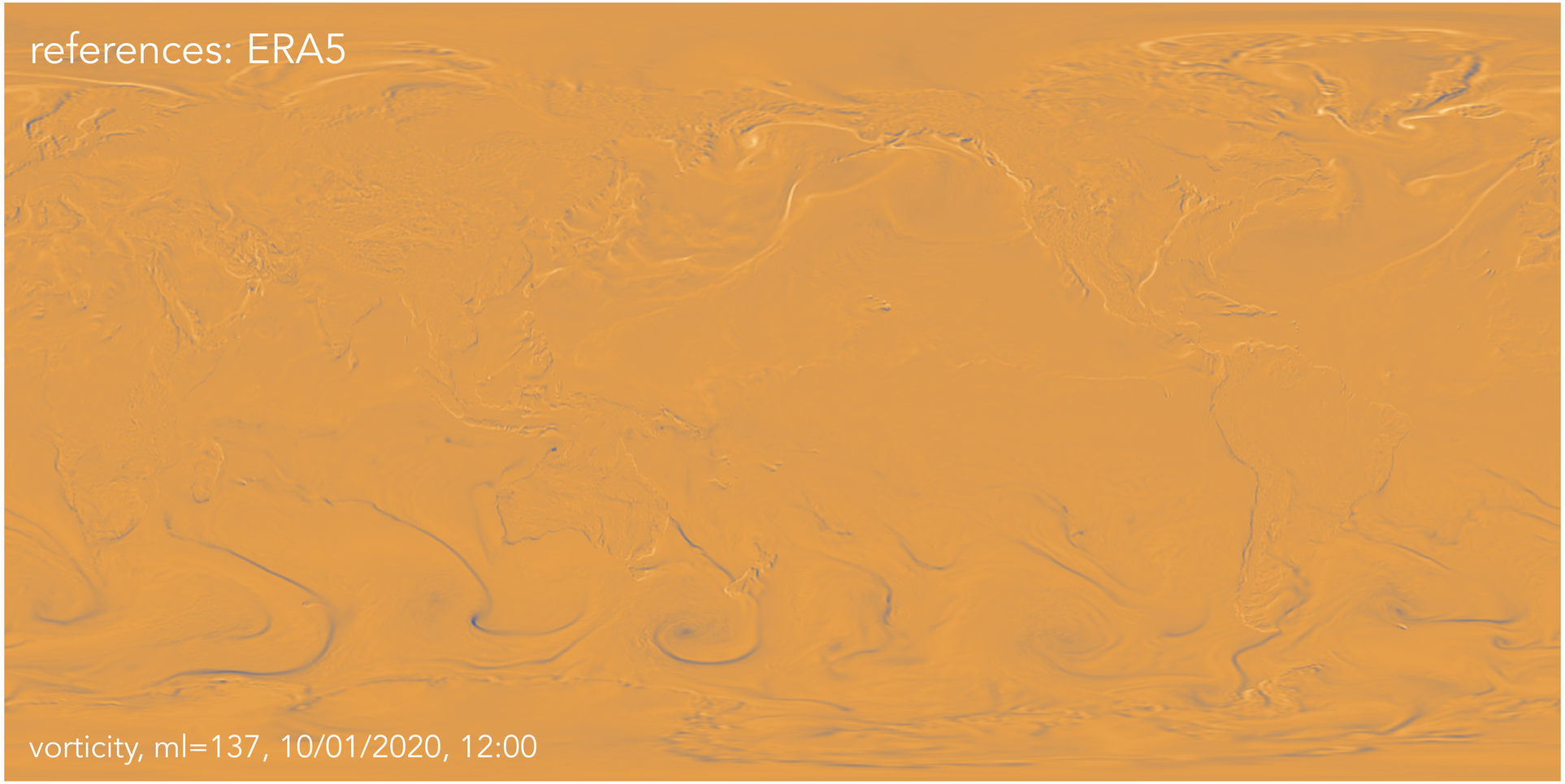
Model correction



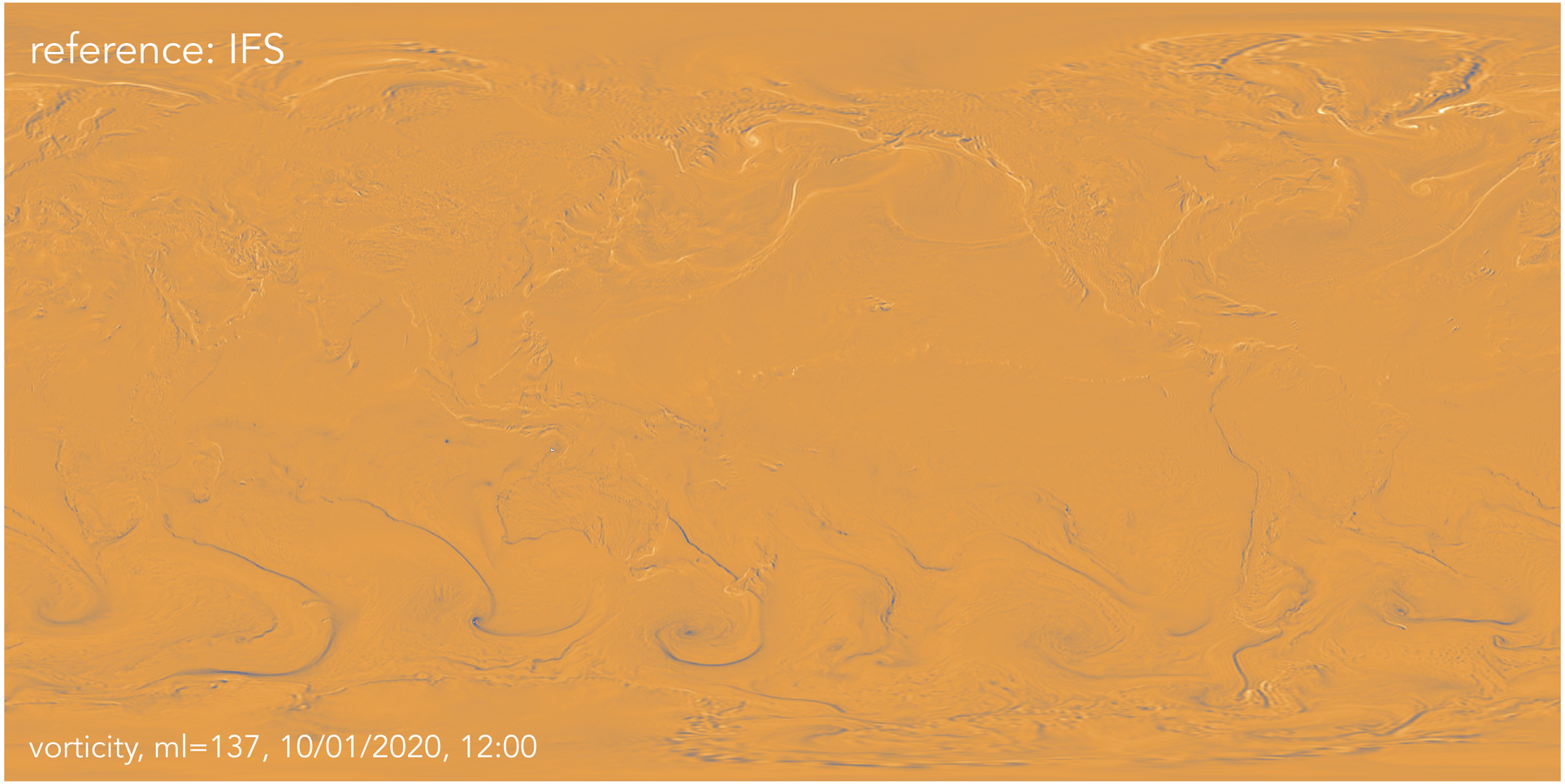
Model correction



Model correction



Model correction



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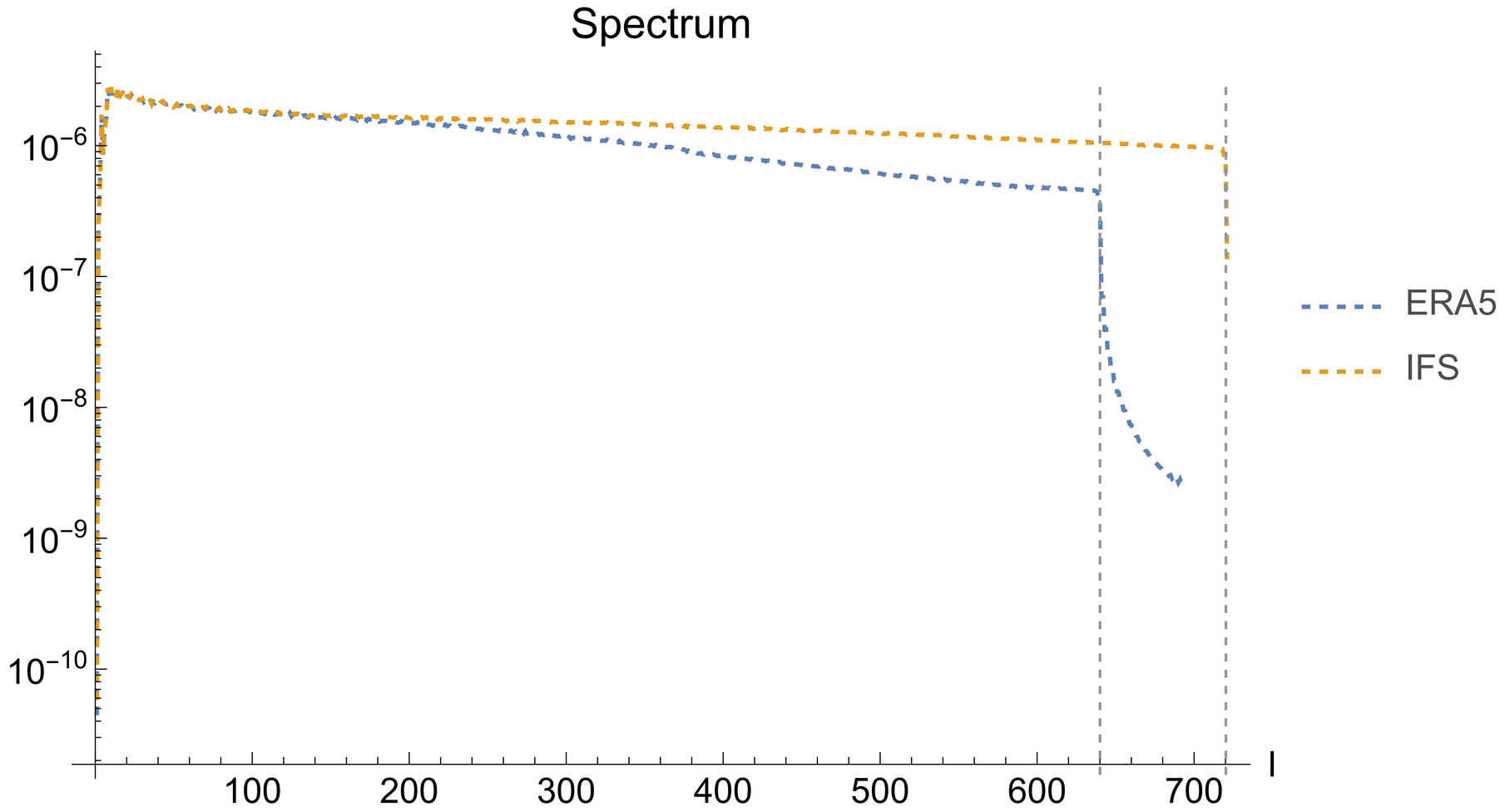

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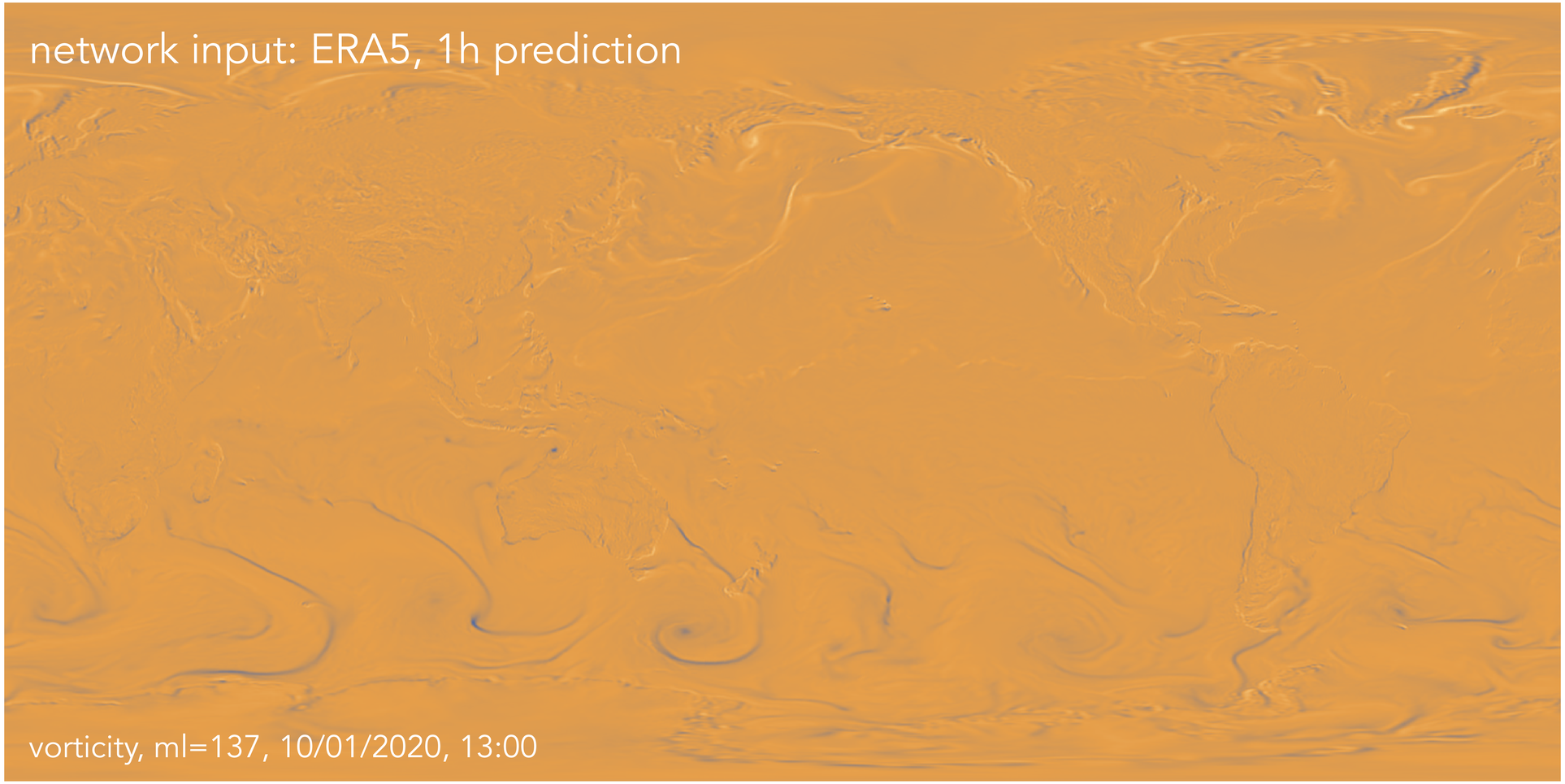

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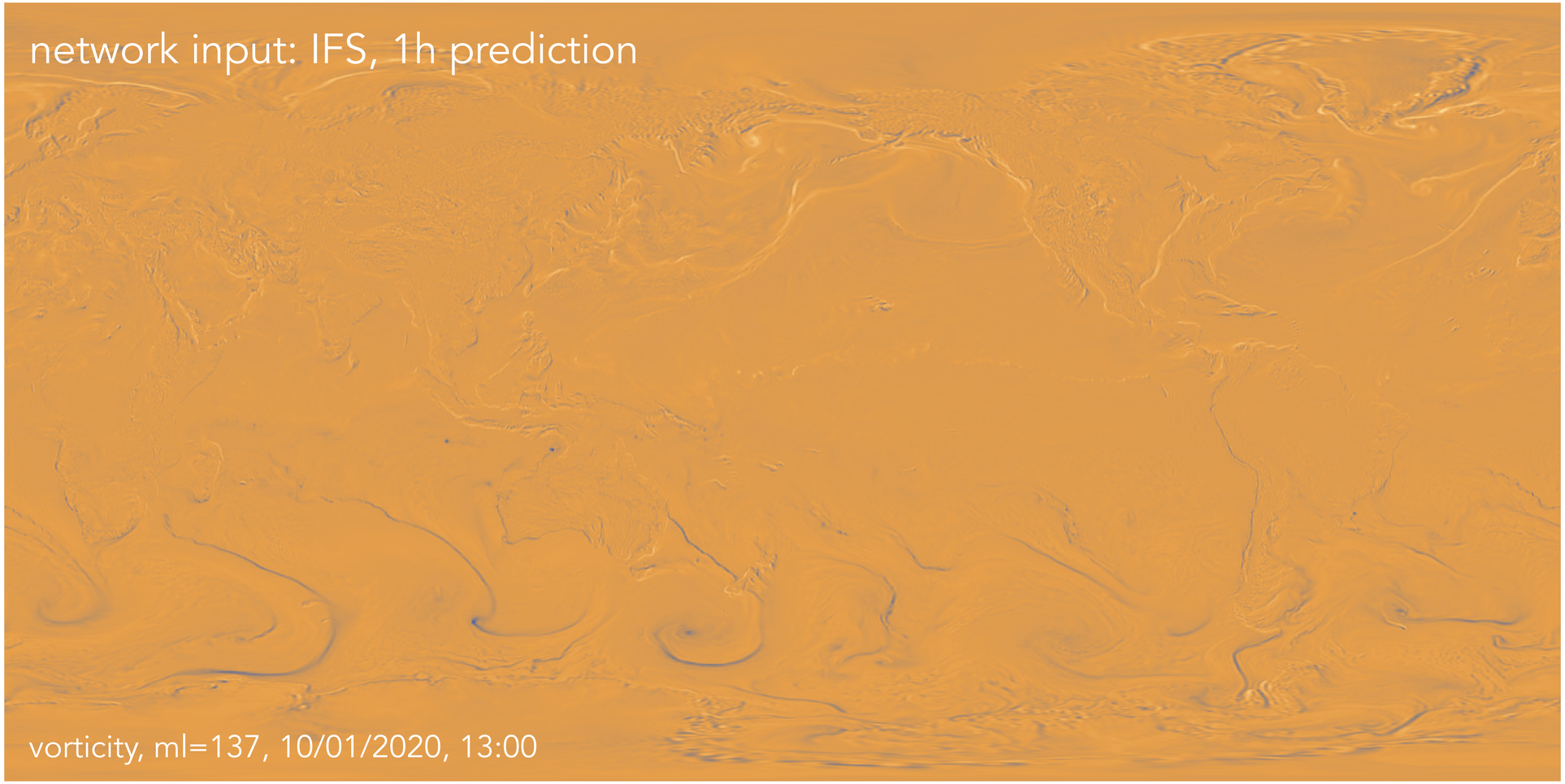
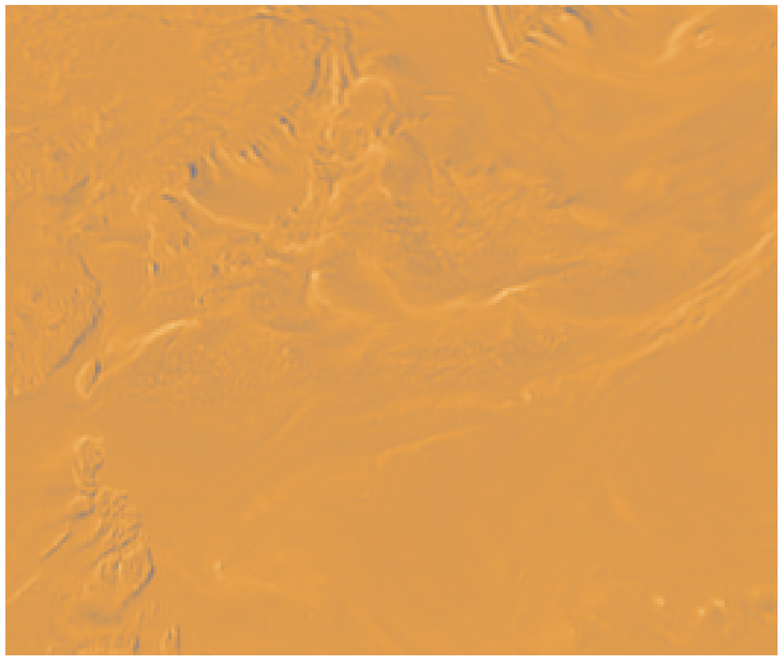


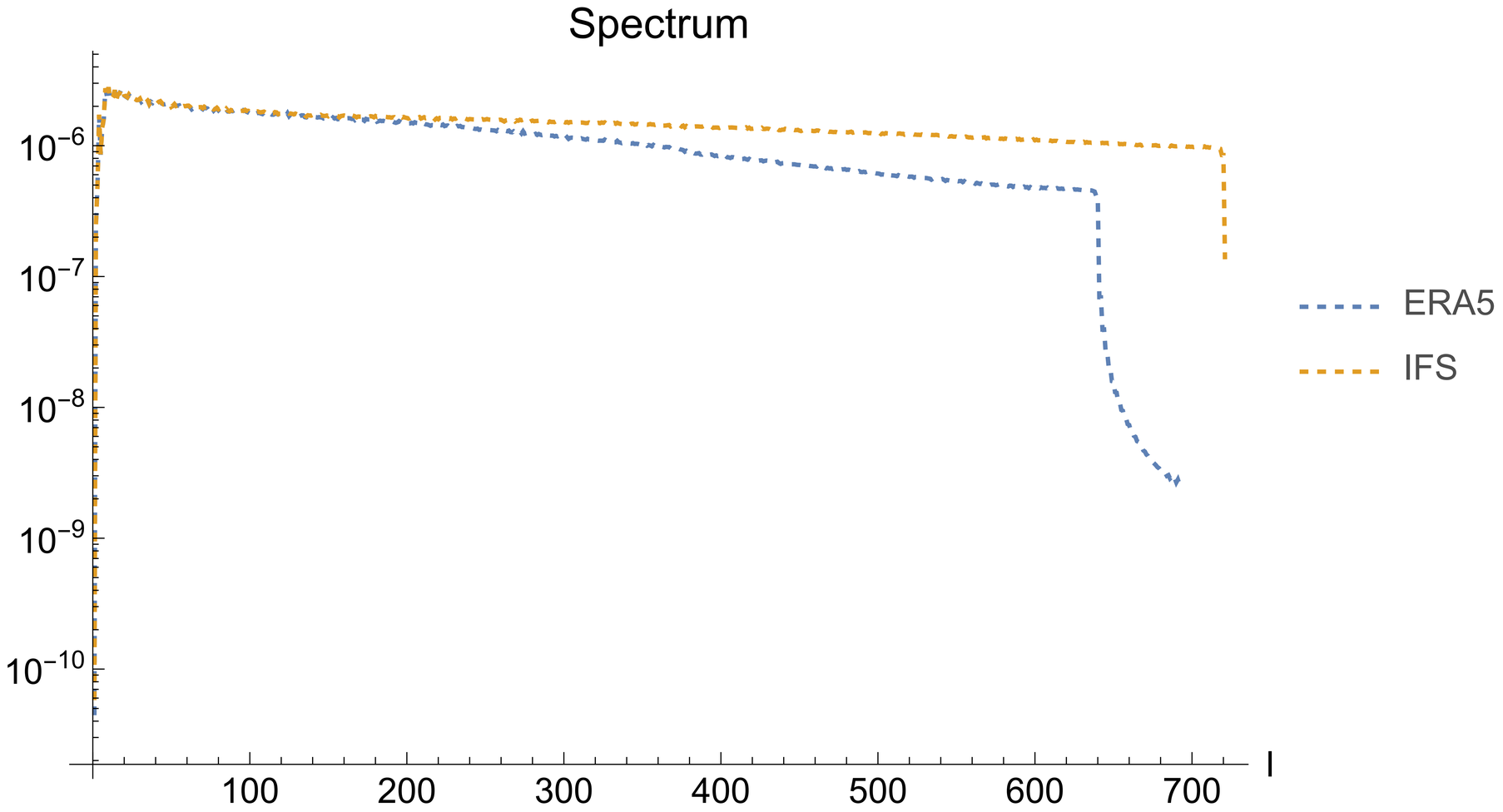
Model correction

network input: ERA5

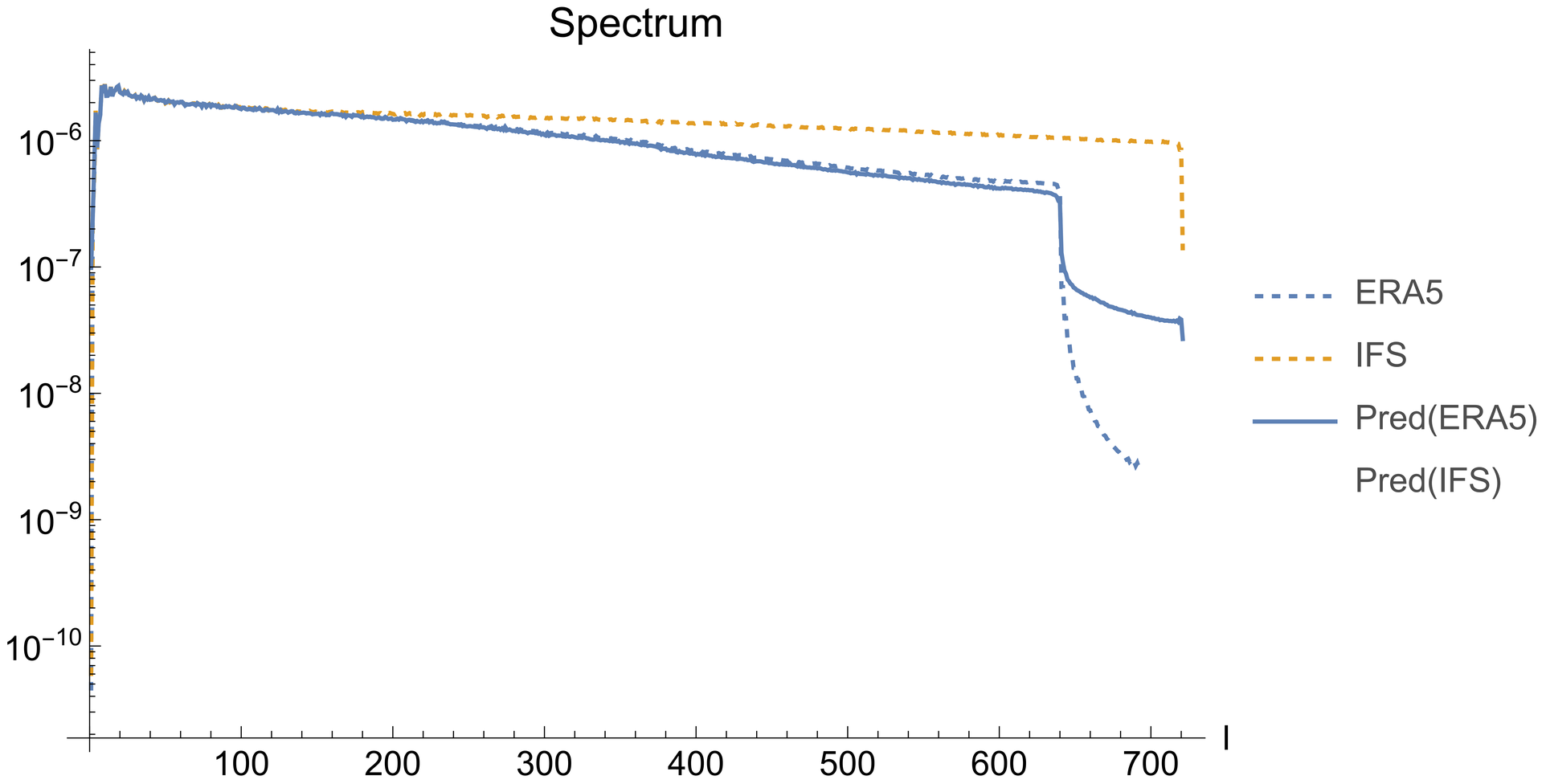
network input: IFS



Model correction



Model correction



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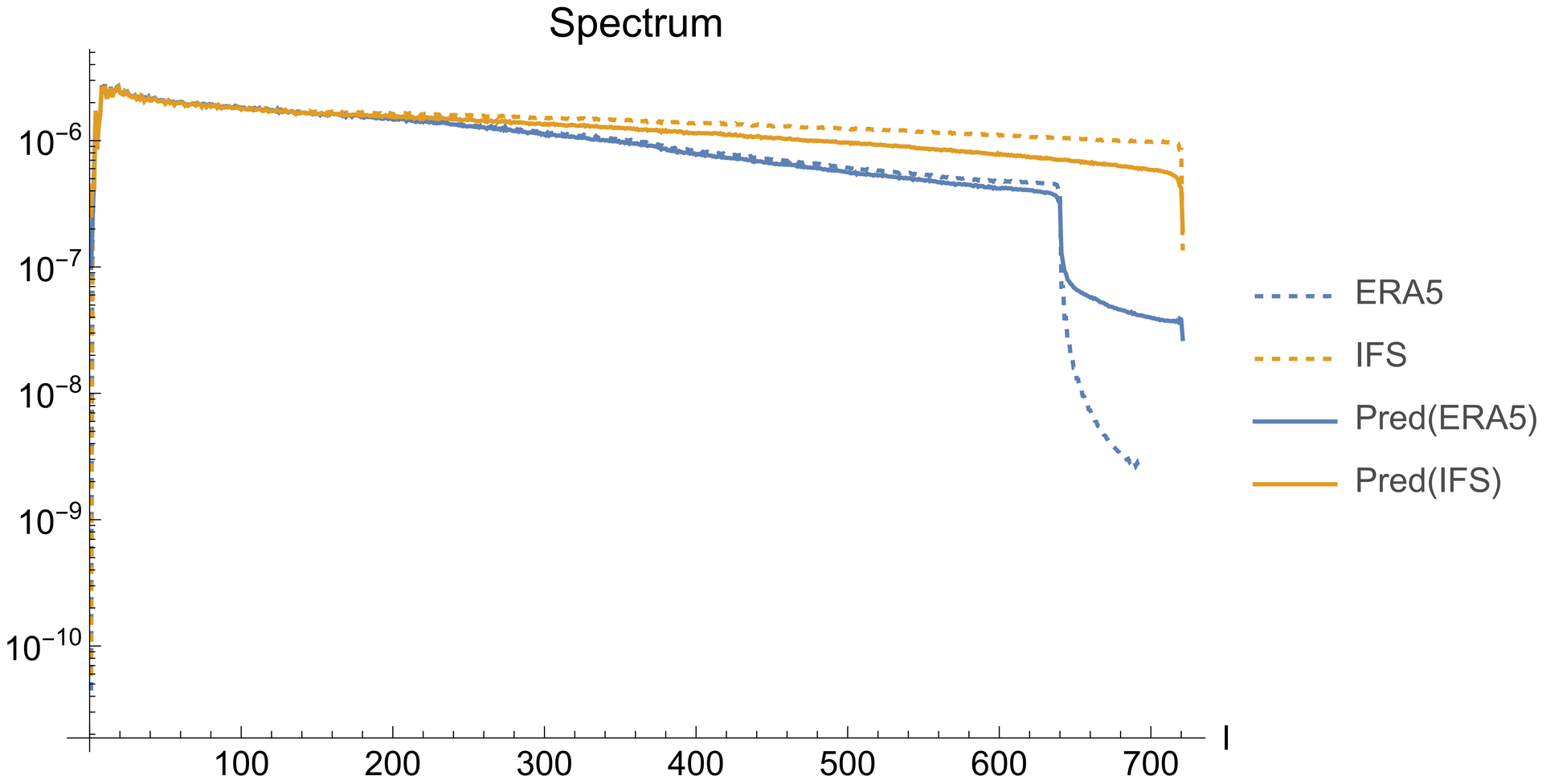

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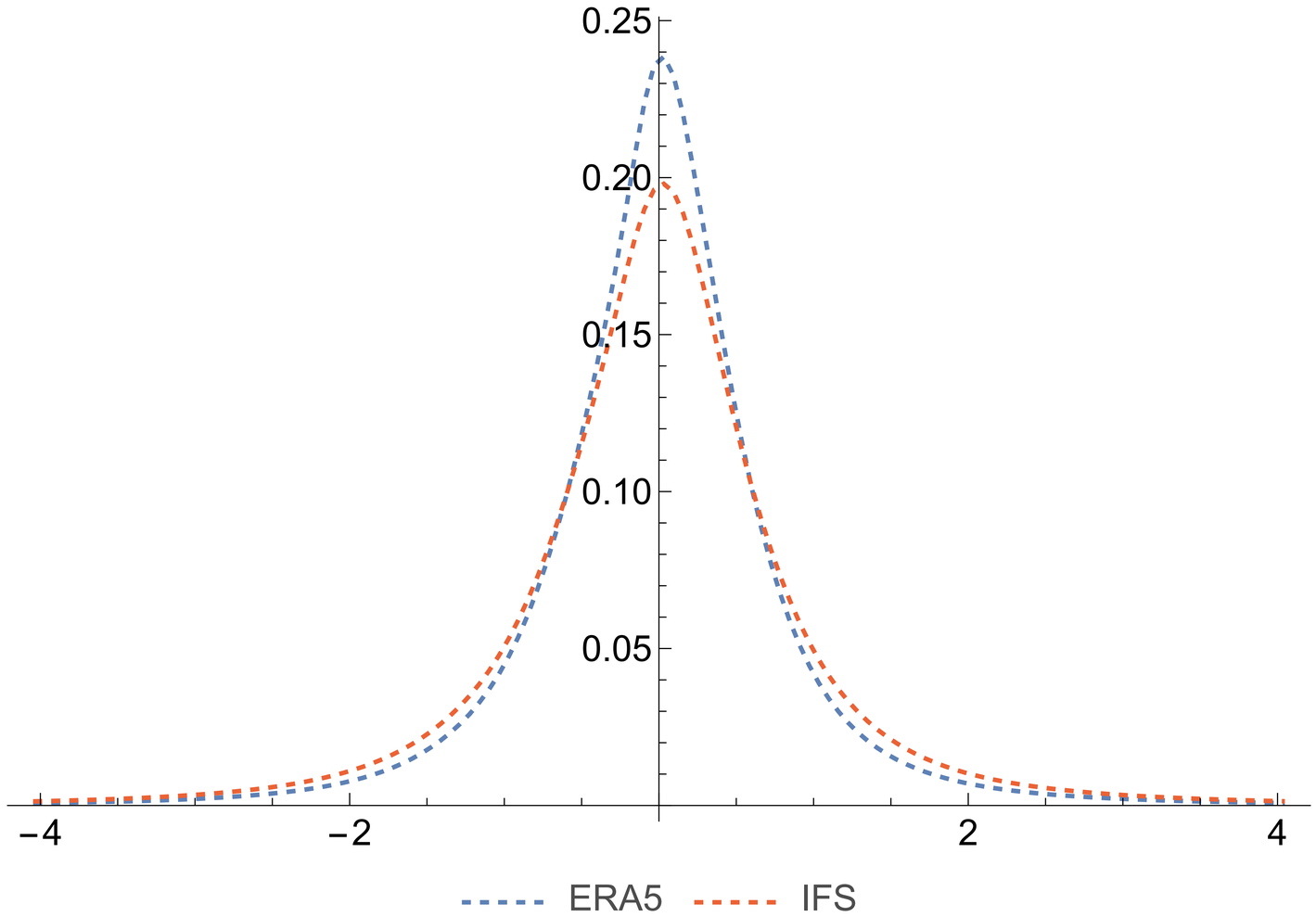

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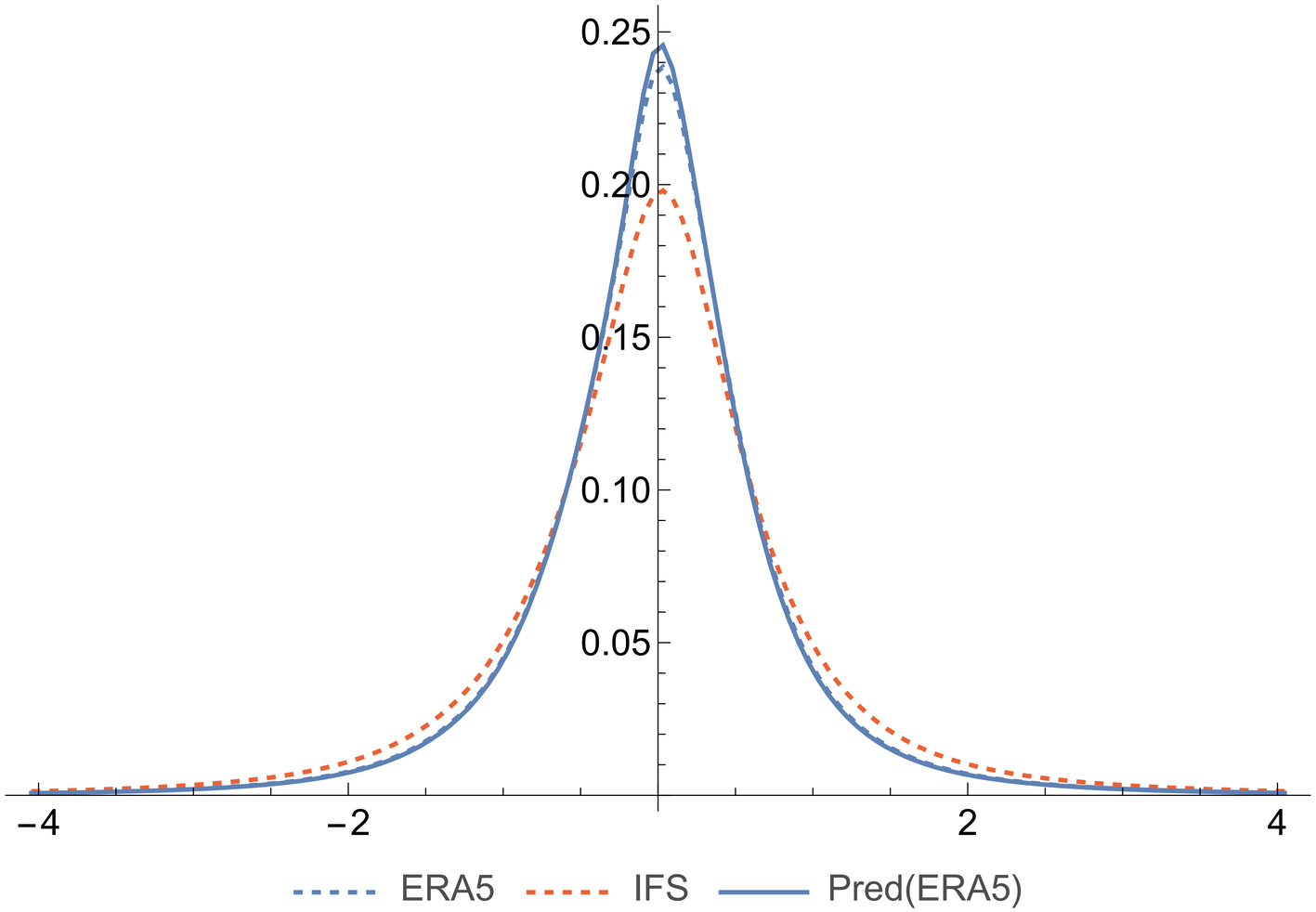

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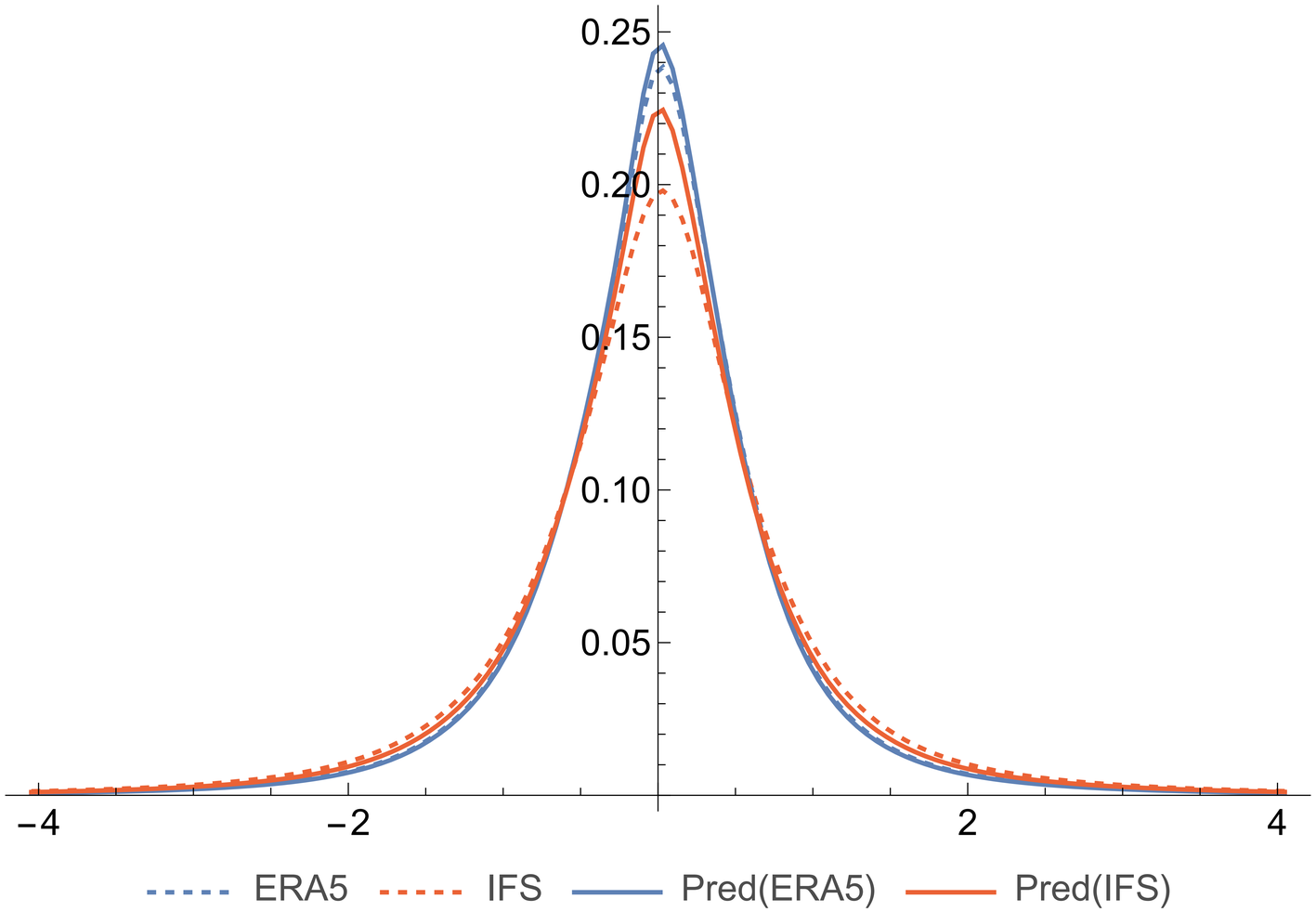


Counterfactuals

- Numerical statistical atmospheric model:

$$p_\theta\left(y|x,\alpha\right)$$

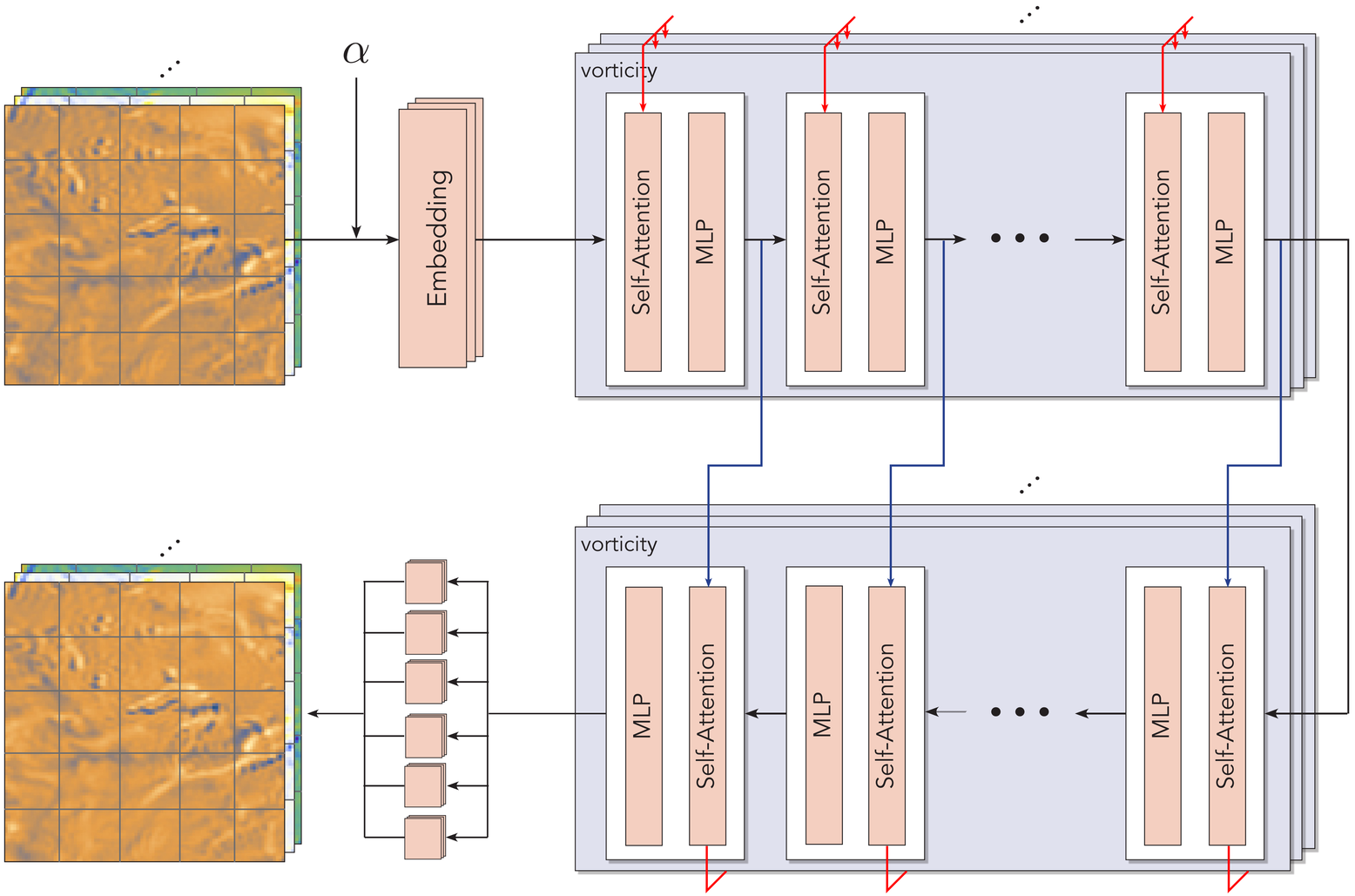
Counterfactuals

- Numerical statistical atmospheric model:

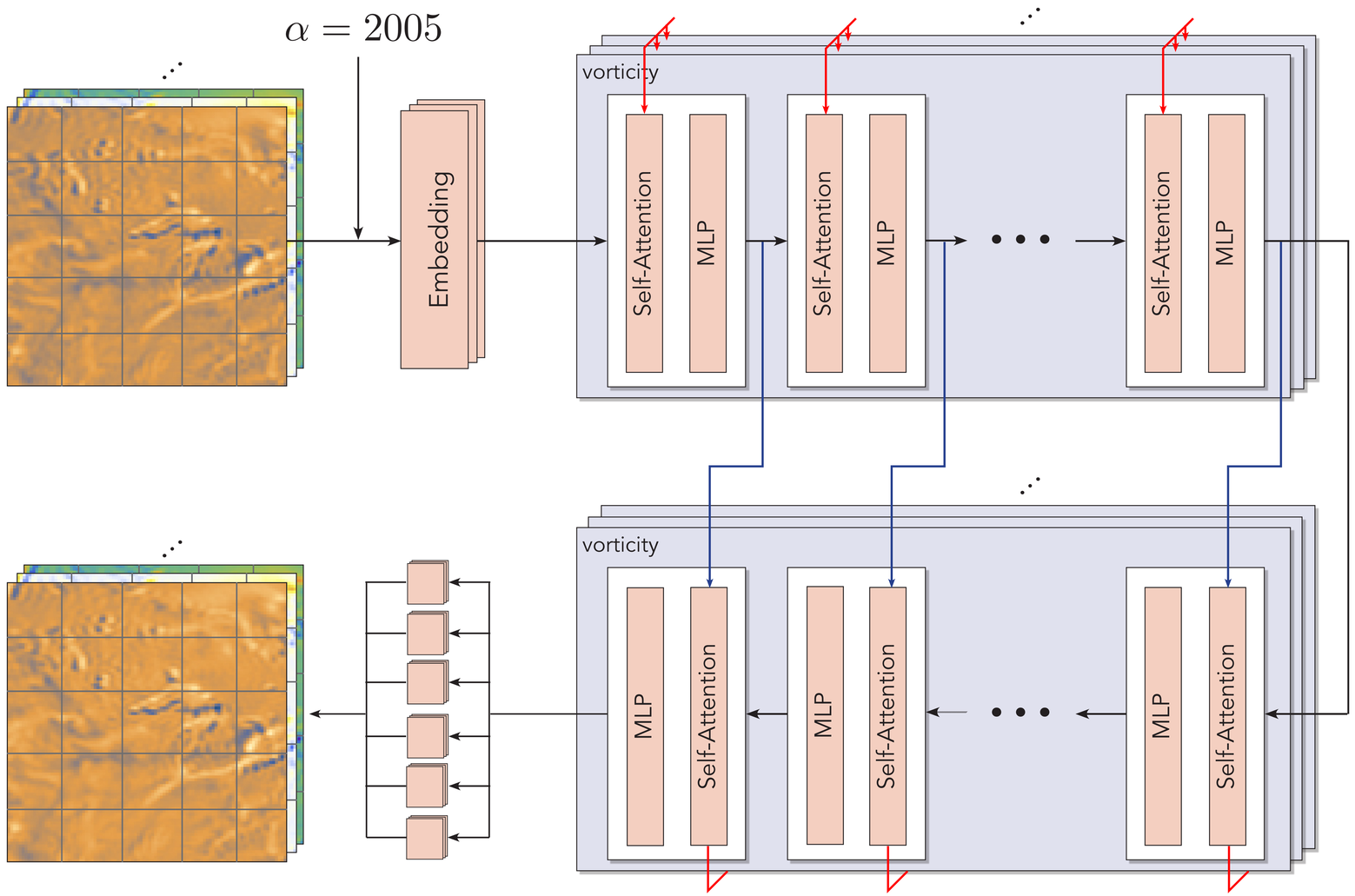
$$p_\theta\left(y|x,\alpha\right)$$

$$\alpha = \left(\mathrm{year}, \mathrm{day}, \mathrm{hour}, \mathrm{ml}, \theta, \phi, \mathrm{res}\right)$$

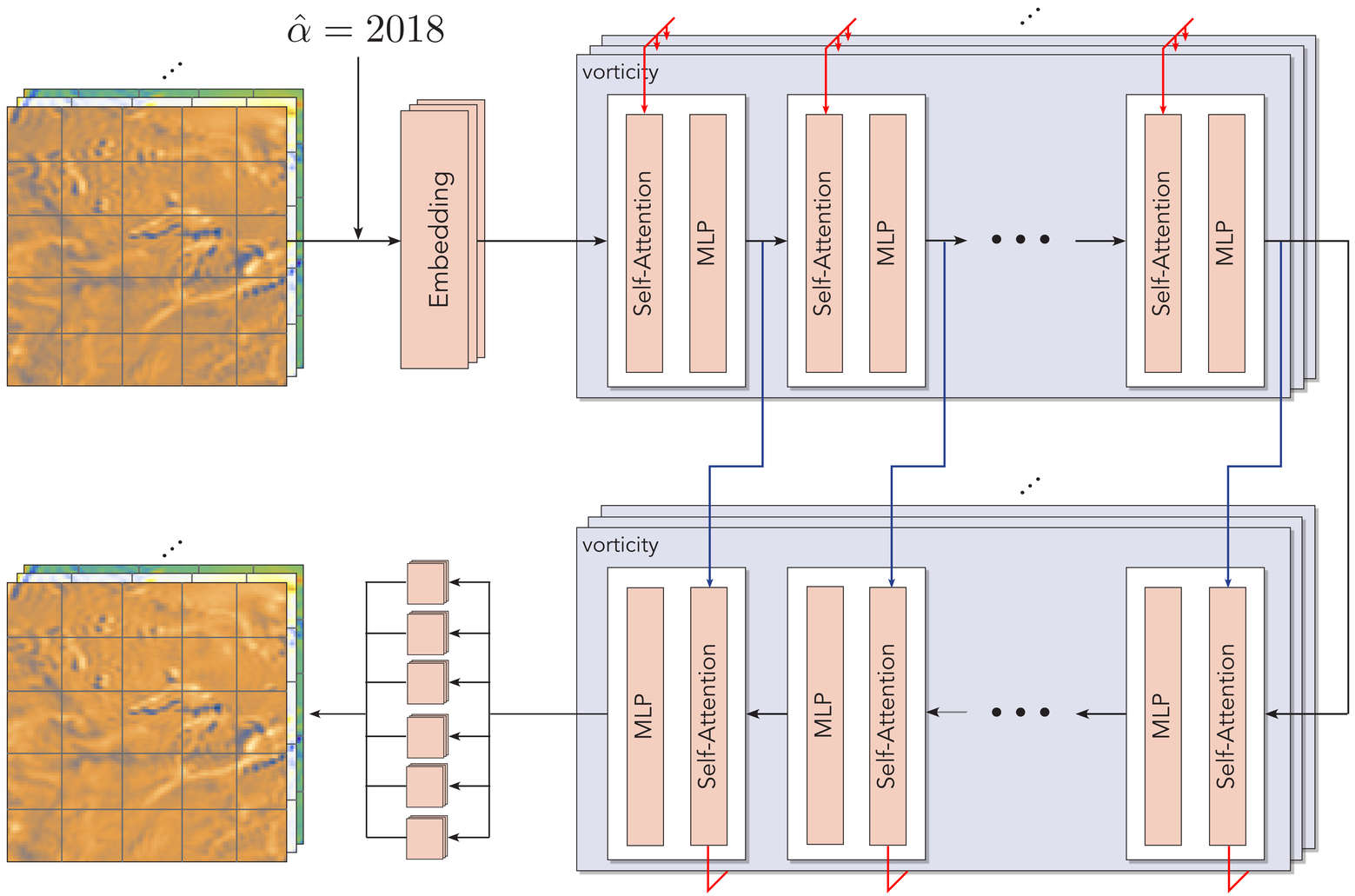
Counterfactuals



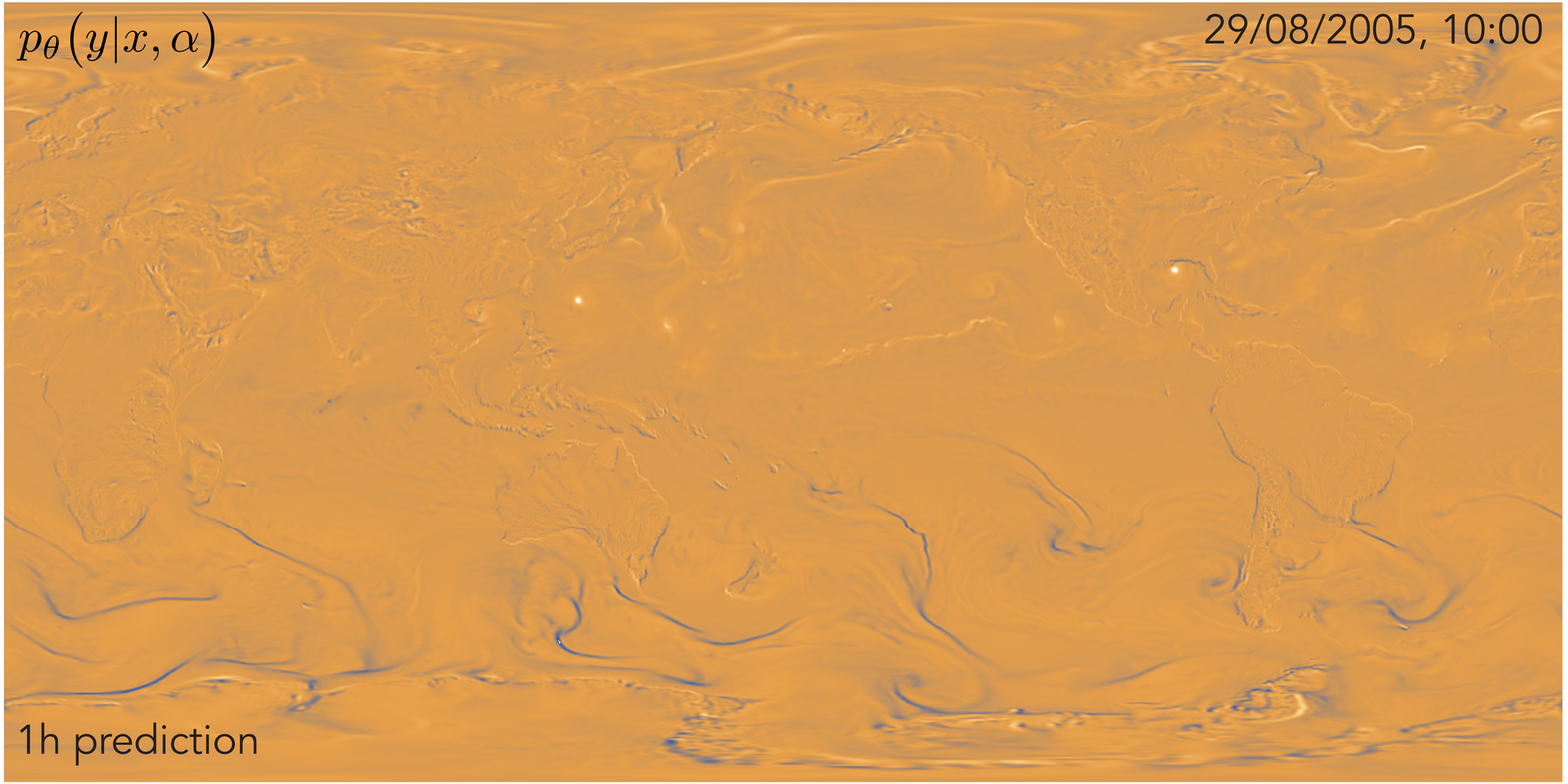
Counterfactuals



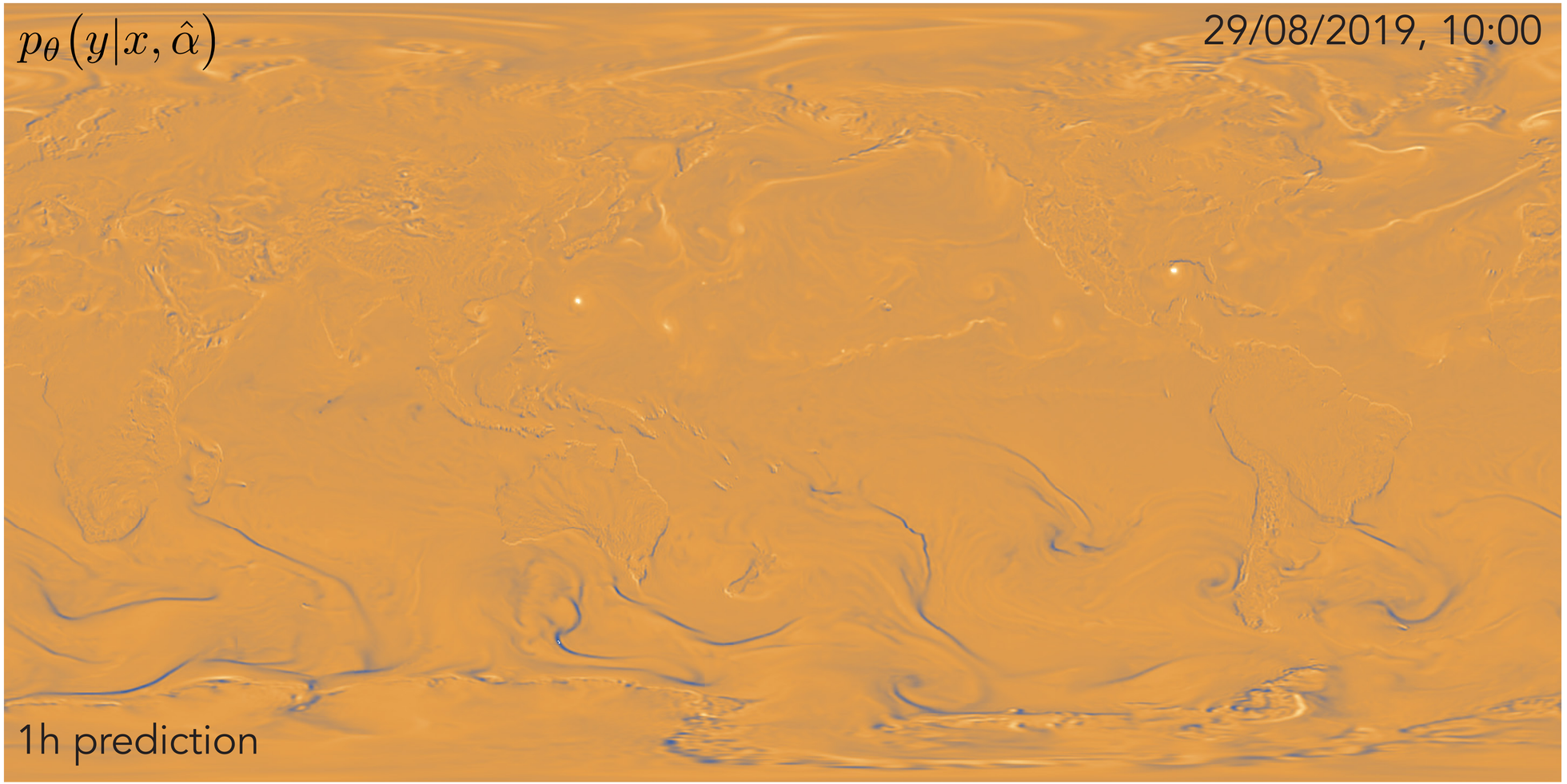
Counterfactuals



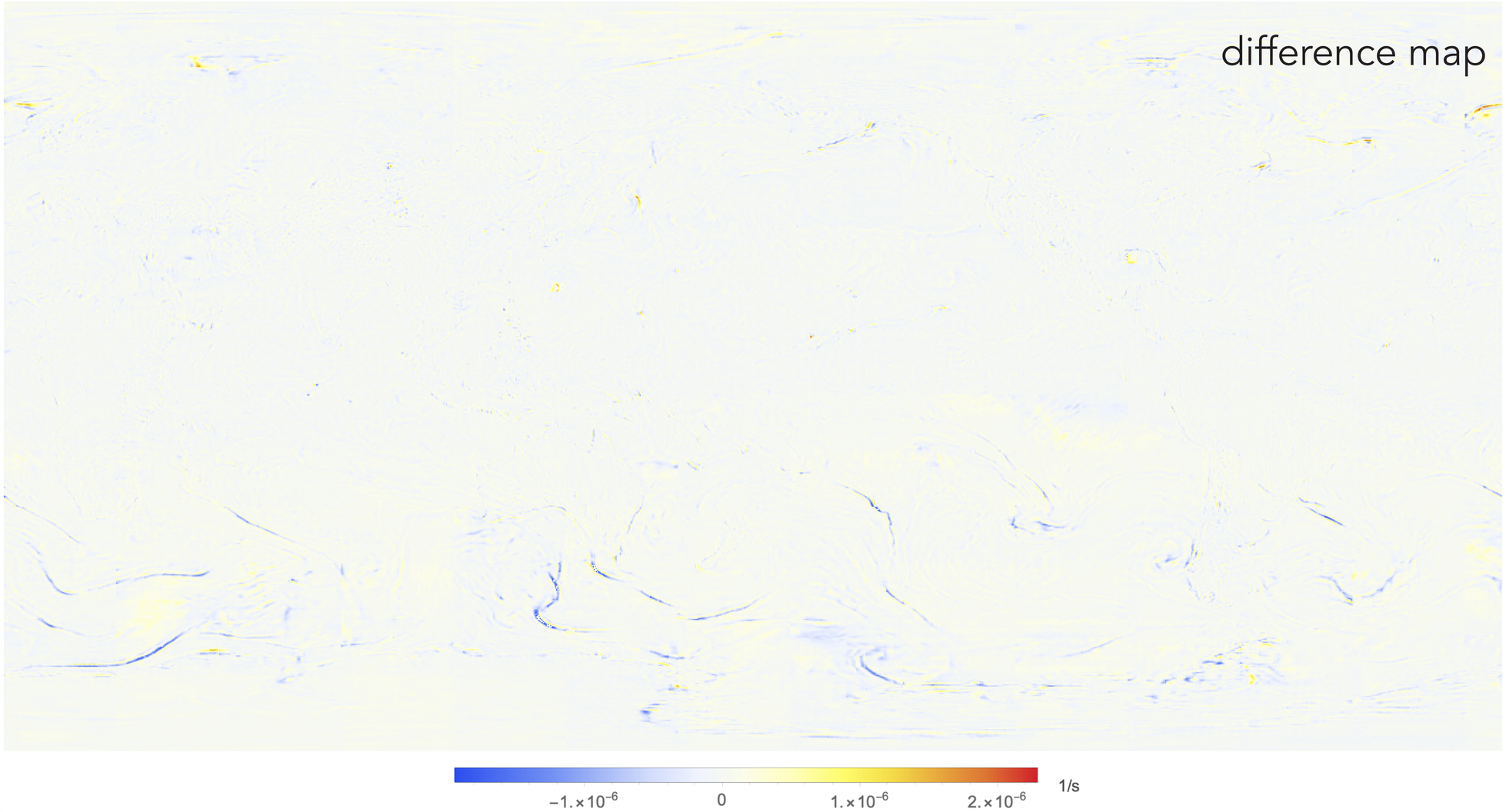
Counterfactuals



Counterfactuals



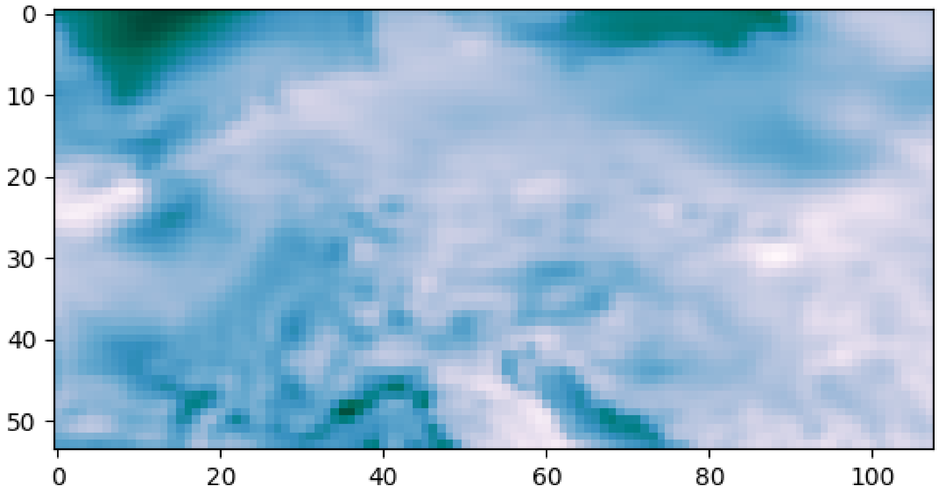
Counterfactuals



Downstream applications

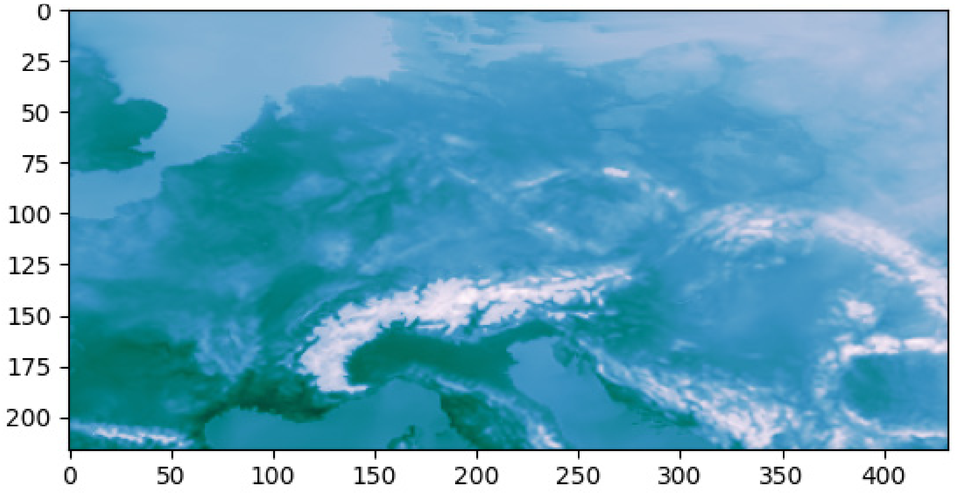
Downscaling

ERA5



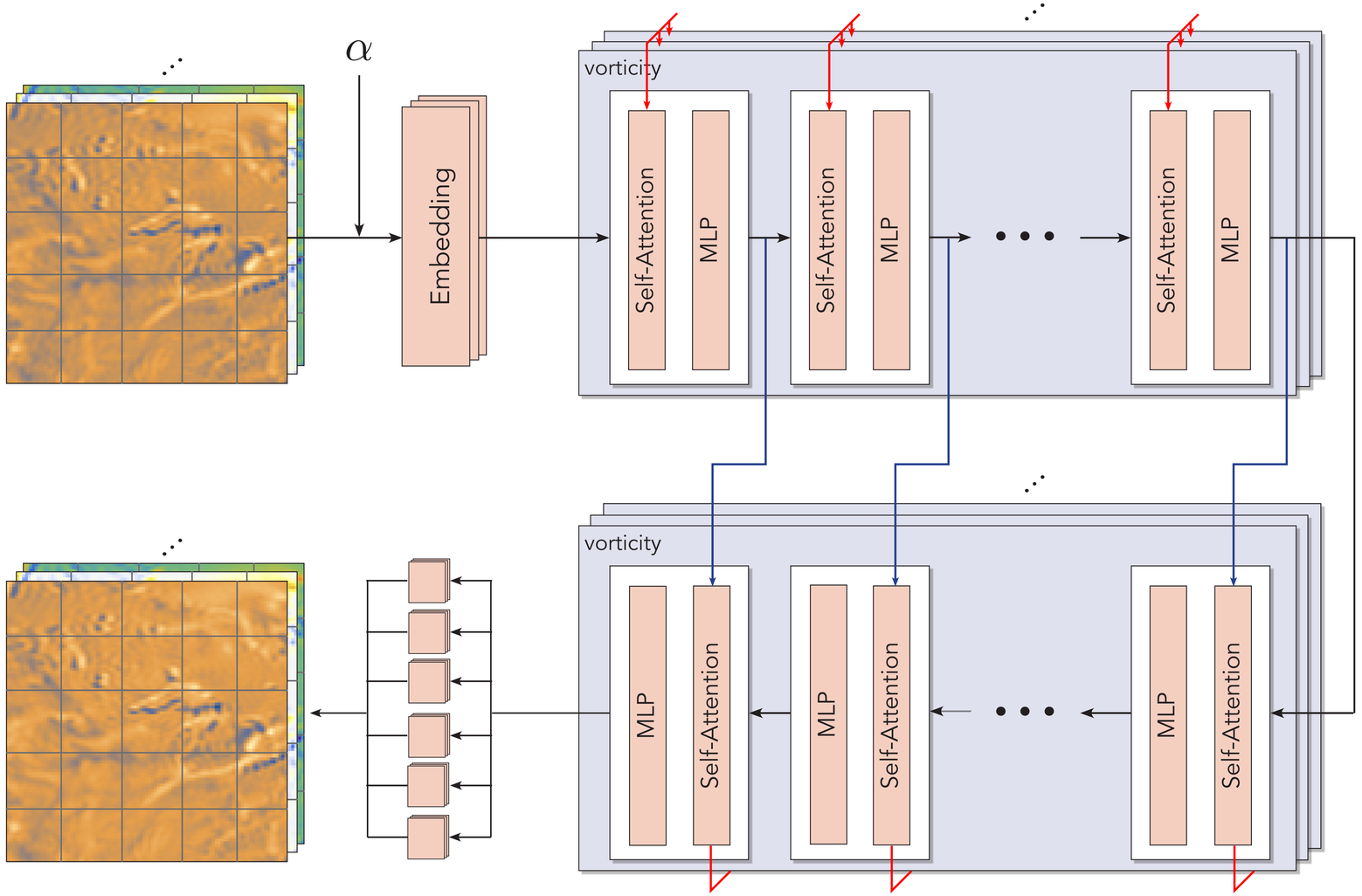
temperature, ml=137

COSMO-REA6

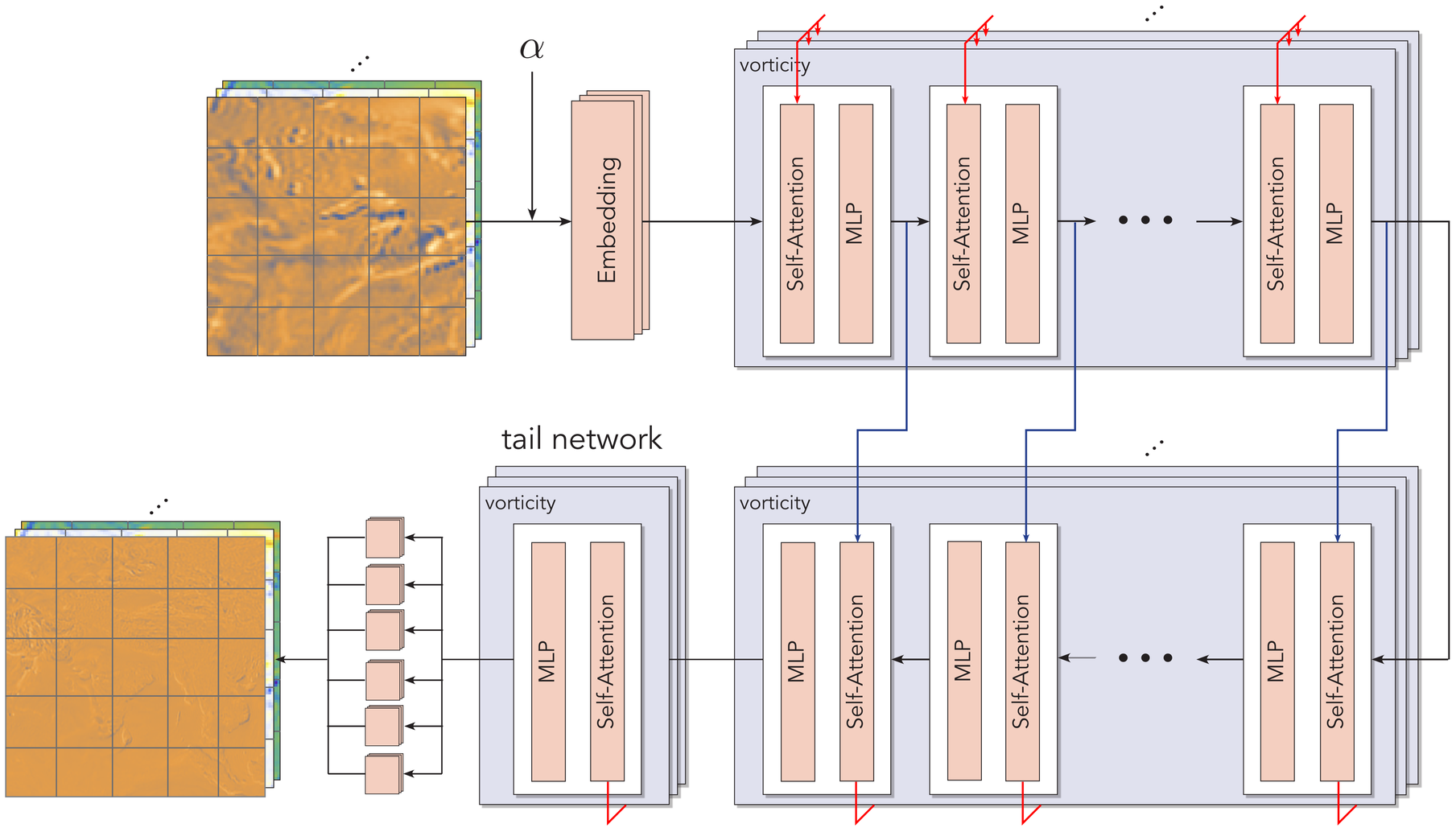


temperature, 2 m

Downscaling



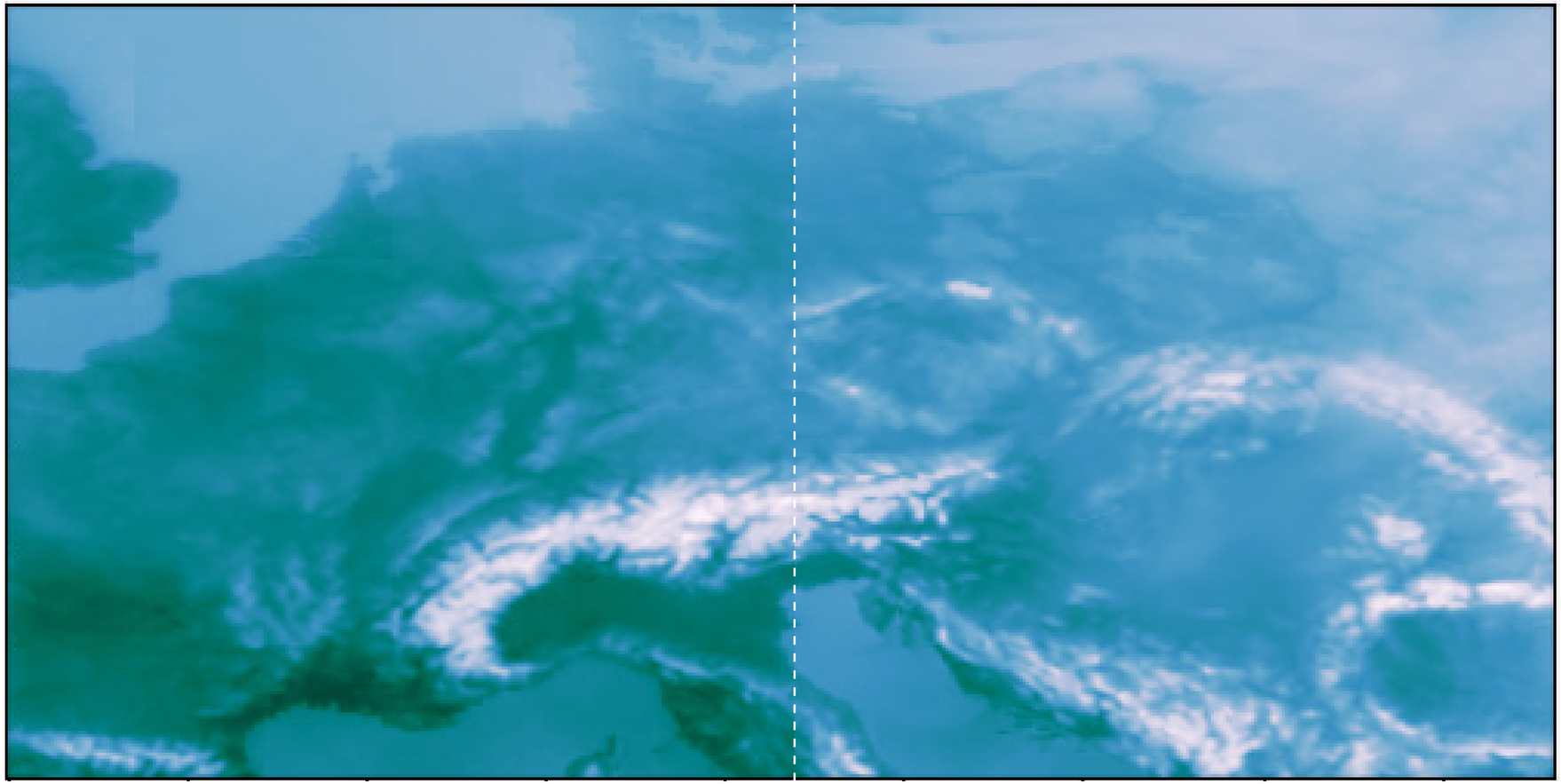
Downscaling



Downscaling

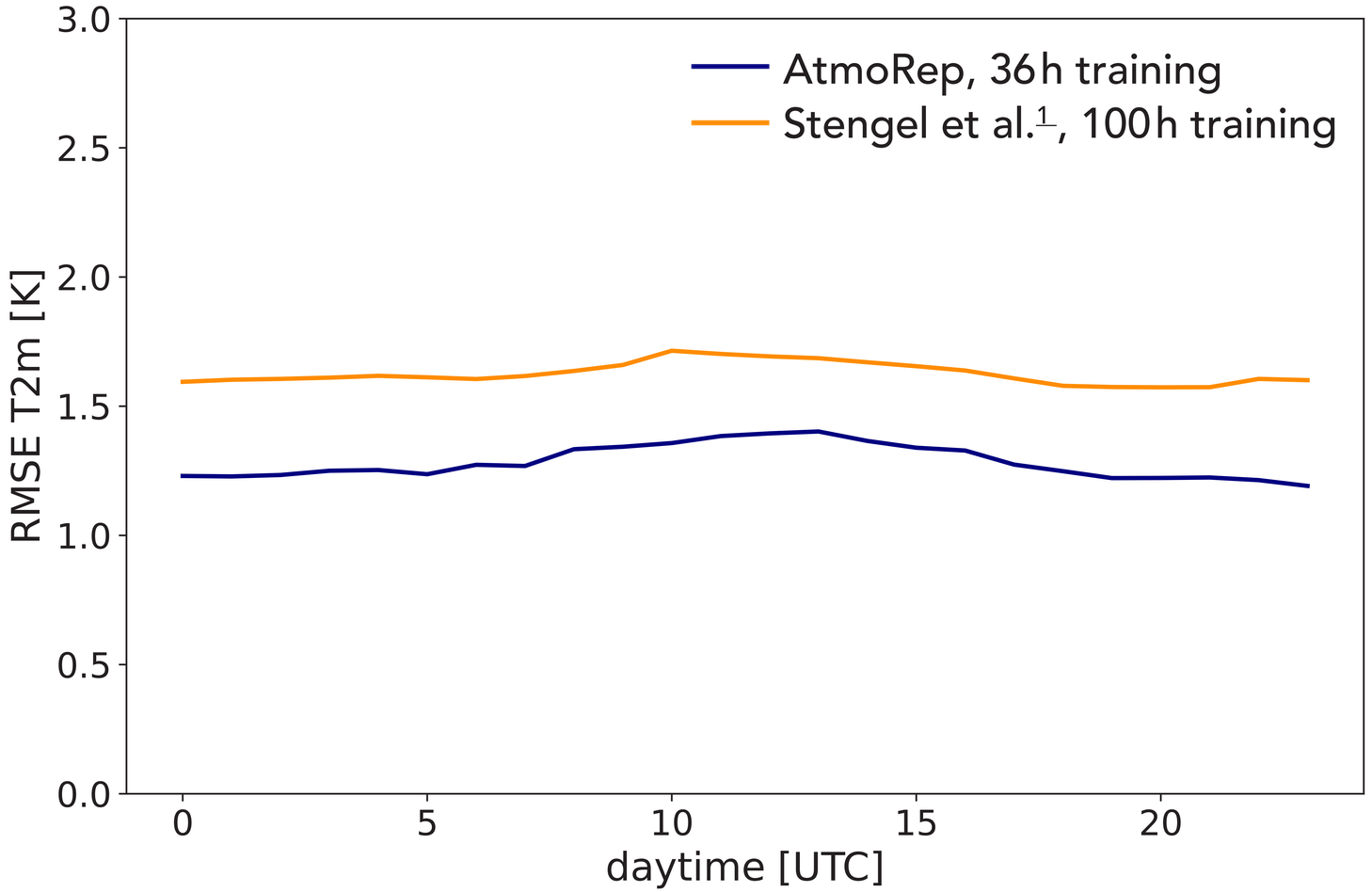
AtmoRep prediction

COSMO-REA6



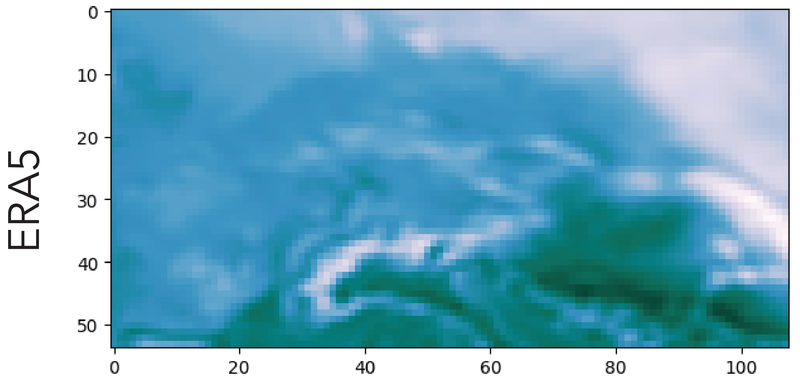
temperature, 2 m

Downscaling

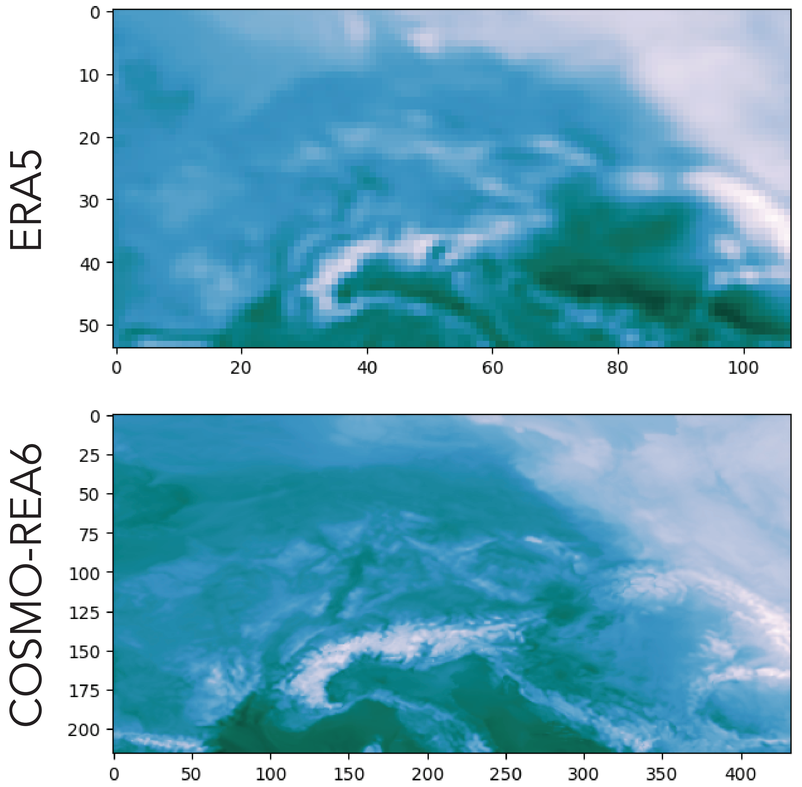


[1] K. Stengel, A. Glaws, D. Hettinger, and R. N. King. Adversarial super-resolution of climatological wind and solar data. Proceedings of the National Academy of Sciences, 117(29):16805–16815, 2020.

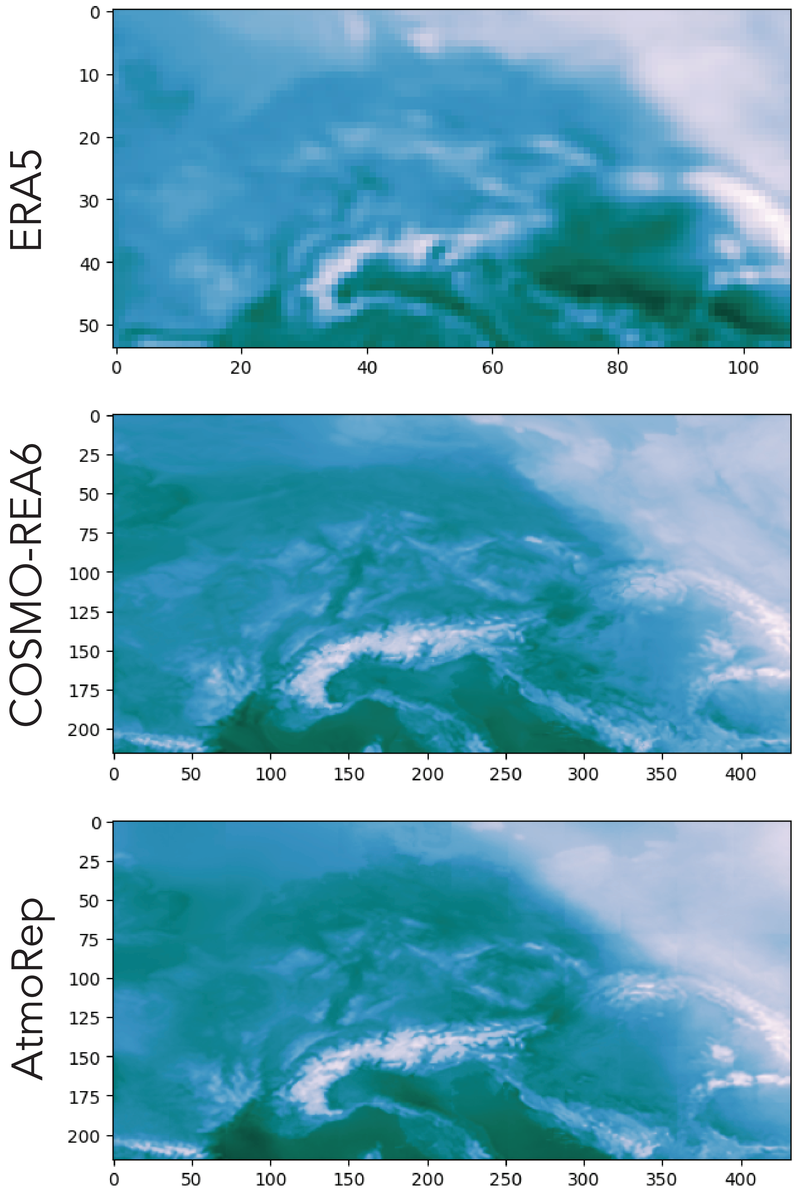
Downscaling



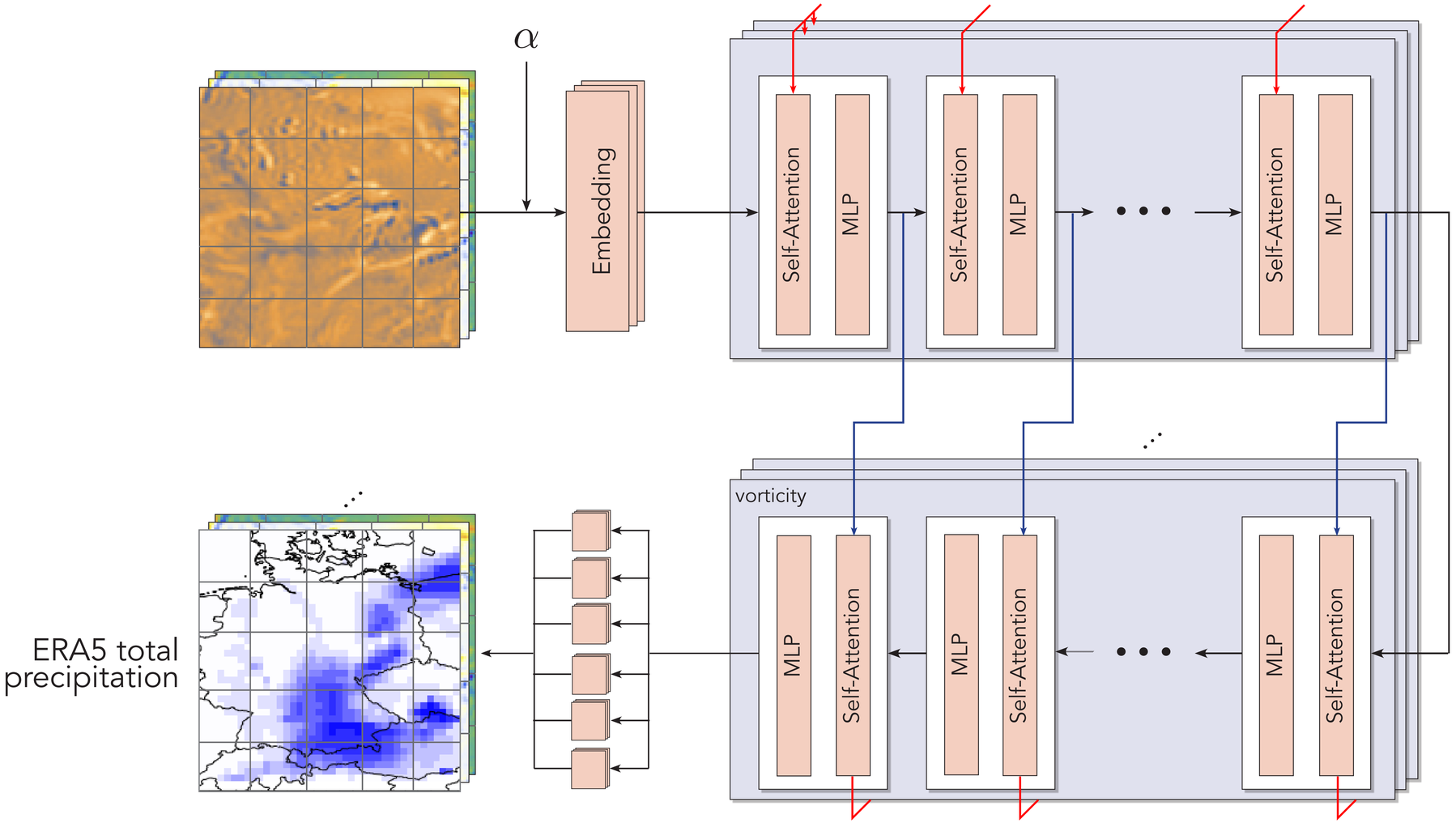
Downscaling



Downscaling



Bias correction



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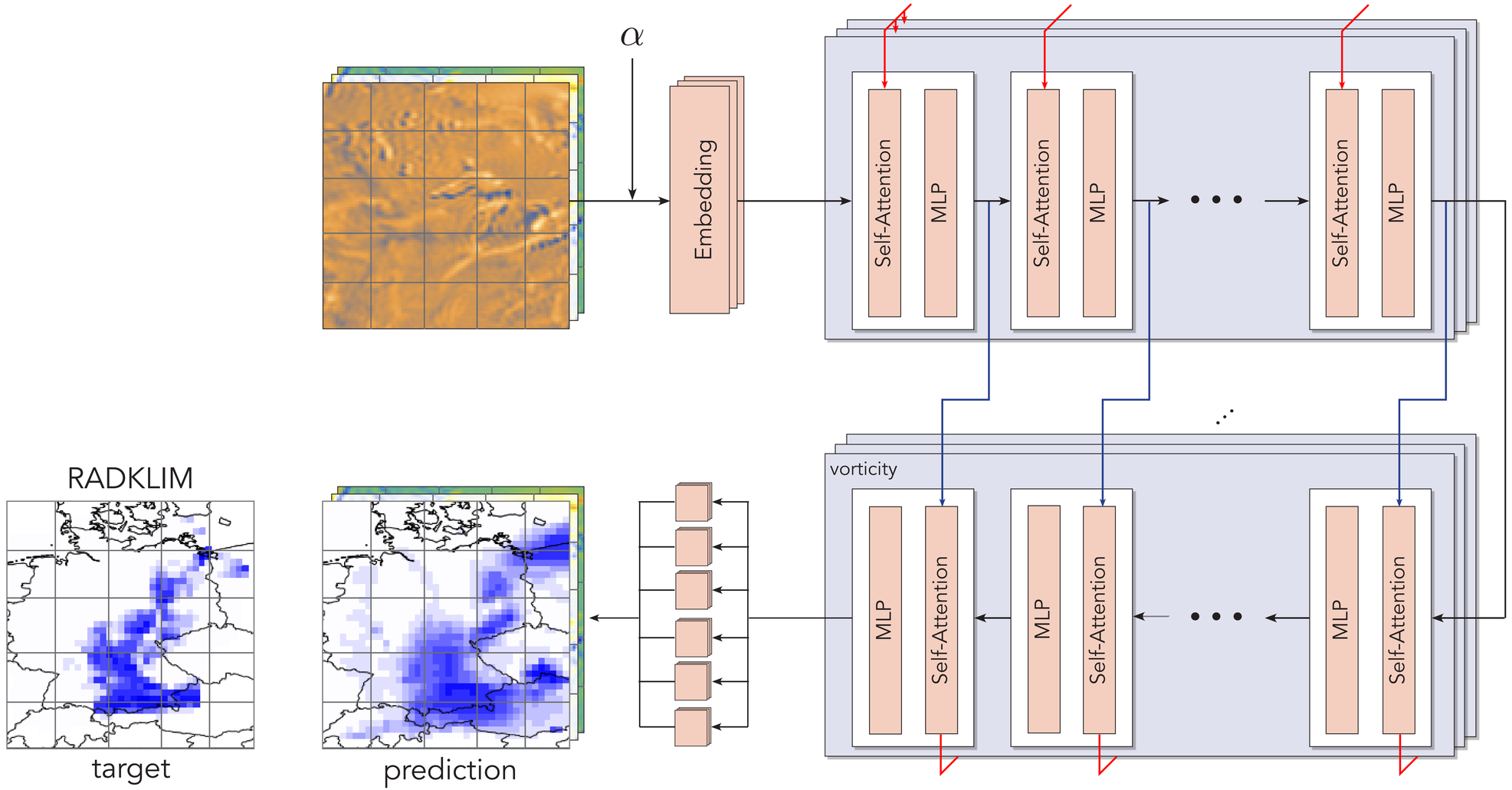

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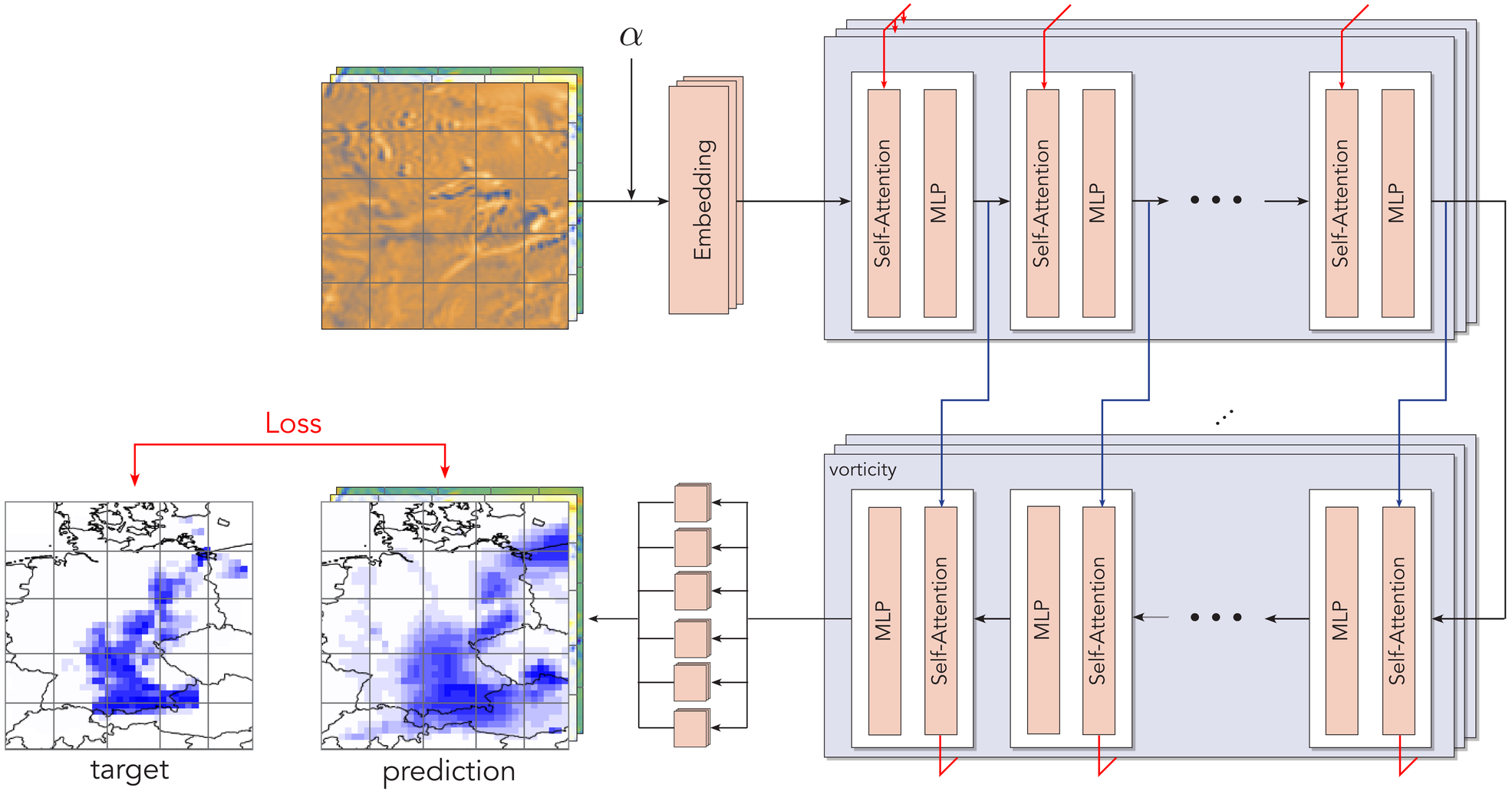

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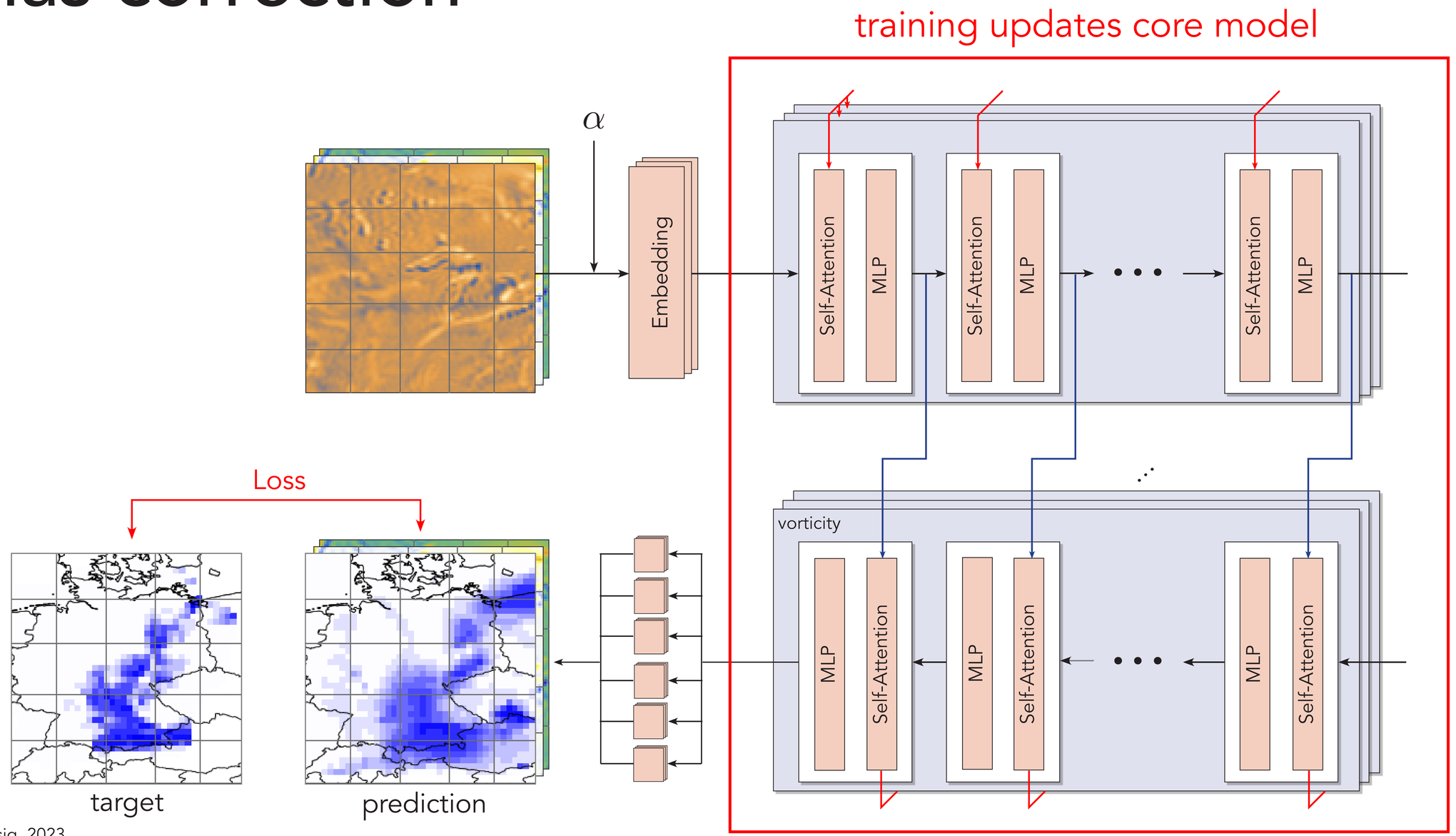

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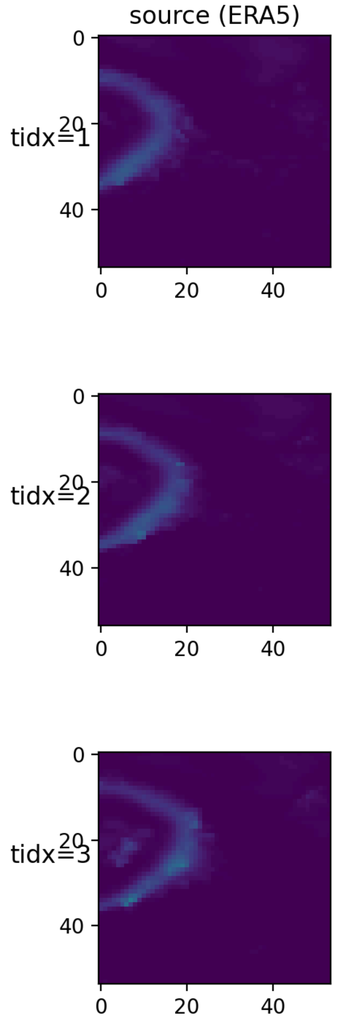

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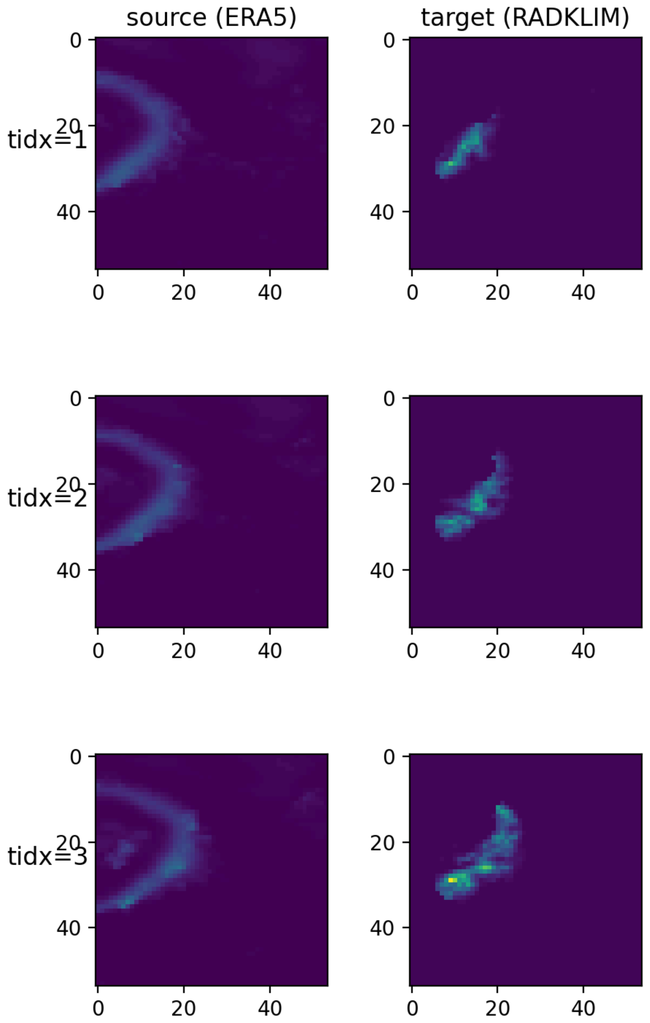

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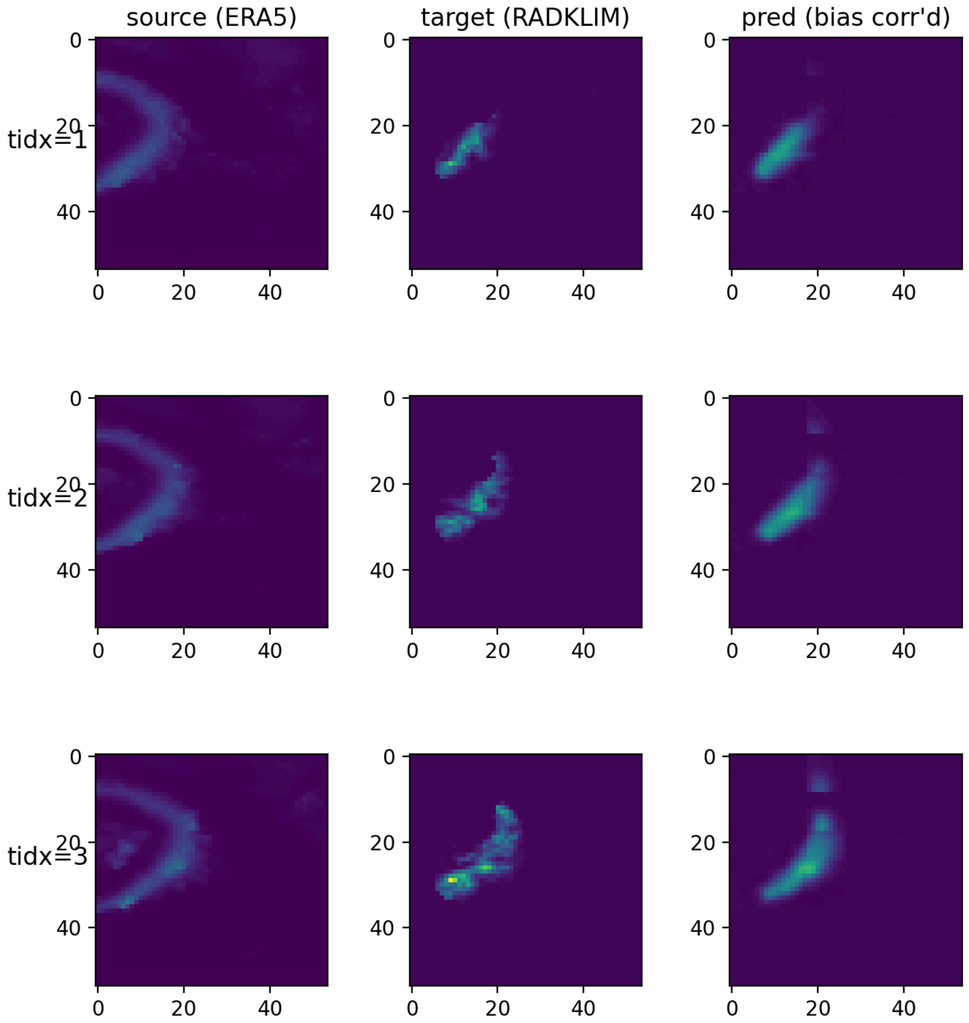

Outlook

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- Train an integrate many different data sources
  - CERRA, NexRAD, ...
  - IFS, ICON, ...
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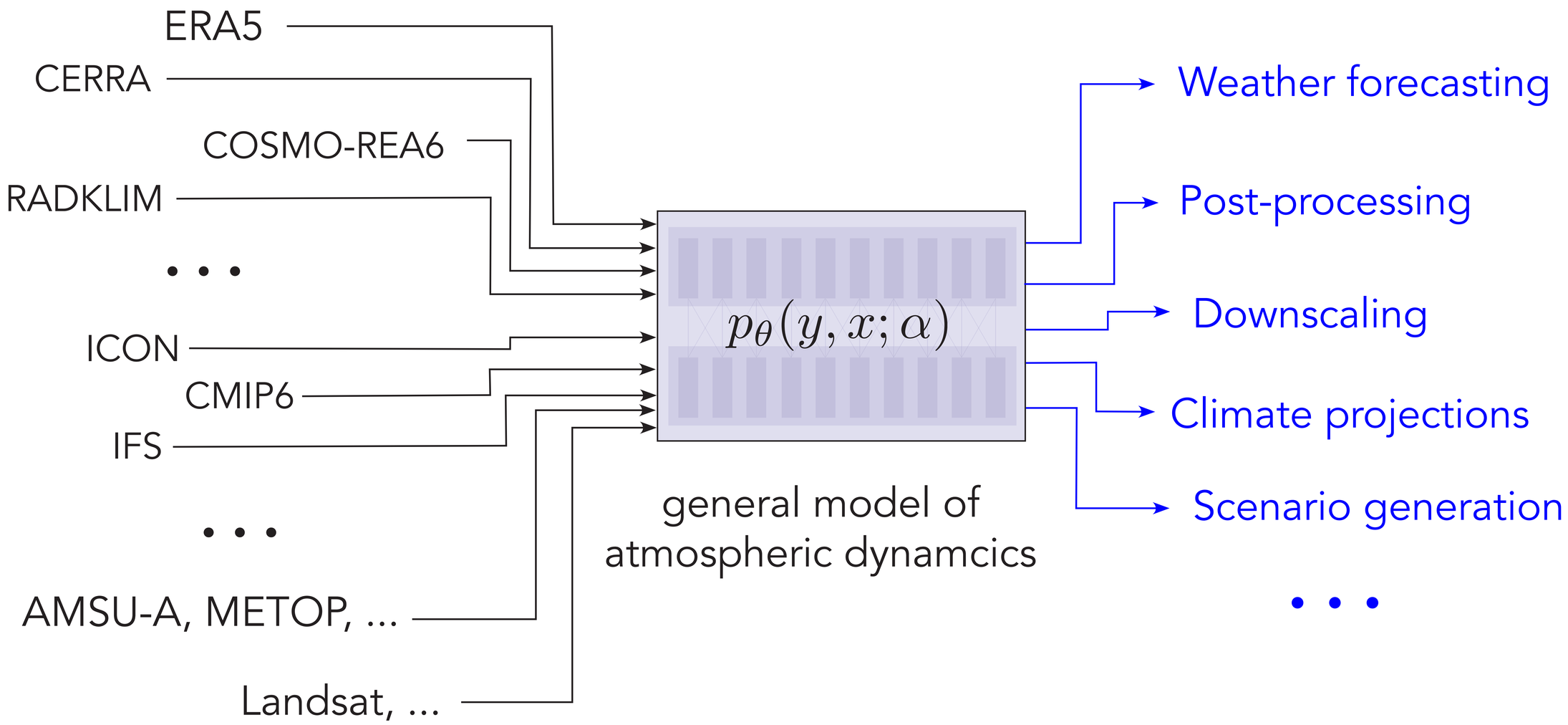
Outlook



Summary

AtmoRep

- Numerical statistical atmospheric model
  - Complementary to classical GCMs and ESMs
  - Represented by very large neural network
  - Very long training leads to continuous improvement

https://arxiv.org/abs/2308.13280

AtmoRep

- Numerical statistical atmospheric model
  - Complementary to classical GCMs and ESMs
  - Represented by very large neural network
  - Very long training leads to continuous improvement
- BERT-type training leads to versatile intrinsic capabilites
  - Forecasting, temporal interpolation, model correction, ...
  - Straight forward extension to various applications

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AtmoRep

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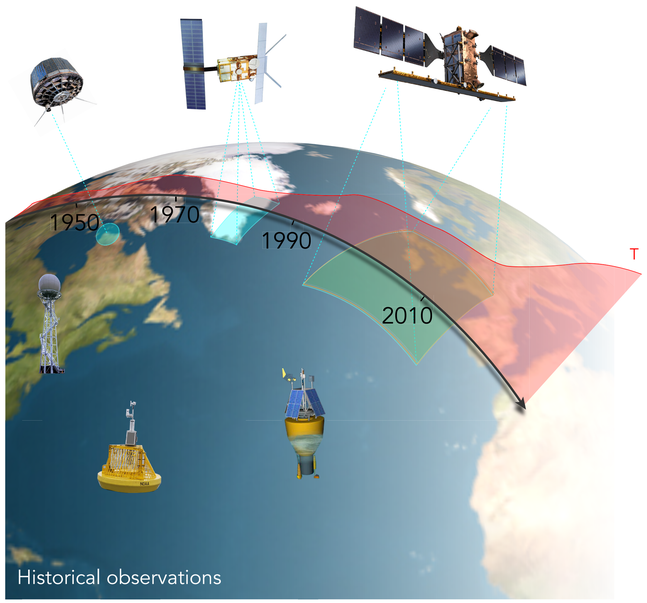

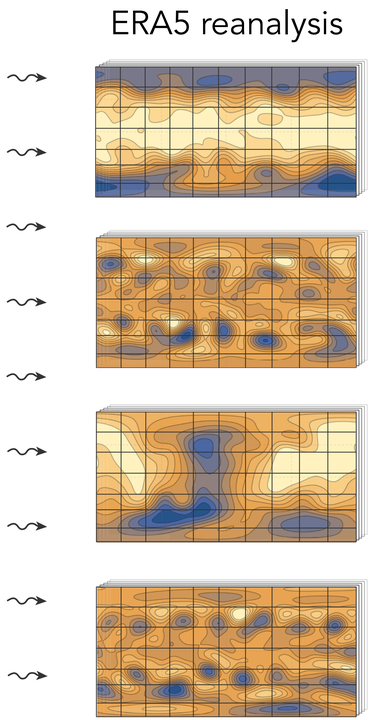

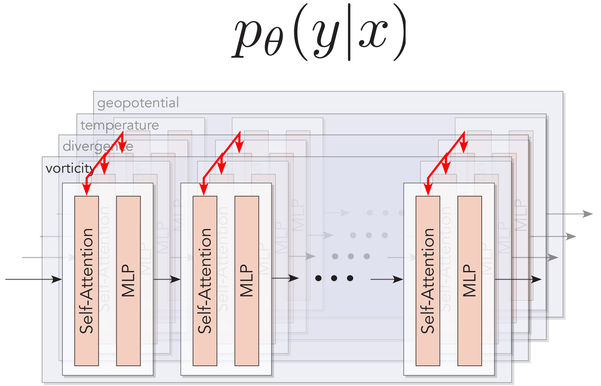

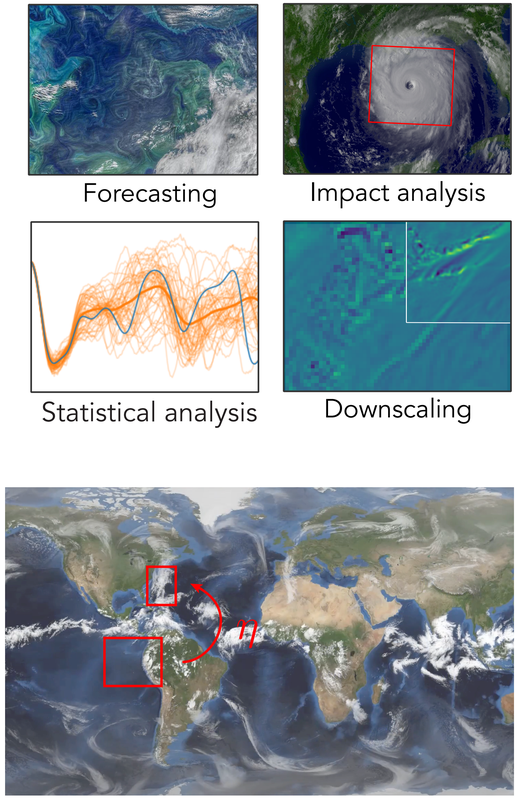

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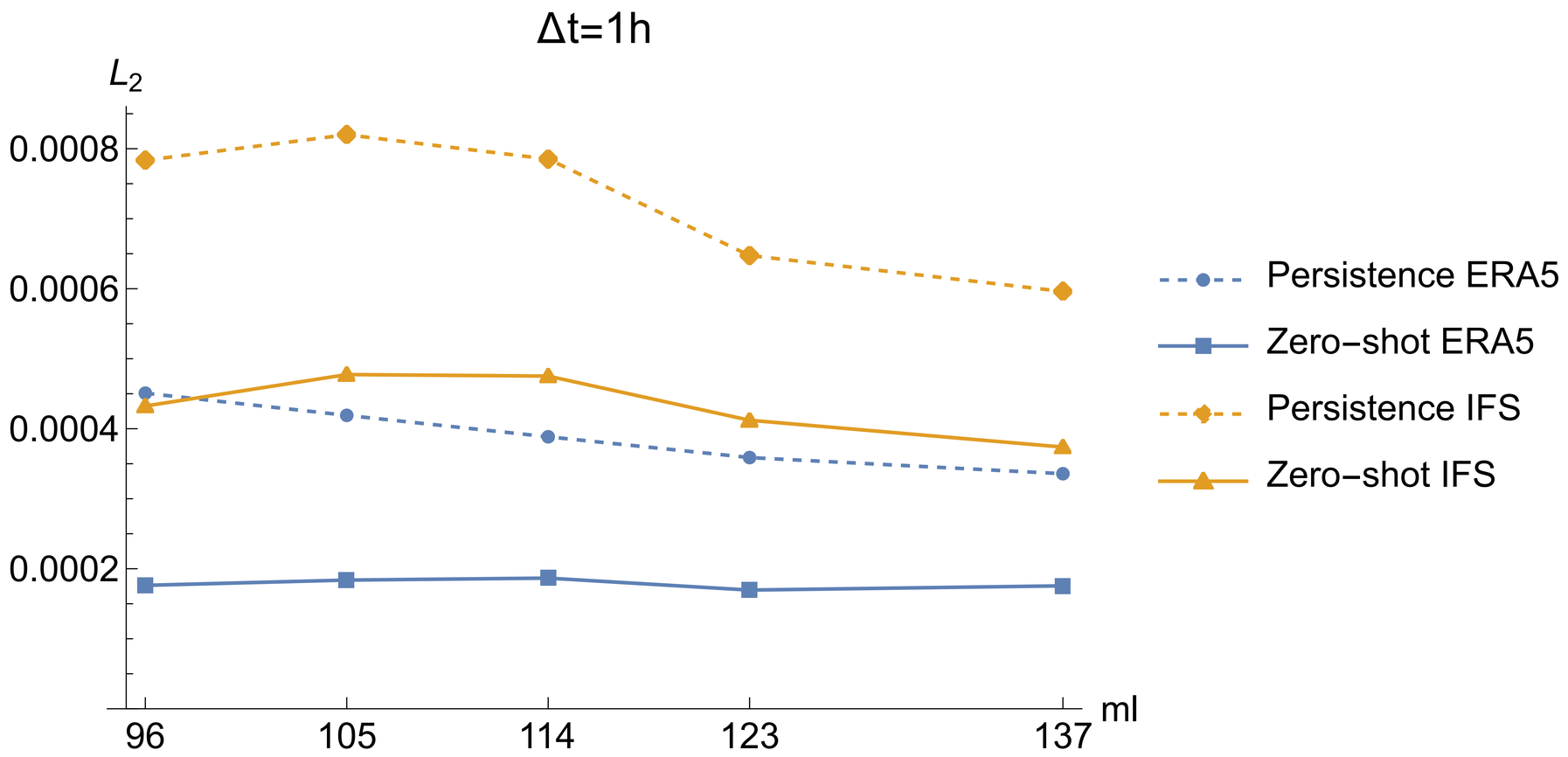
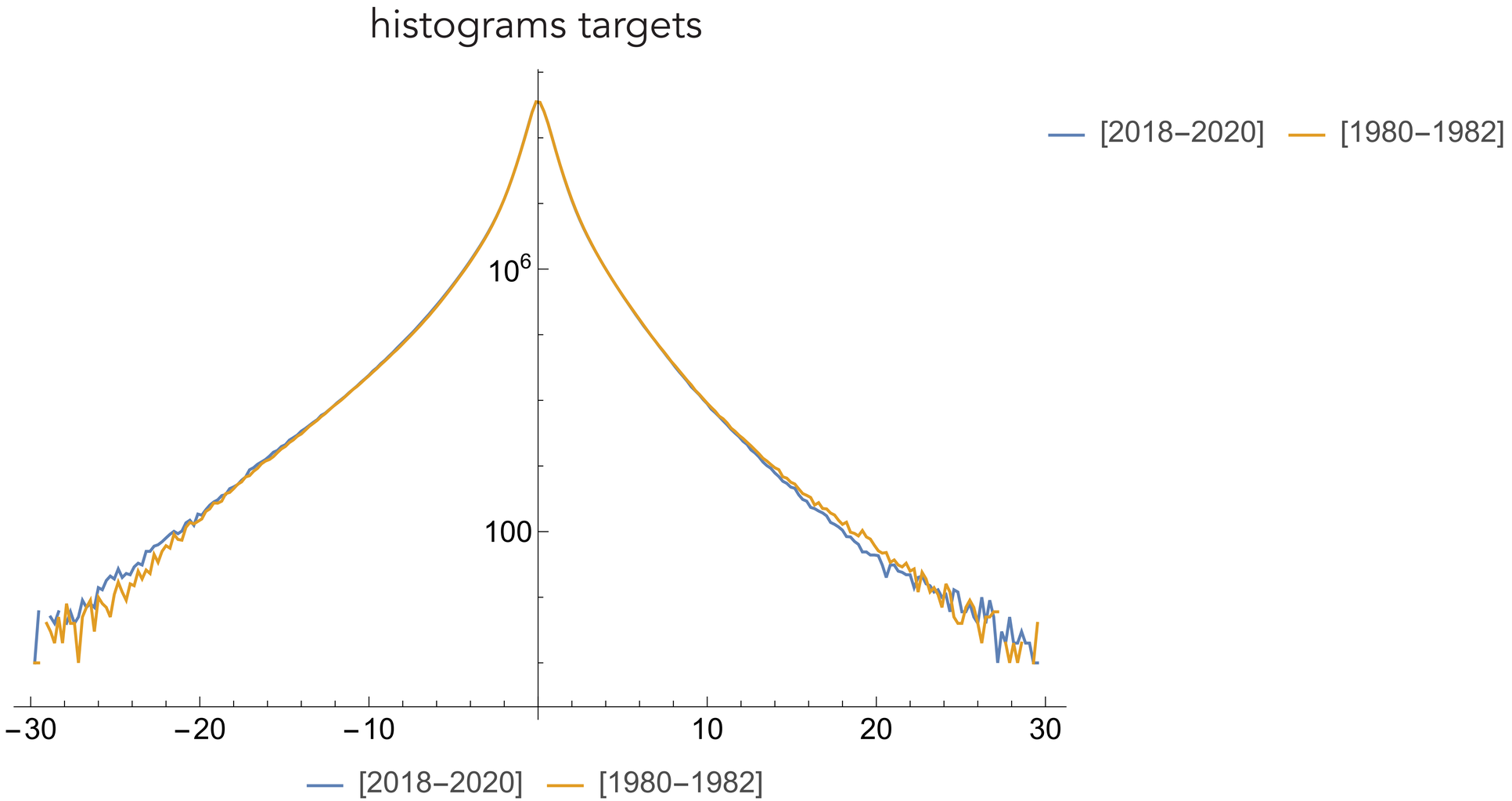


Counterfactuals



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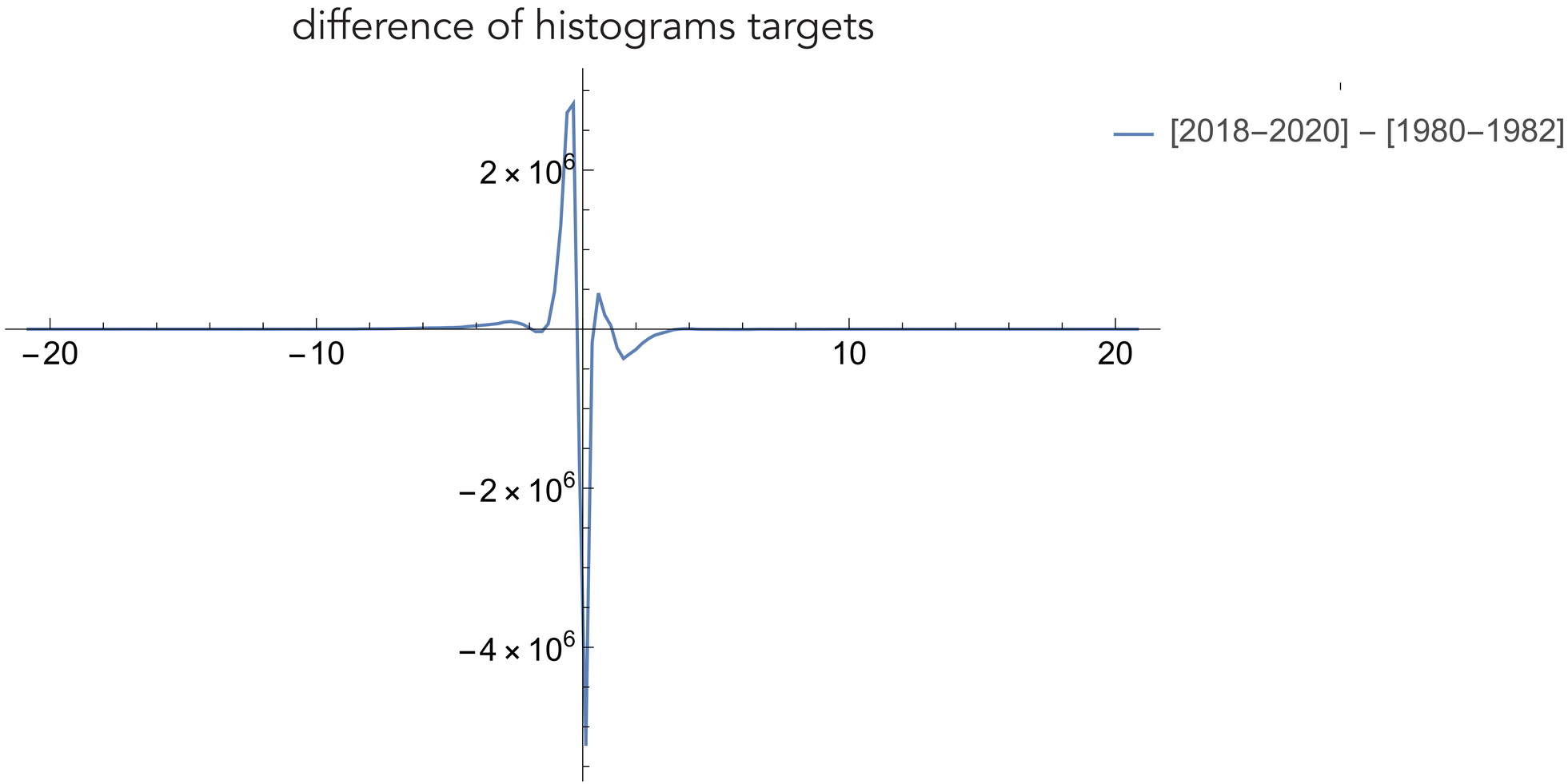

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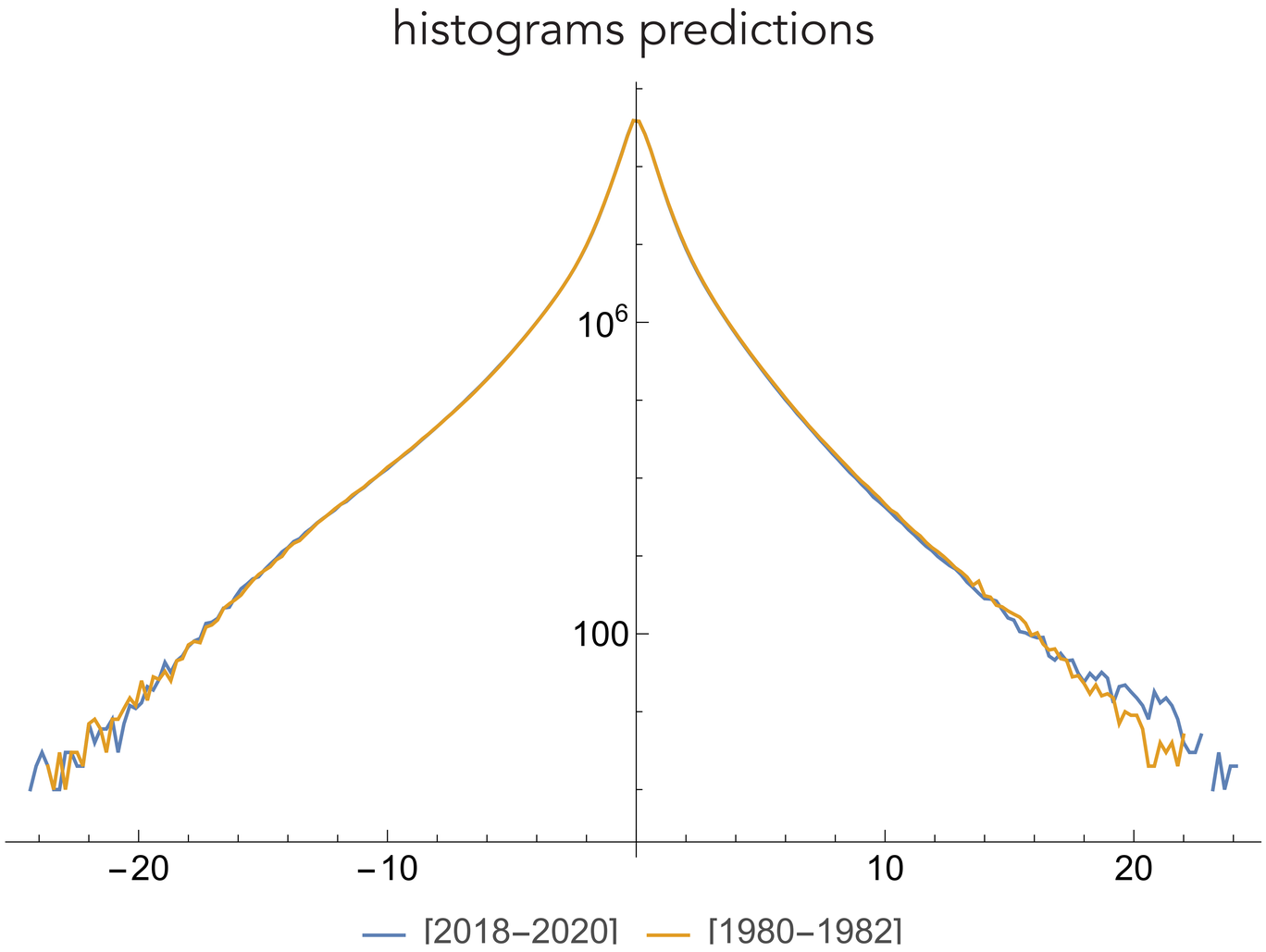

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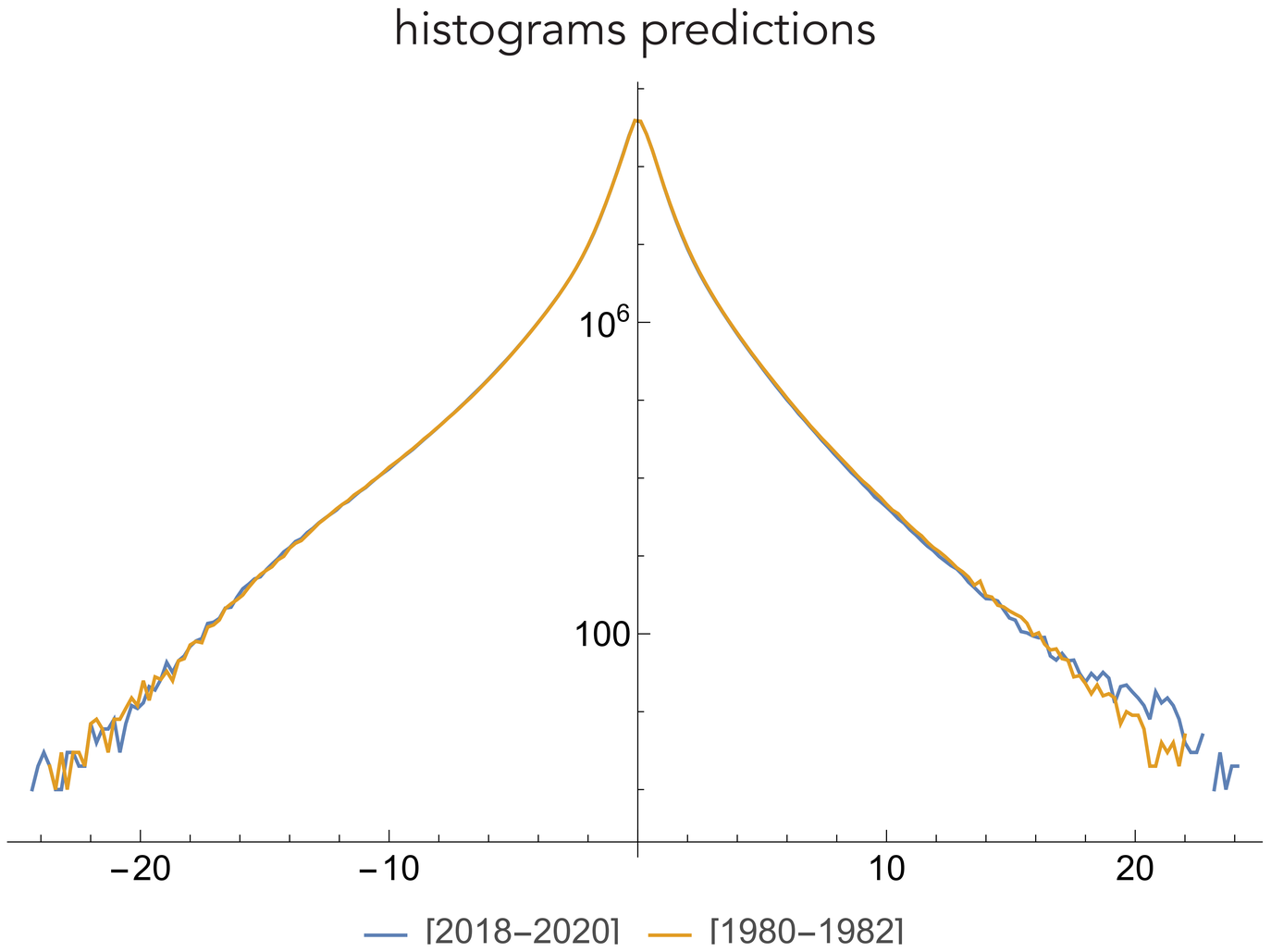

[2018–2020]

initial conditions *but*
$\alpha_{\text{year}} = [1980, 1982]$

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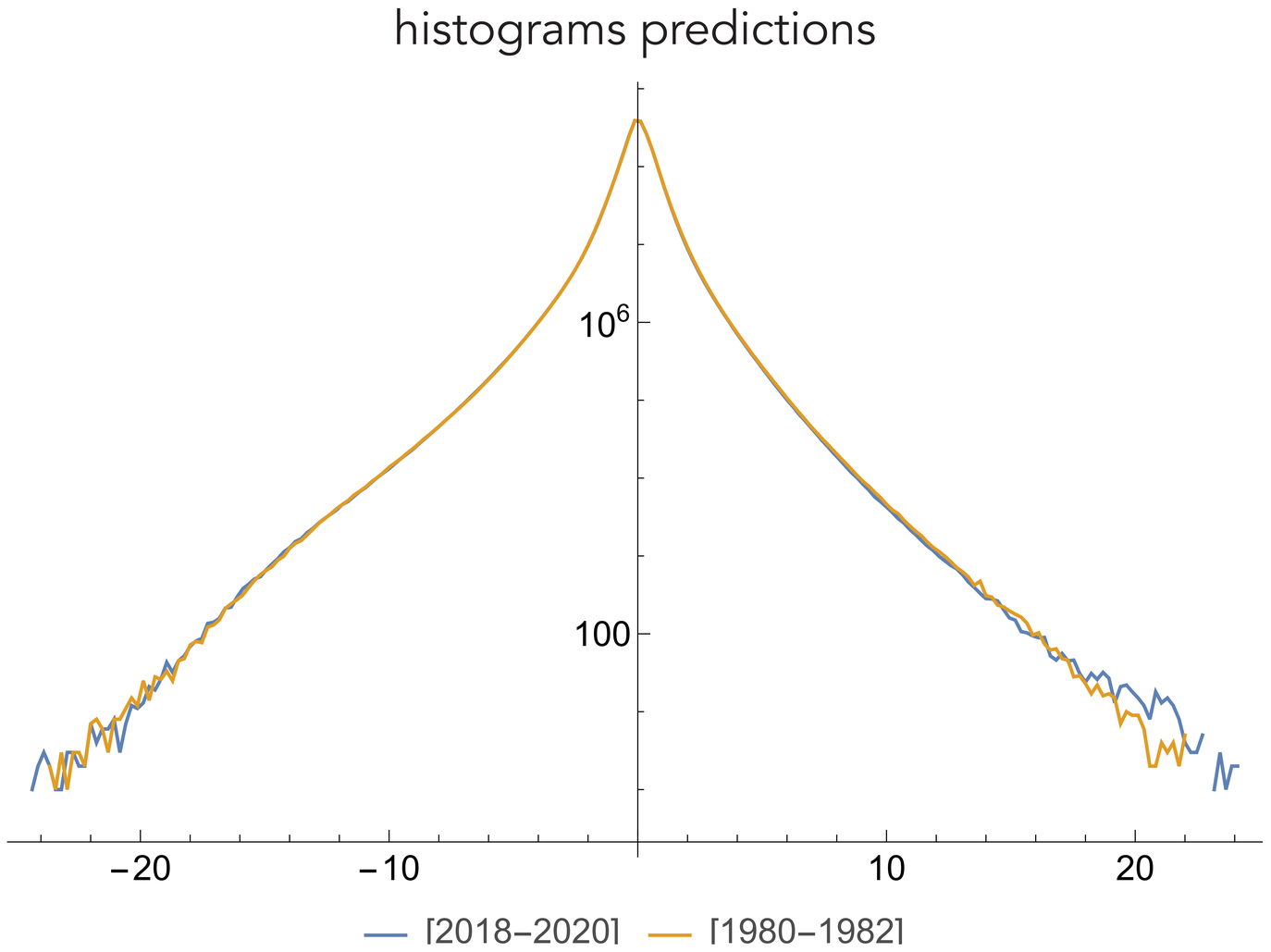

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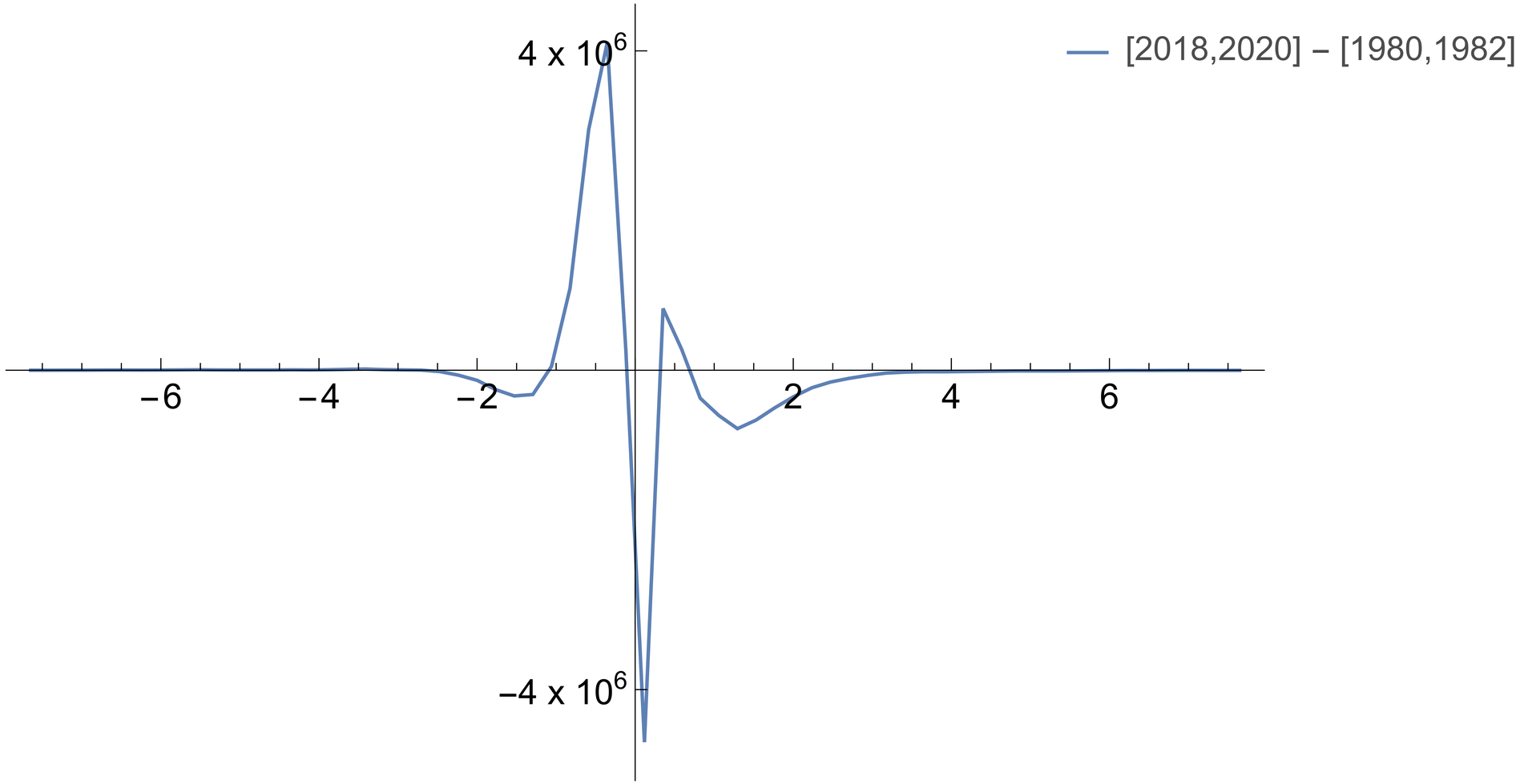

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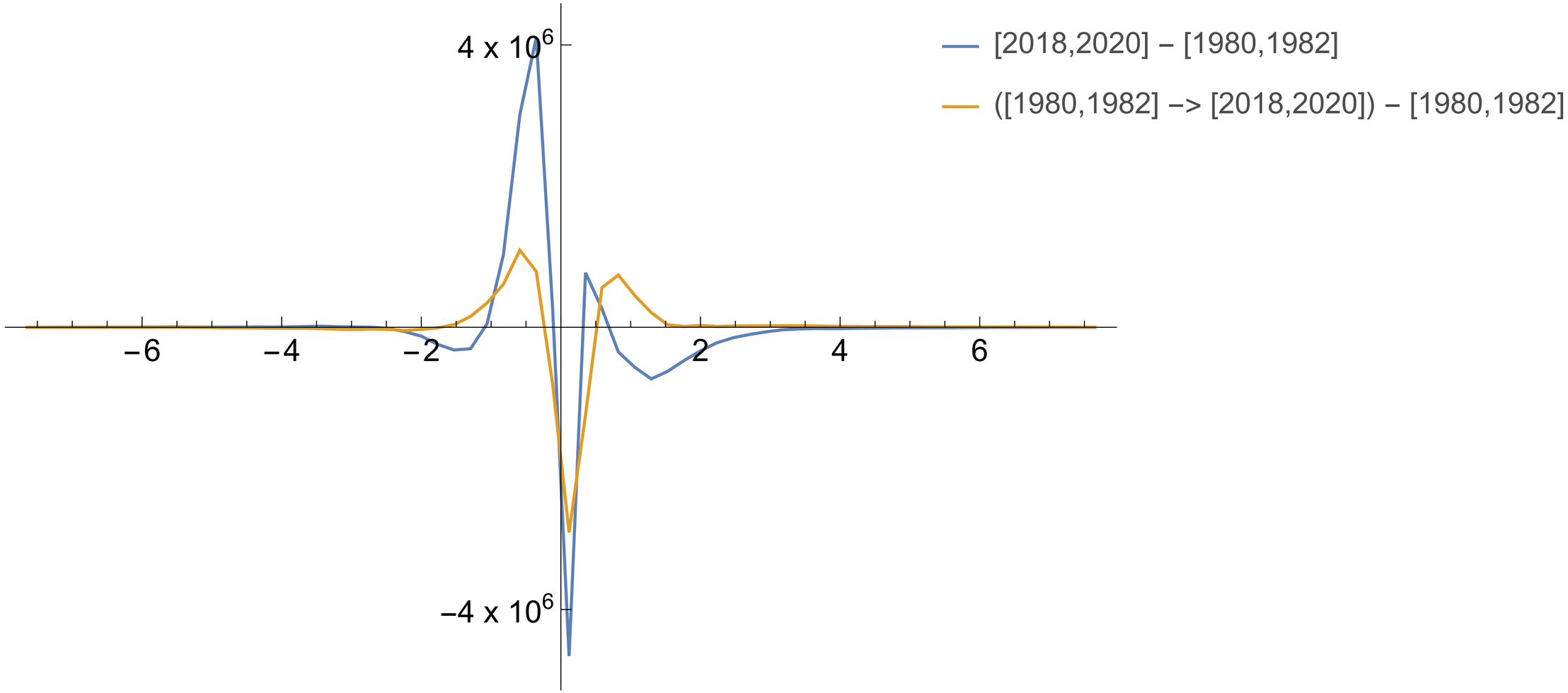

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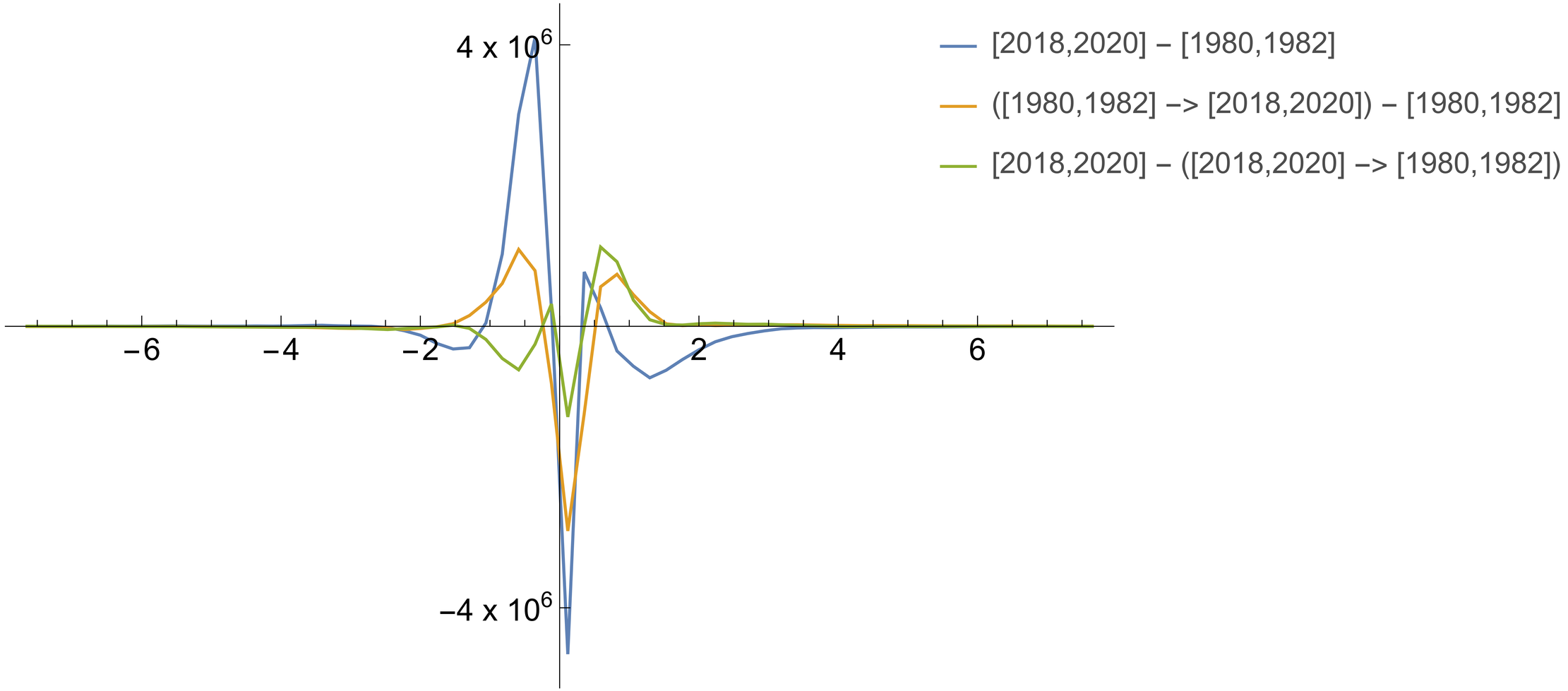
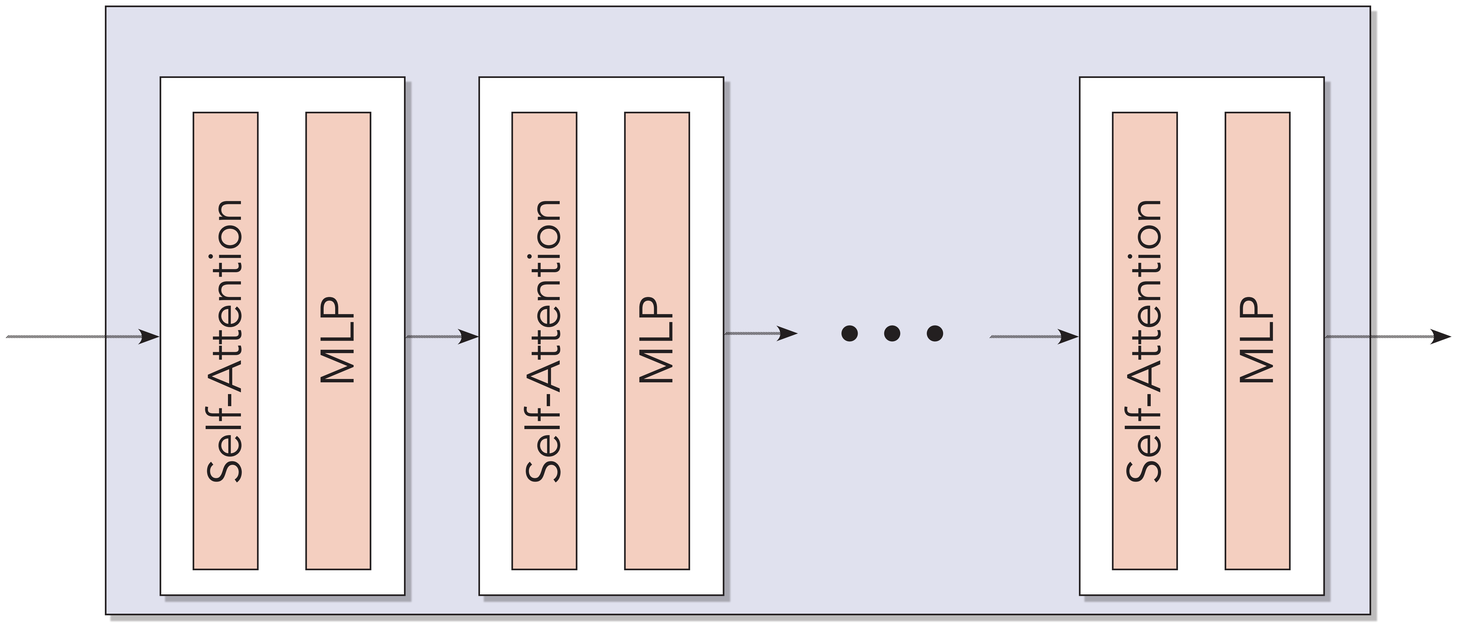


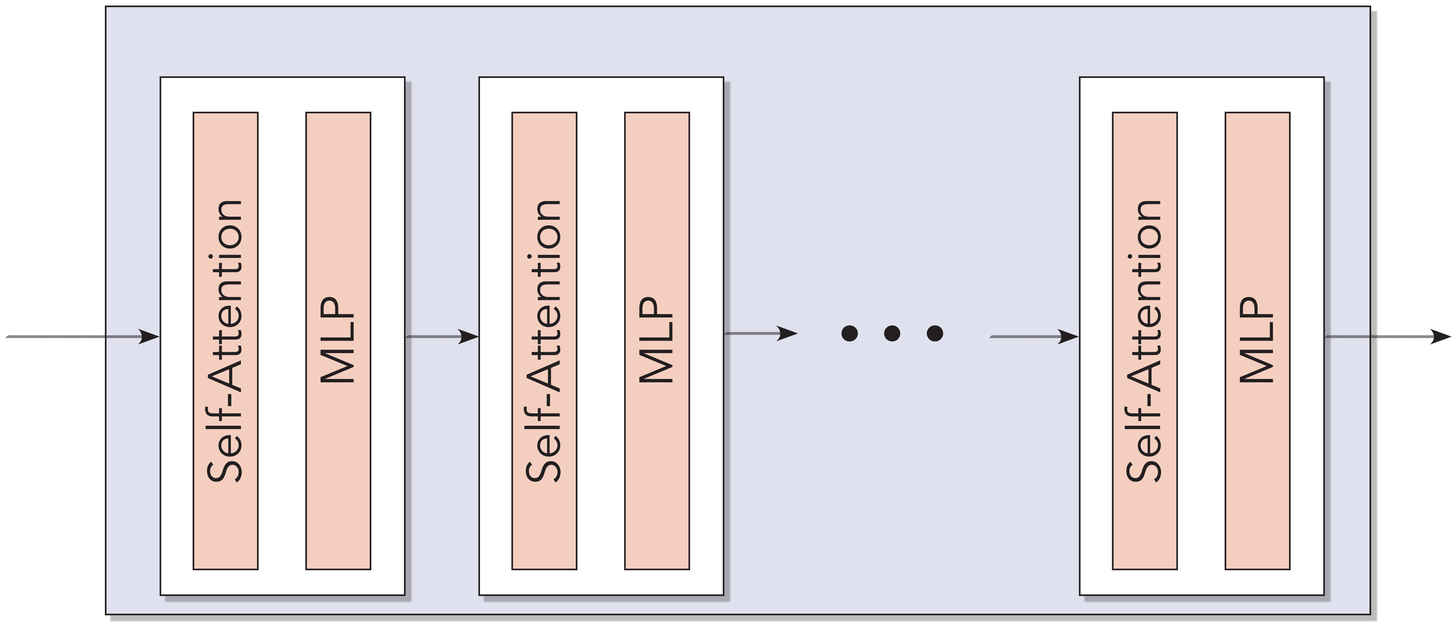
Multiformer



Multiformer

Self
attention

$$\sigma\left(Q\,K^T\right)V$$



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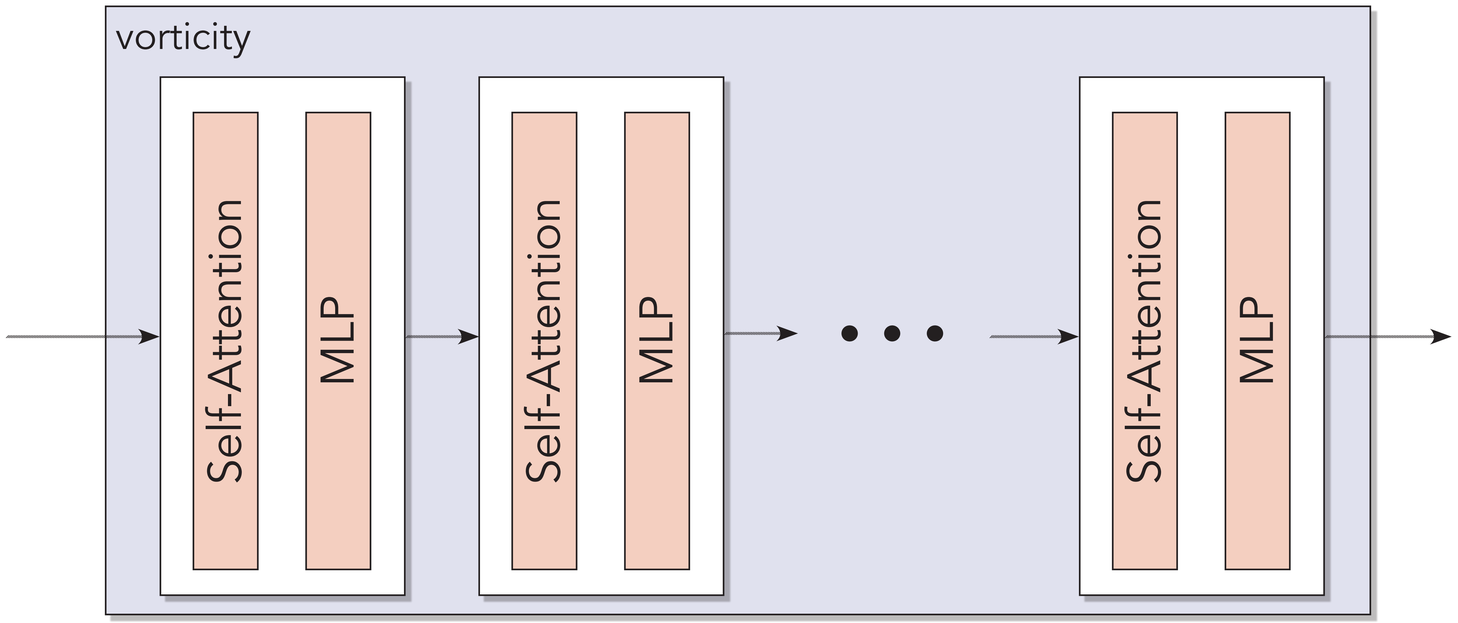

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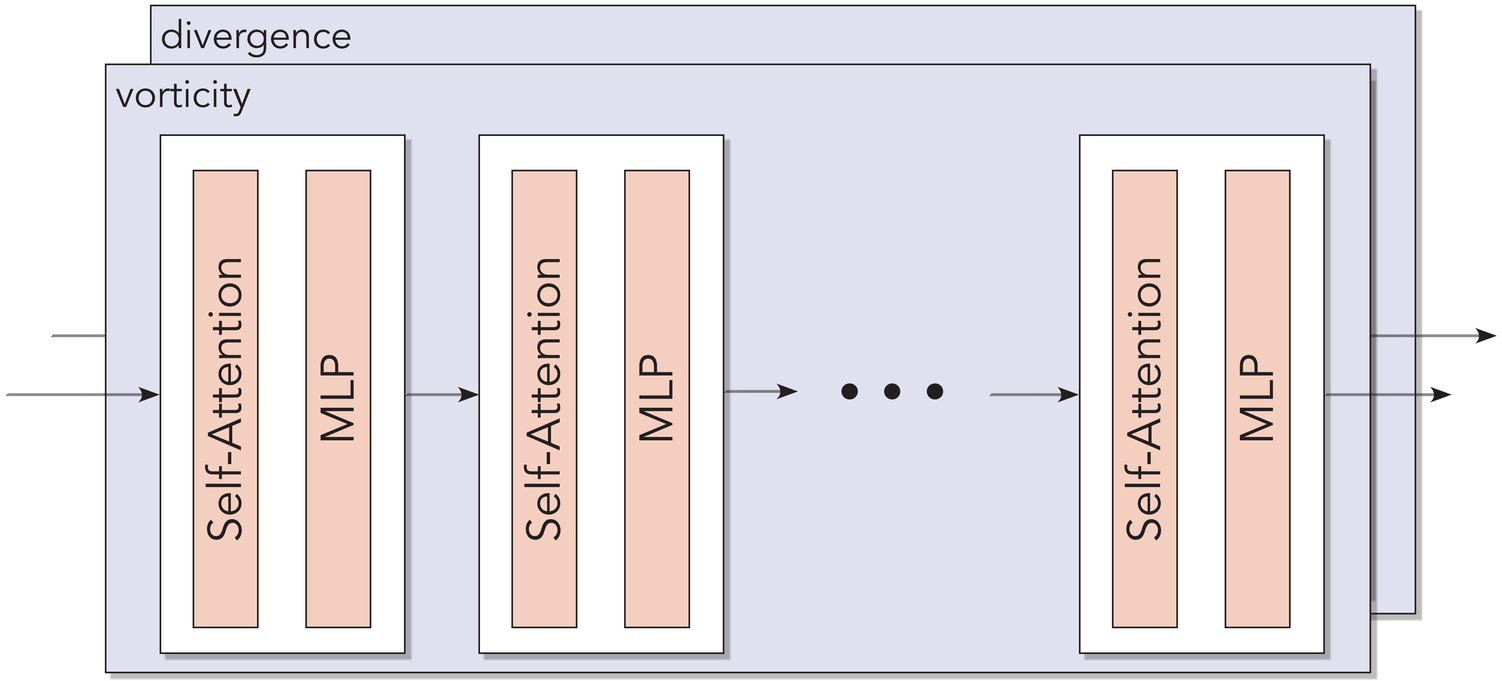

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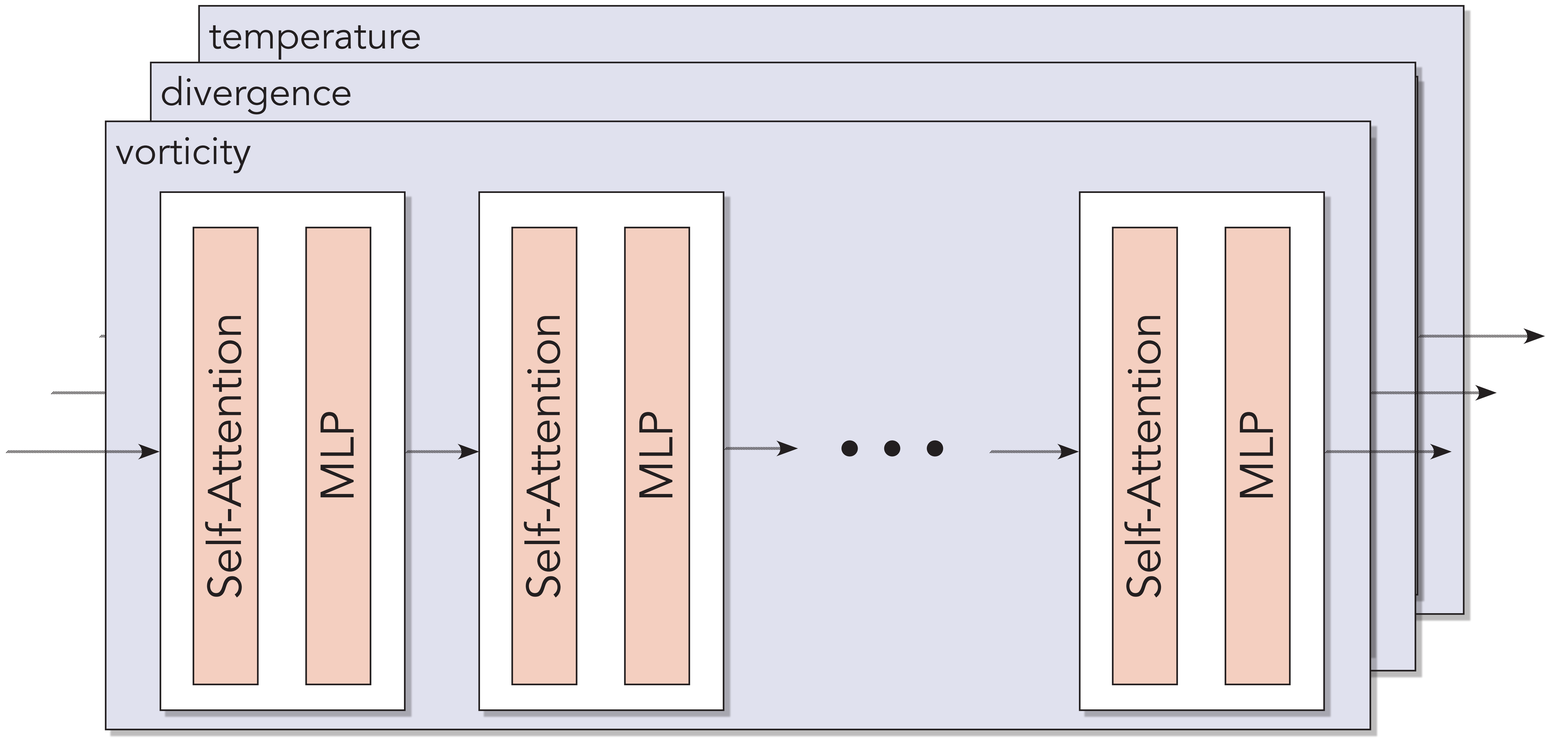

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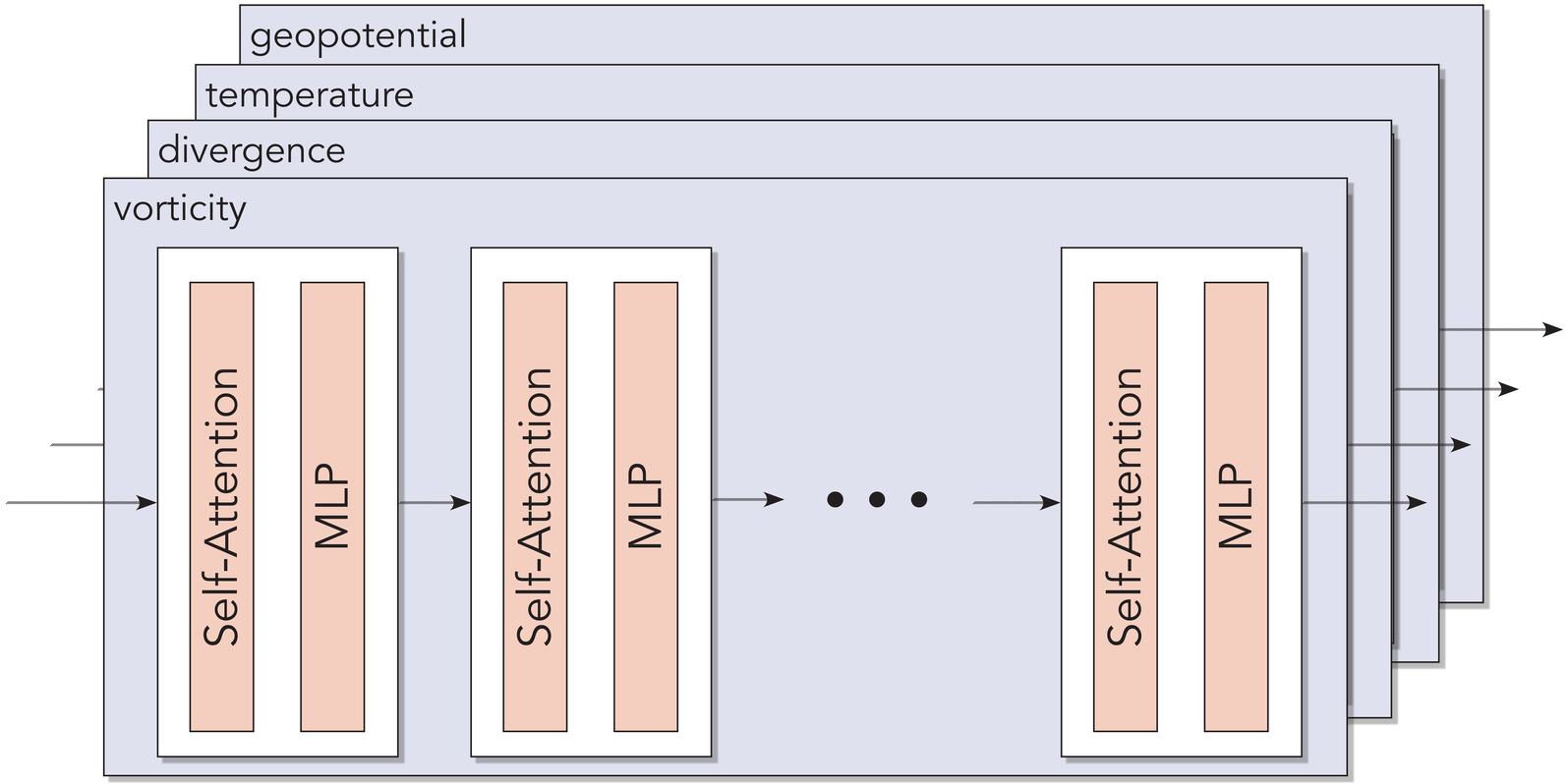

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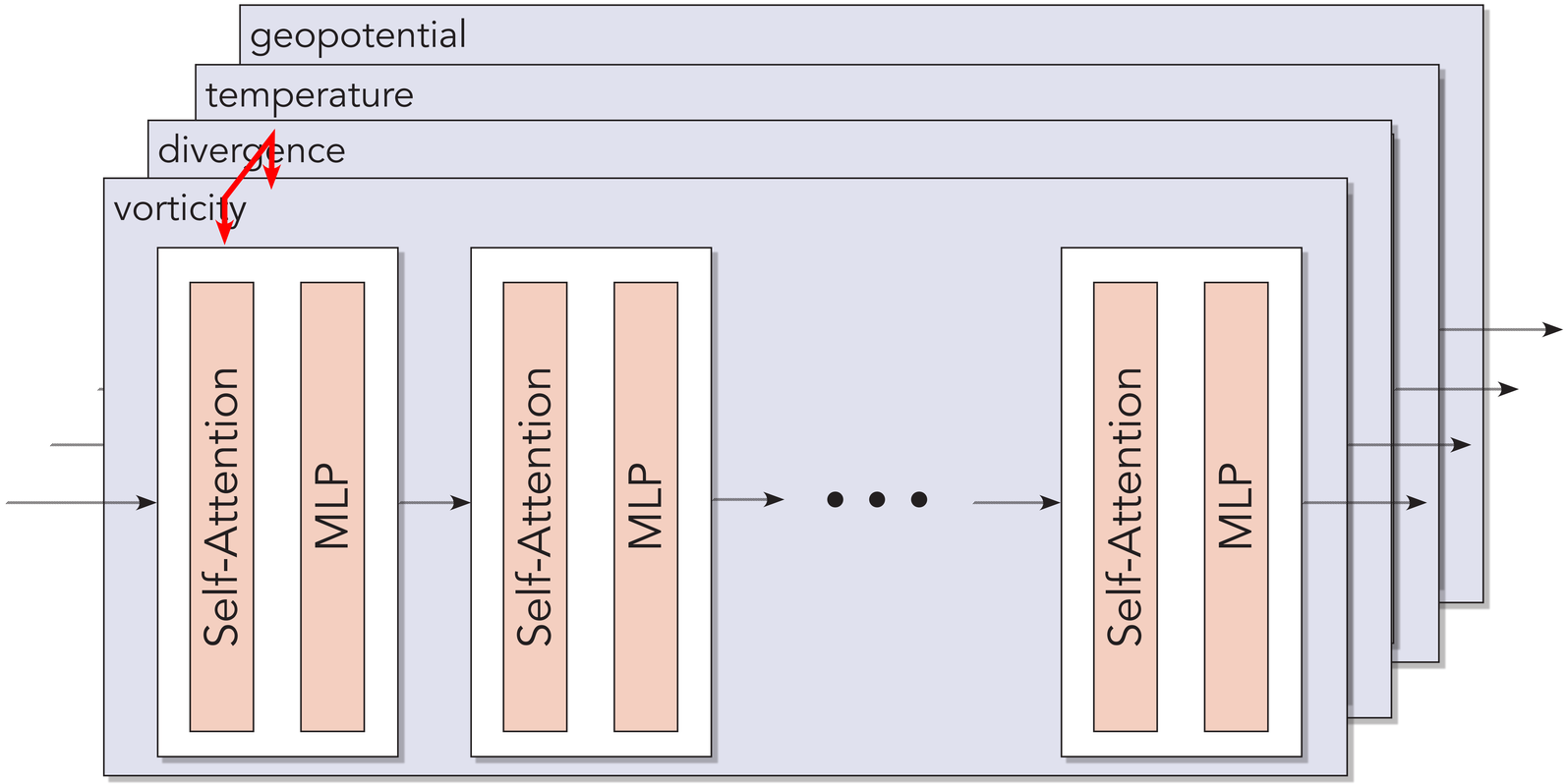

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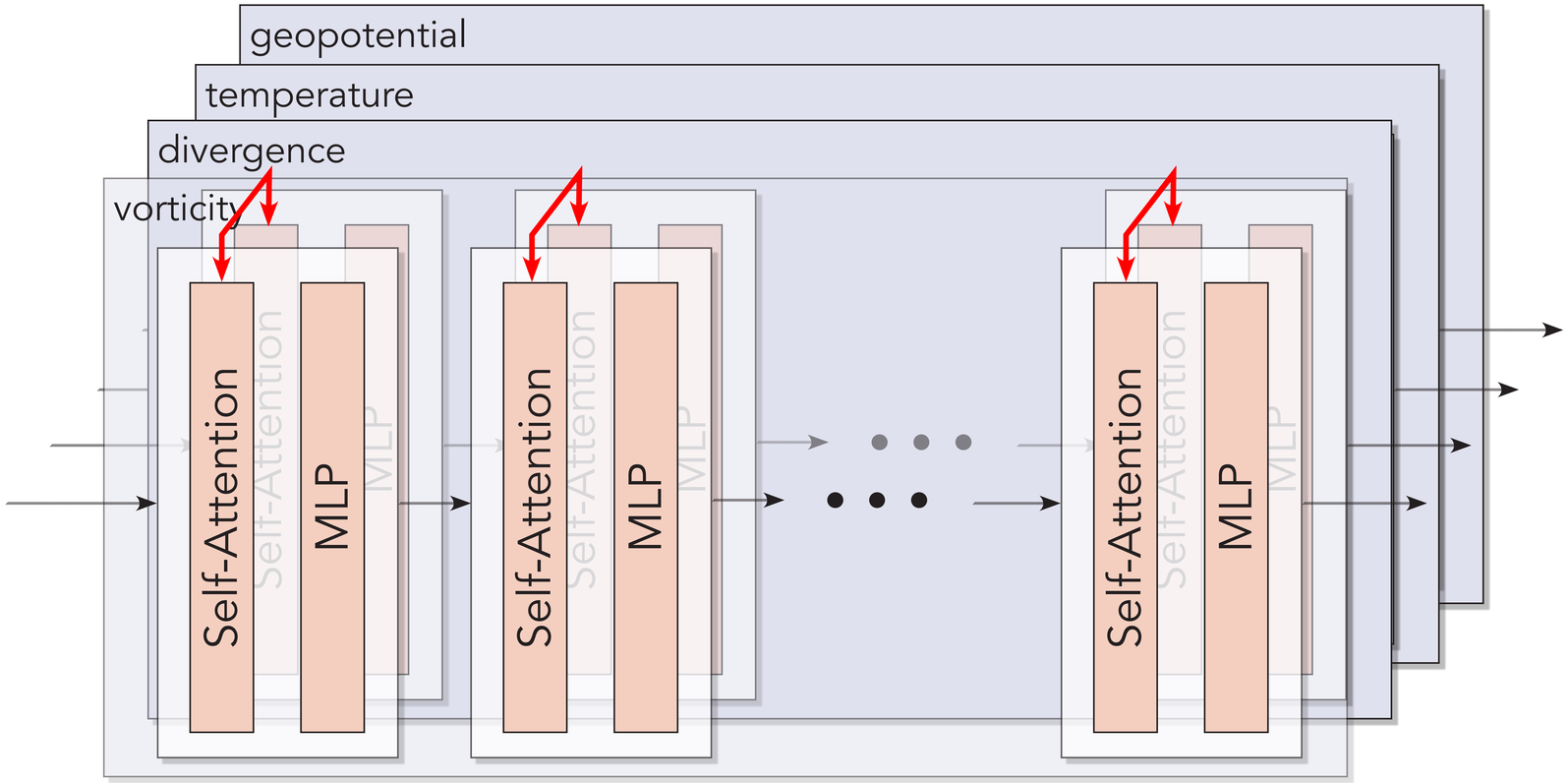

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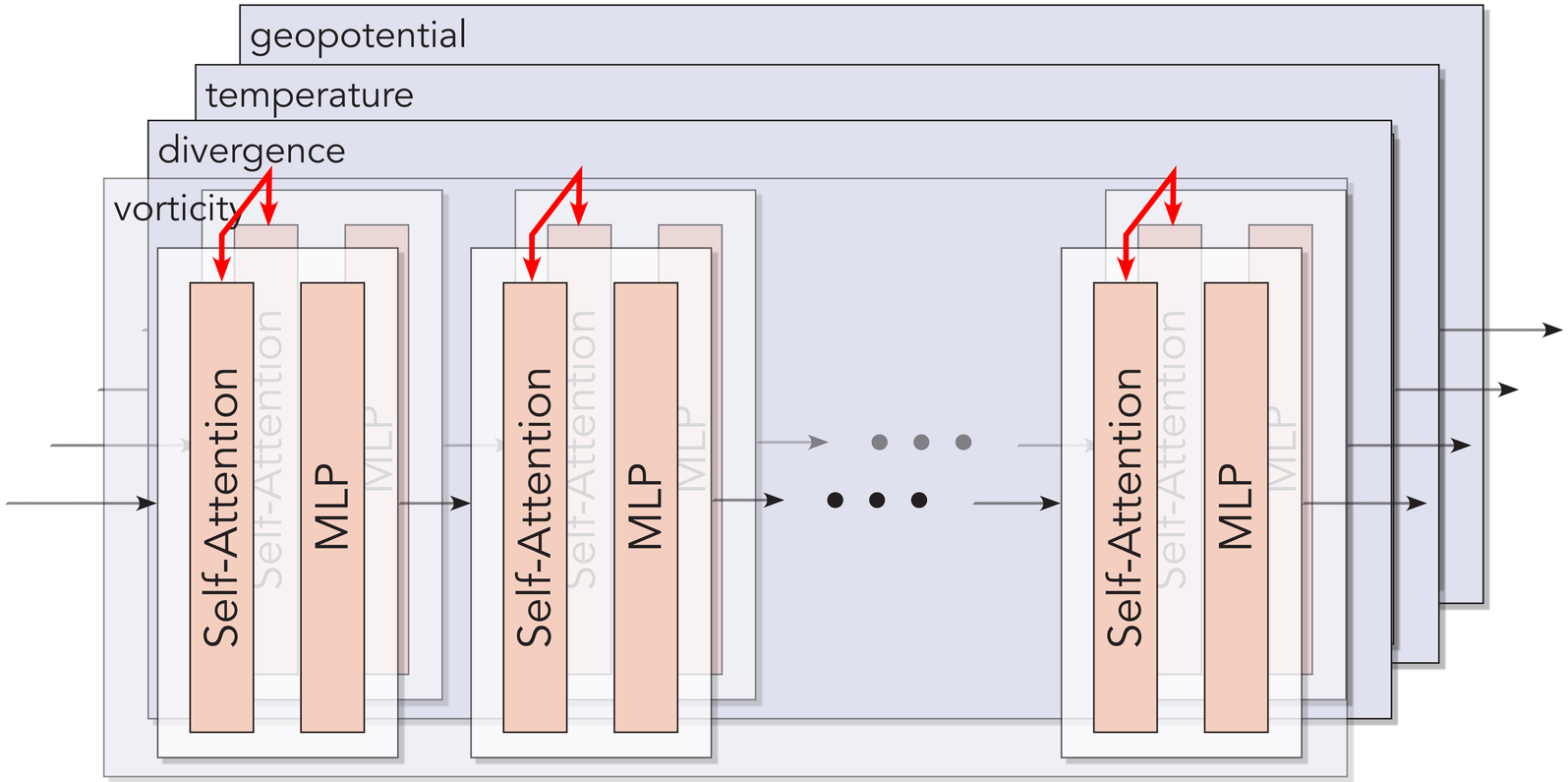

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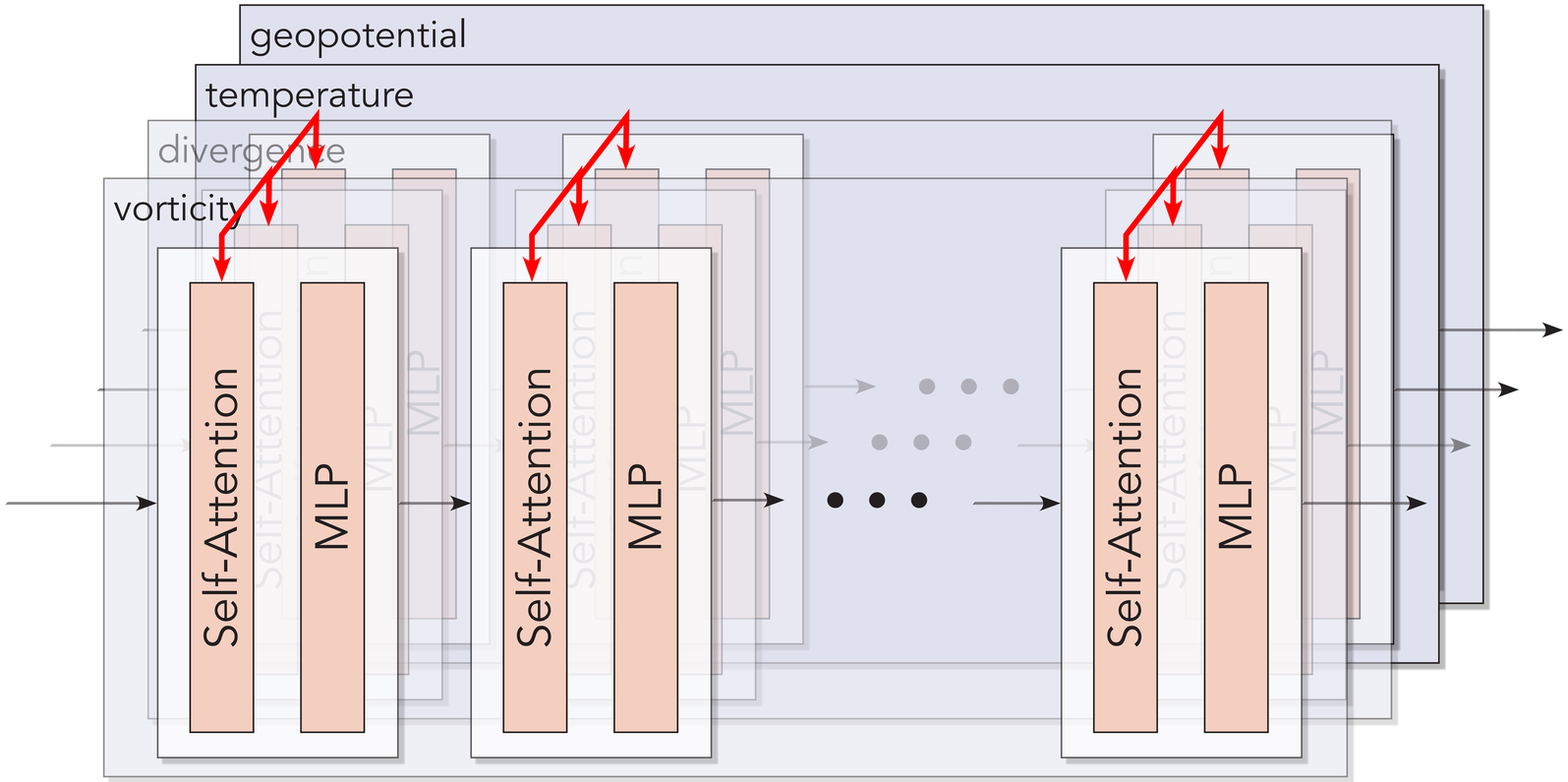

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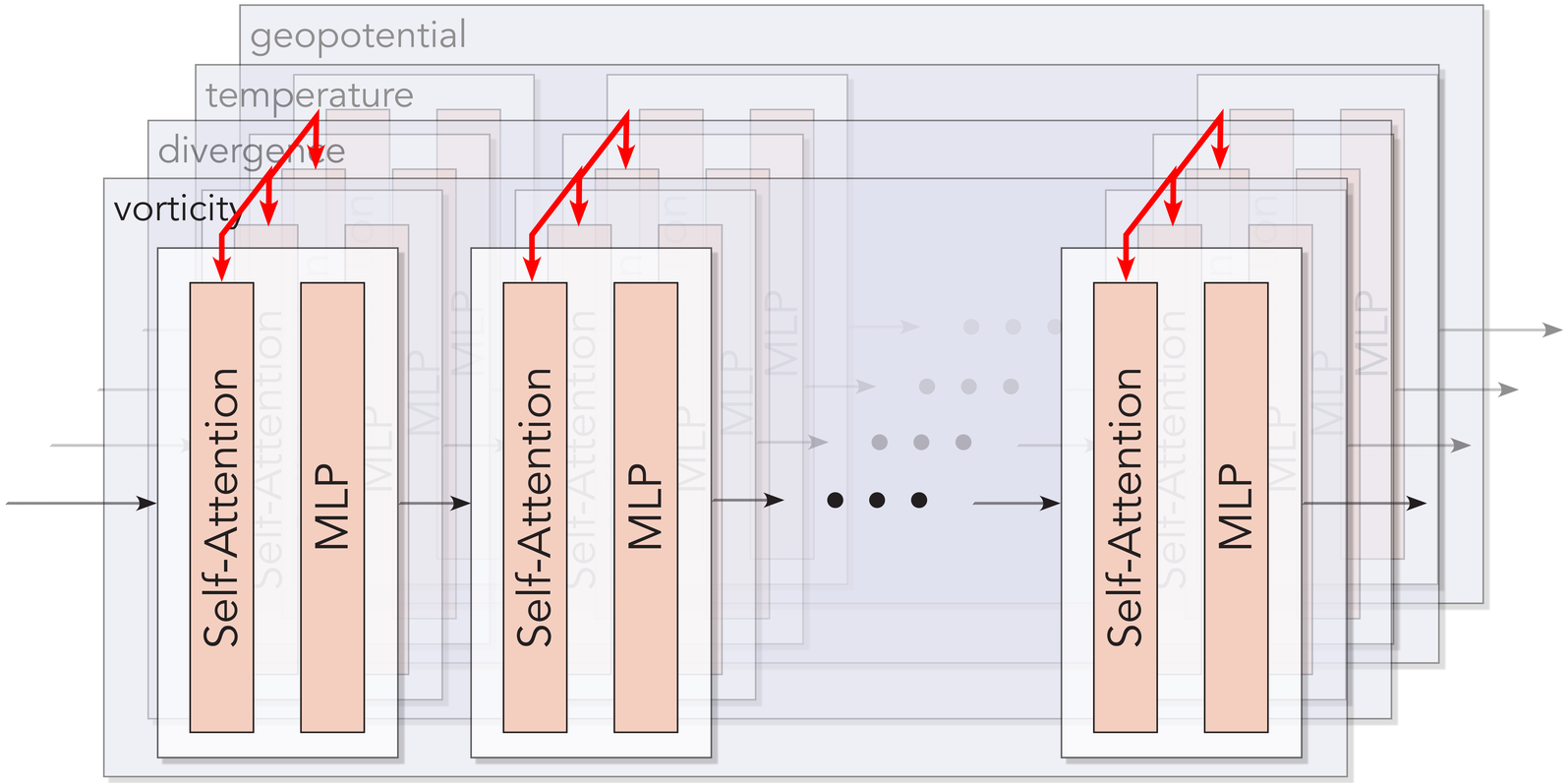

Multiformer

- Plug-and-play of fields
  - Fields can be added/removed with limited (or no) computational effort

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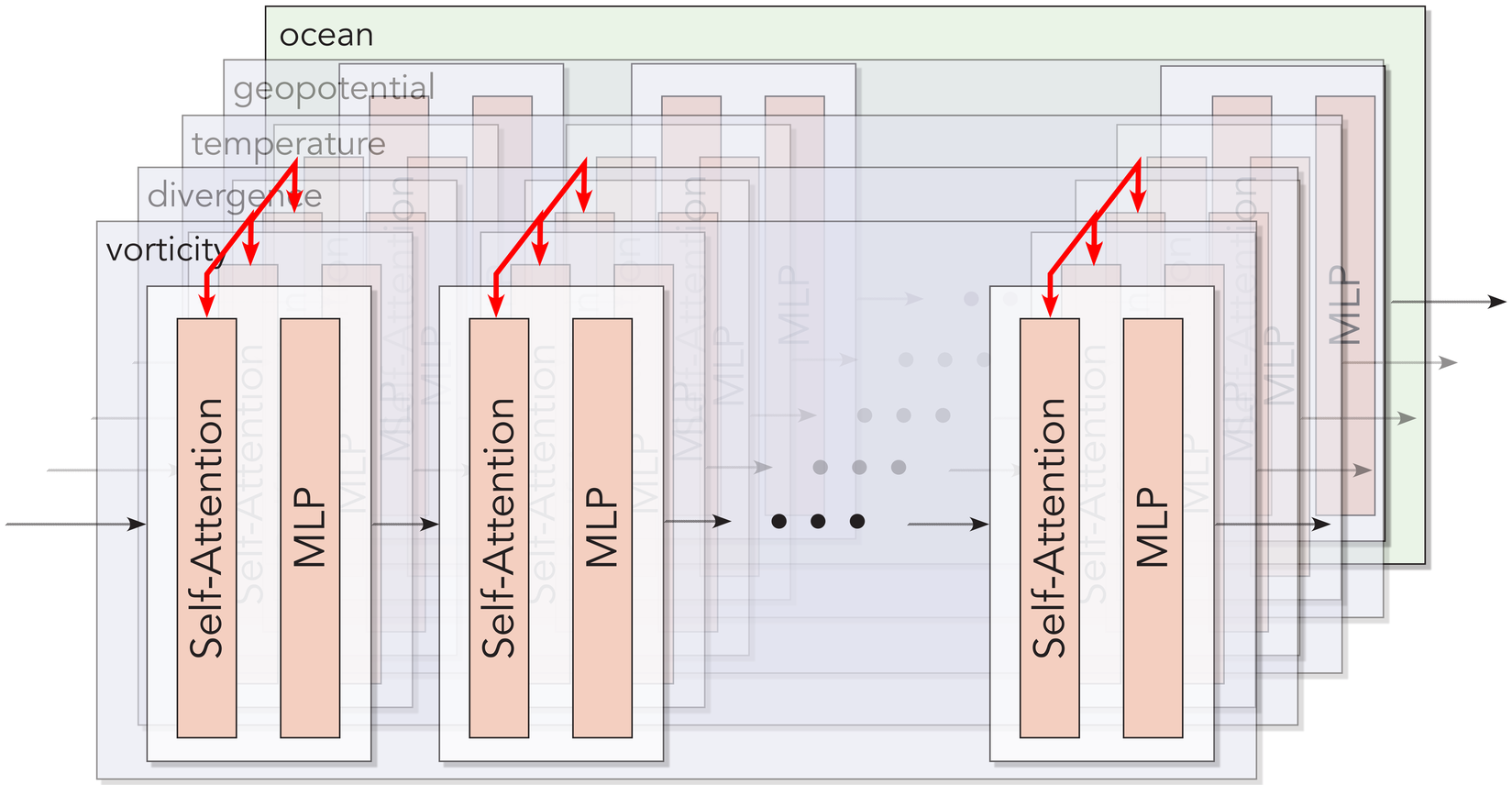

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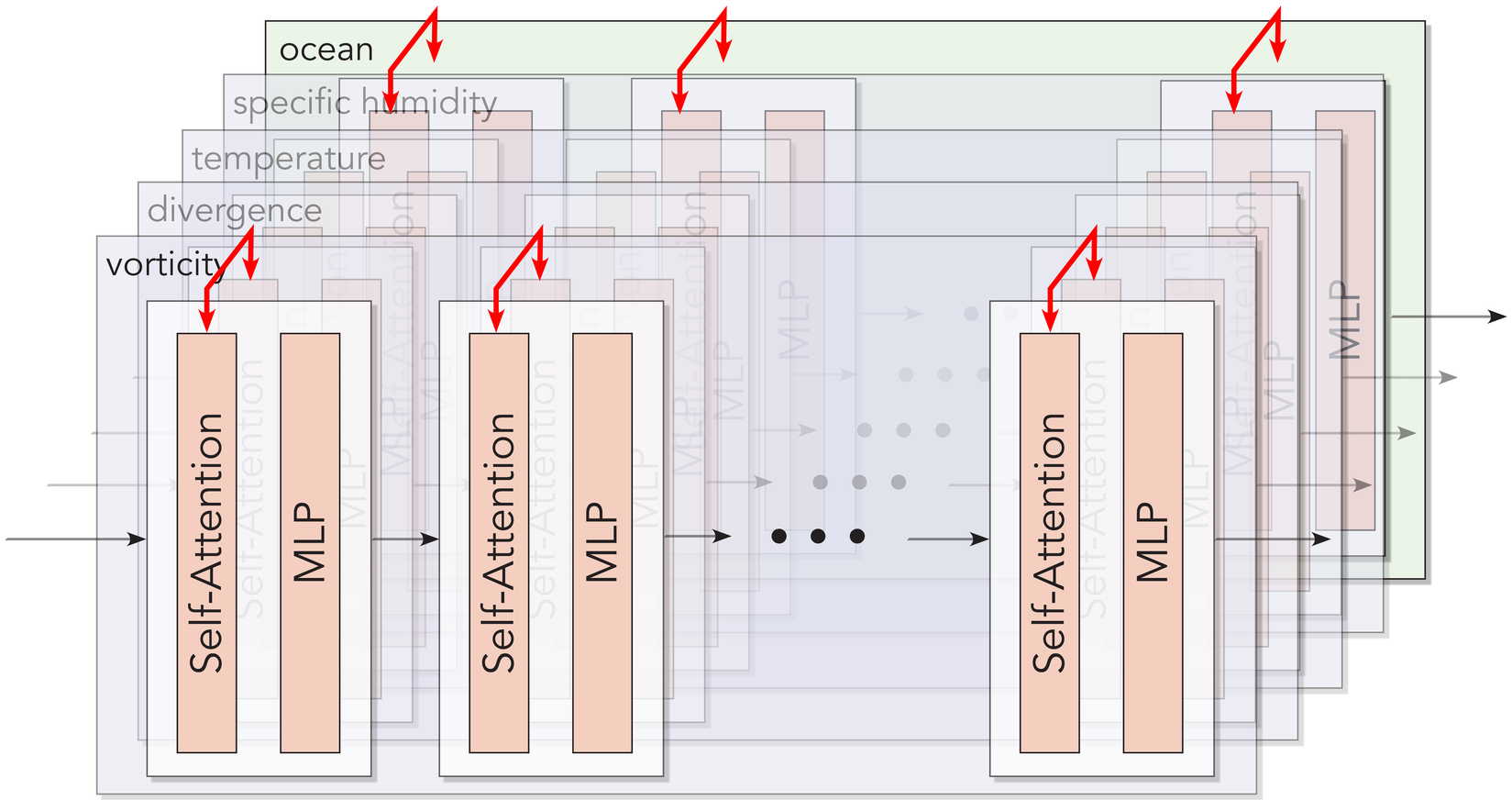
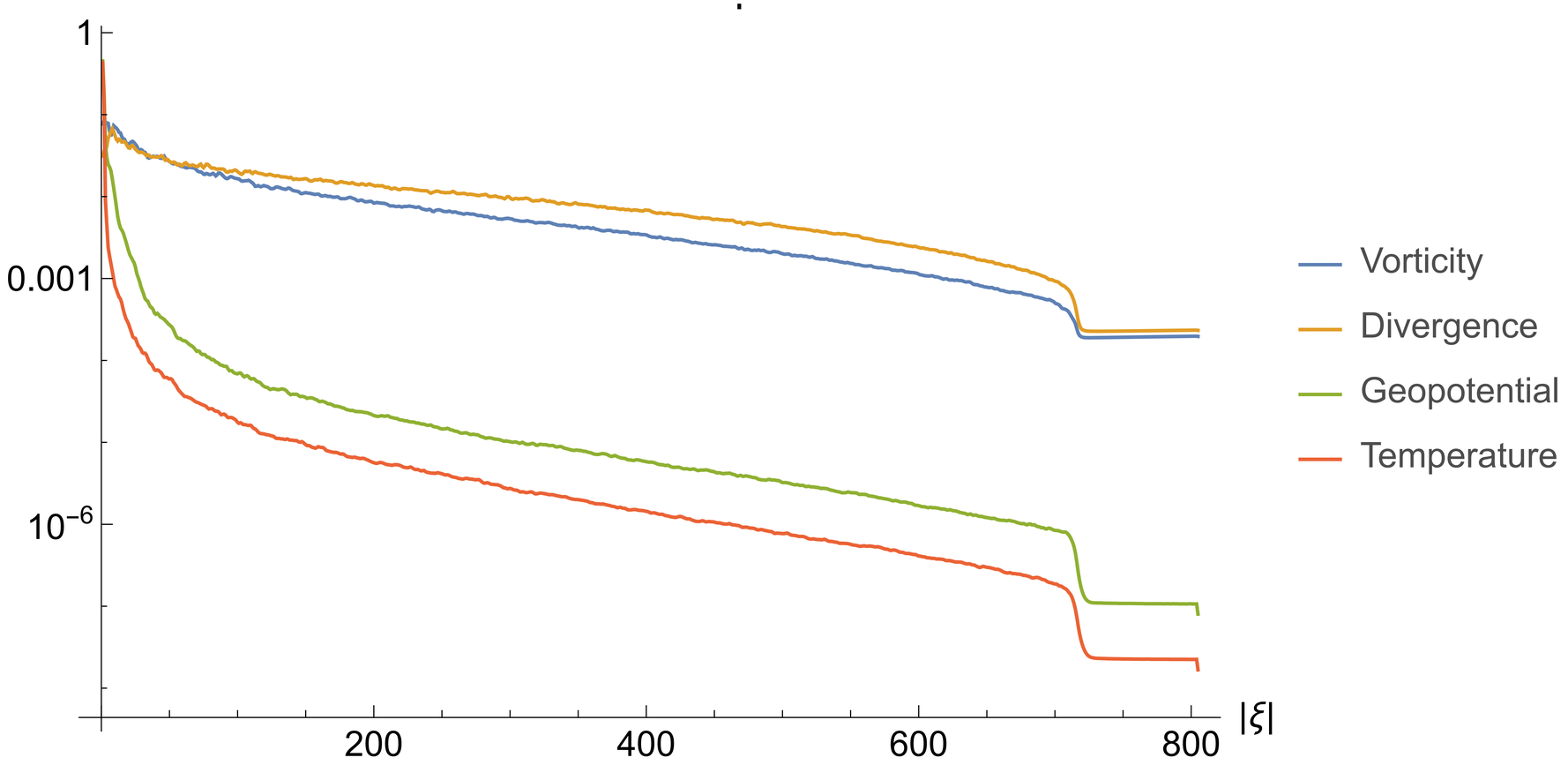


Multiformer

- Plug-and-play of fields
  - Fields can be added/removed with very limited computational effort
- Cross-attention allows for explicit introspection of interaction between fields
- Different physical fields with different properties have separate latent spaces (and transformations for these)

AtmoRep data



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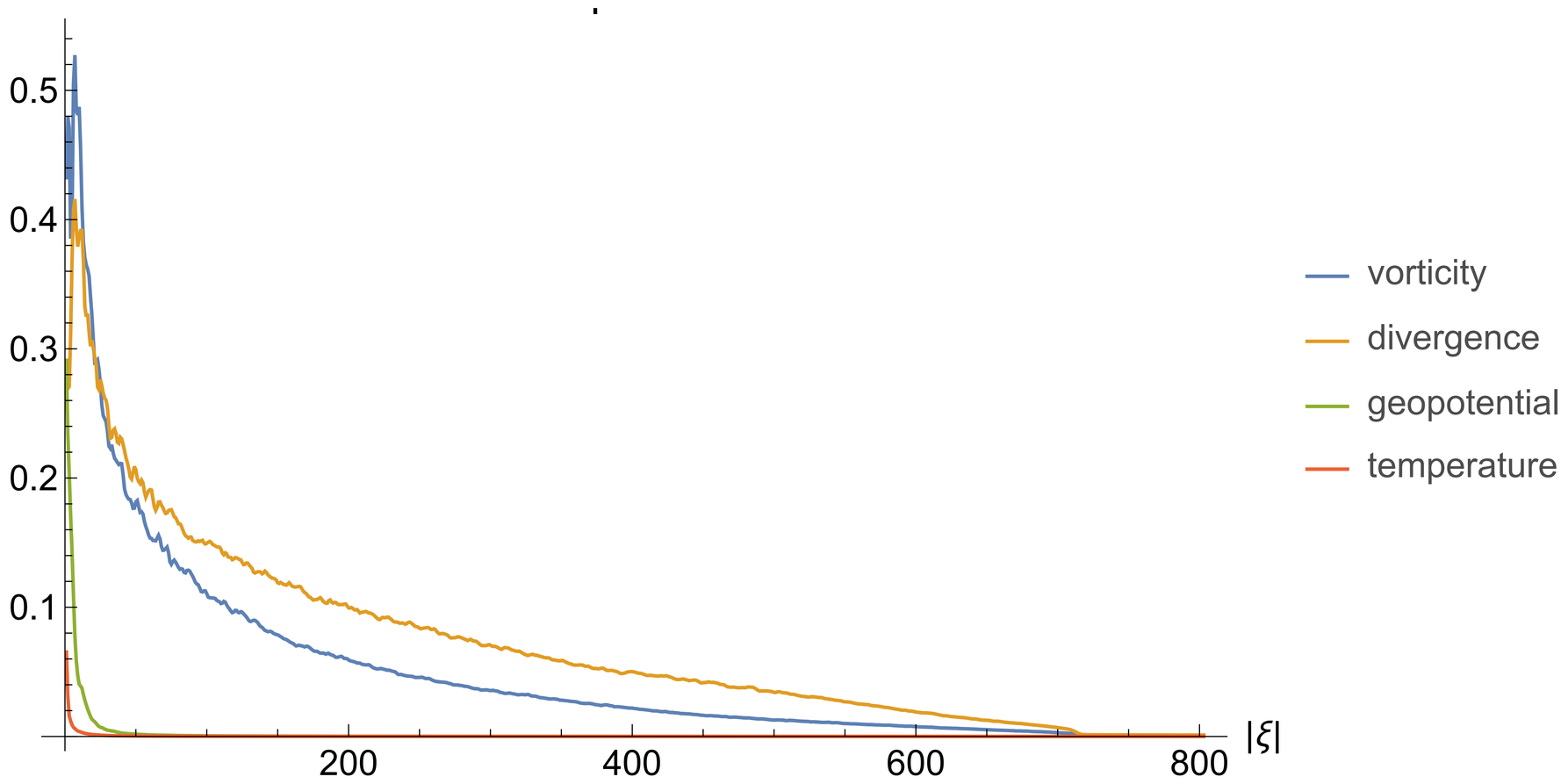
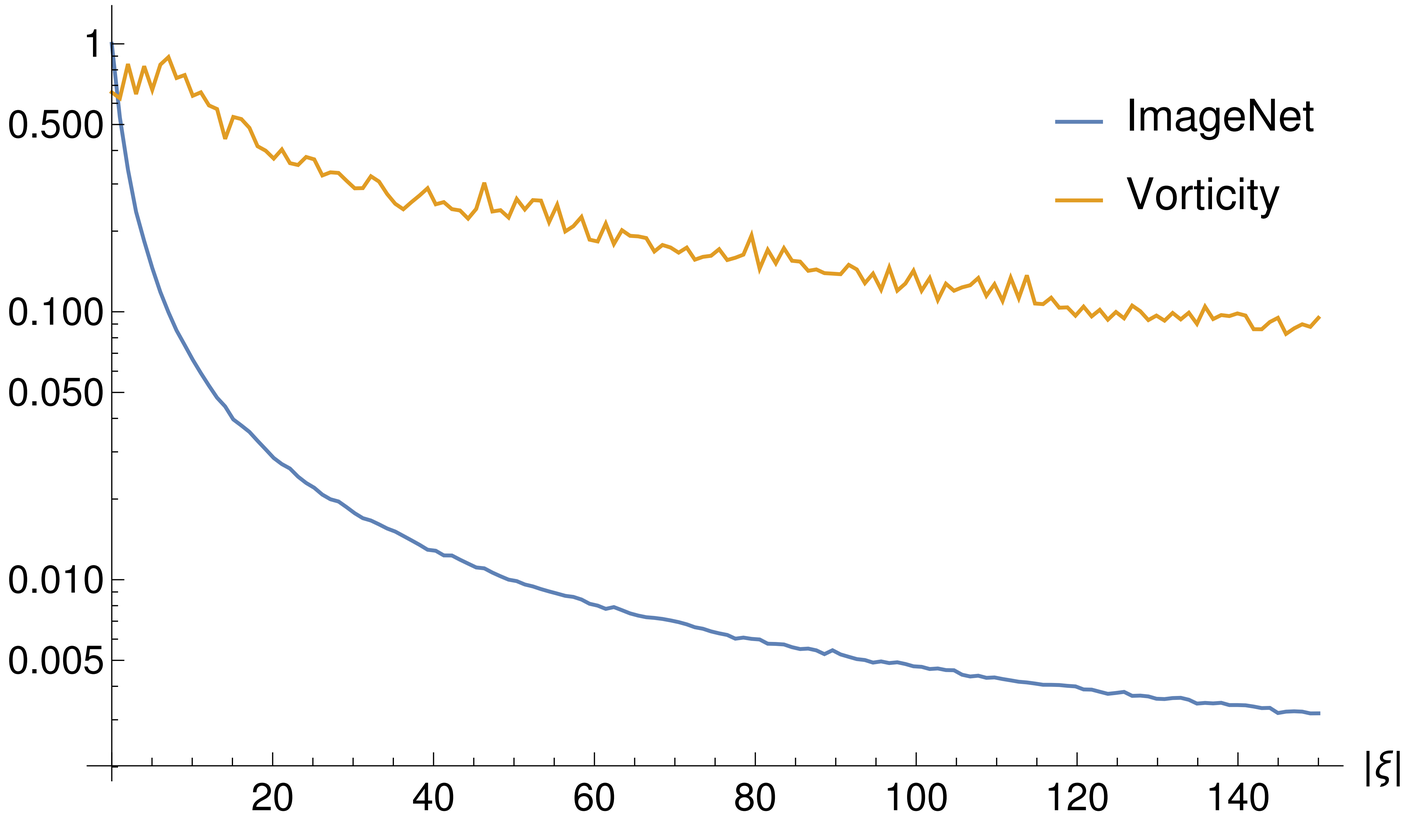


ERA5 versus ImageNet



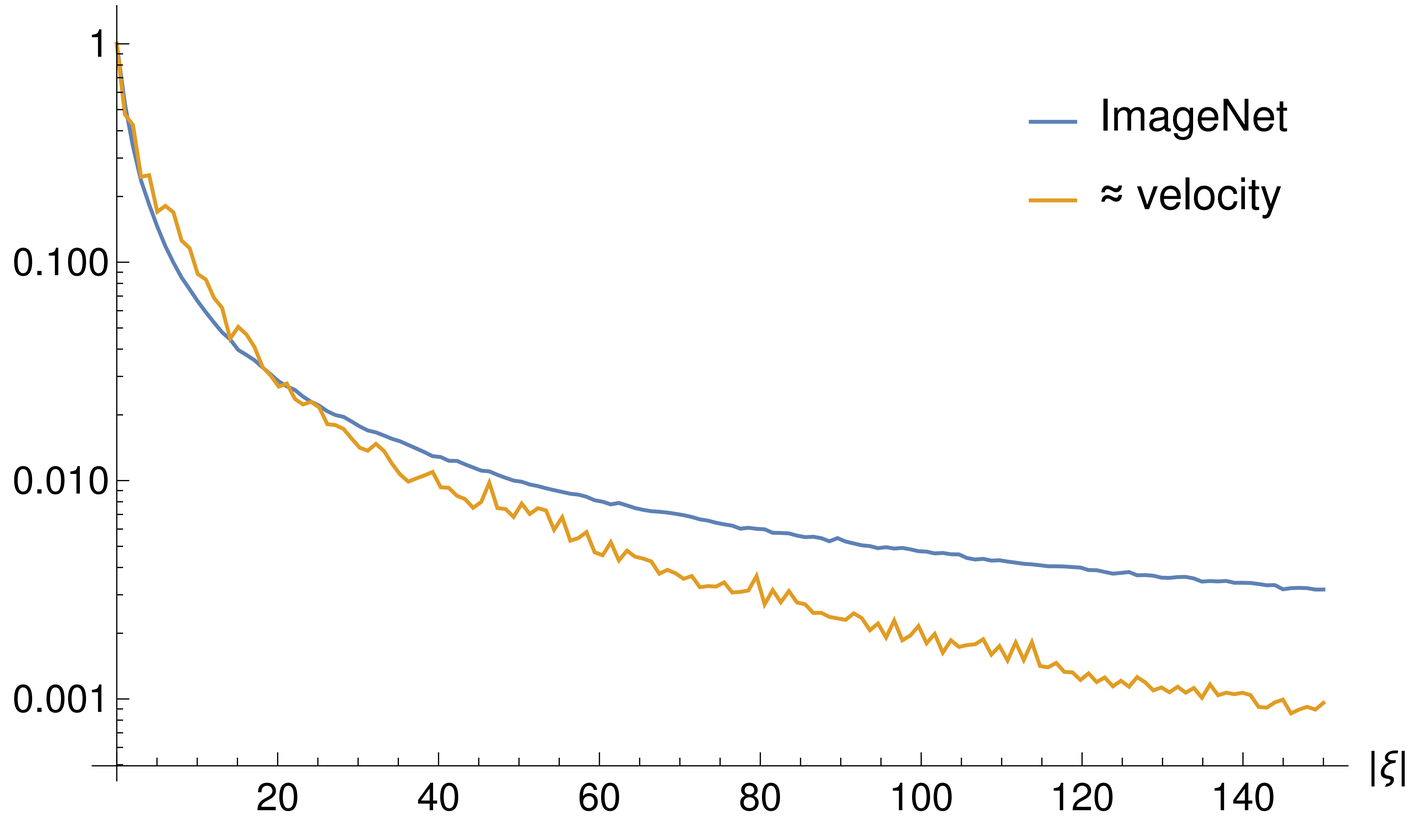
ERA5 versus ImageNet

stream function
velocity potential

velocity
vector field

vorticity
divergence

ERA5 versus ImageNet



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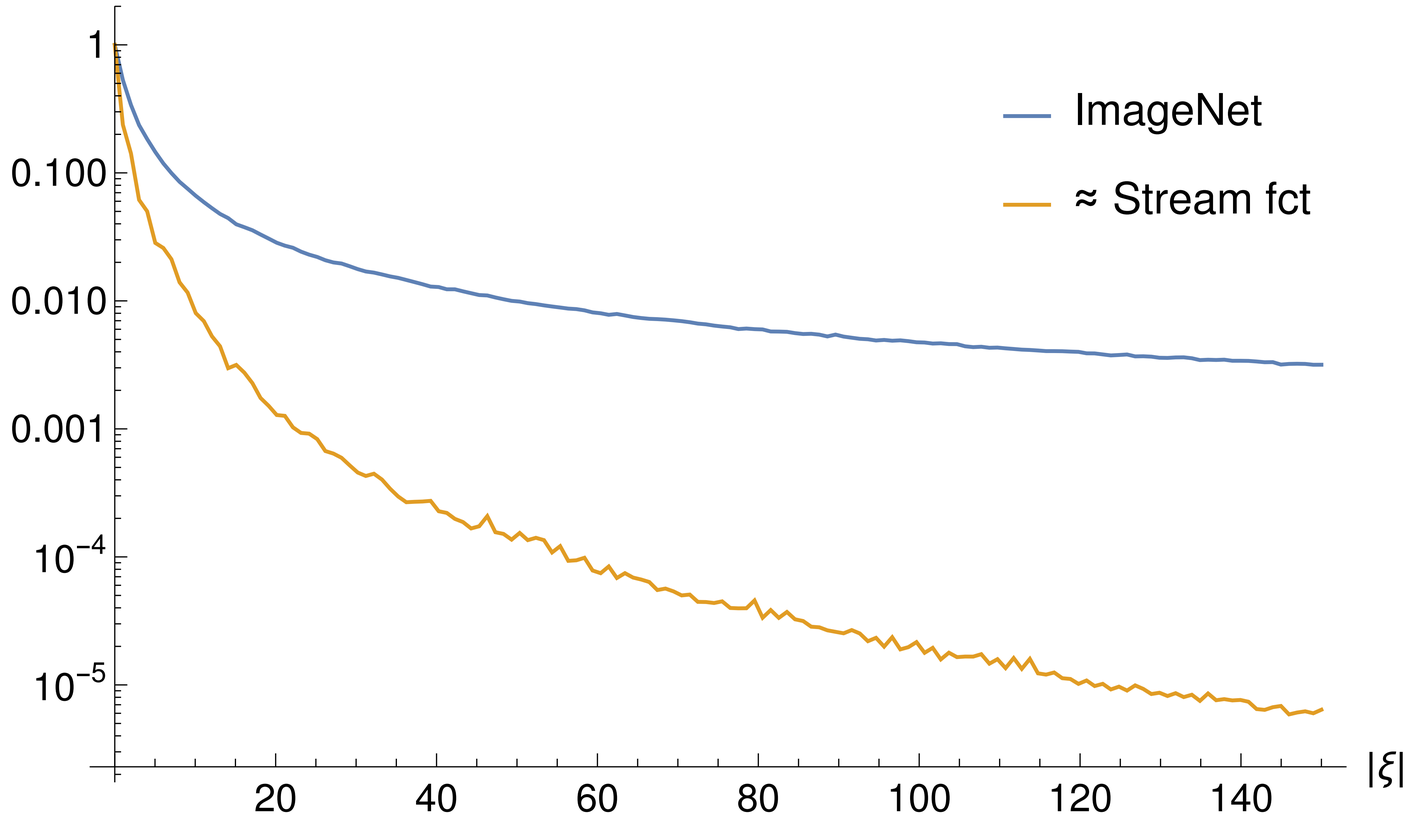

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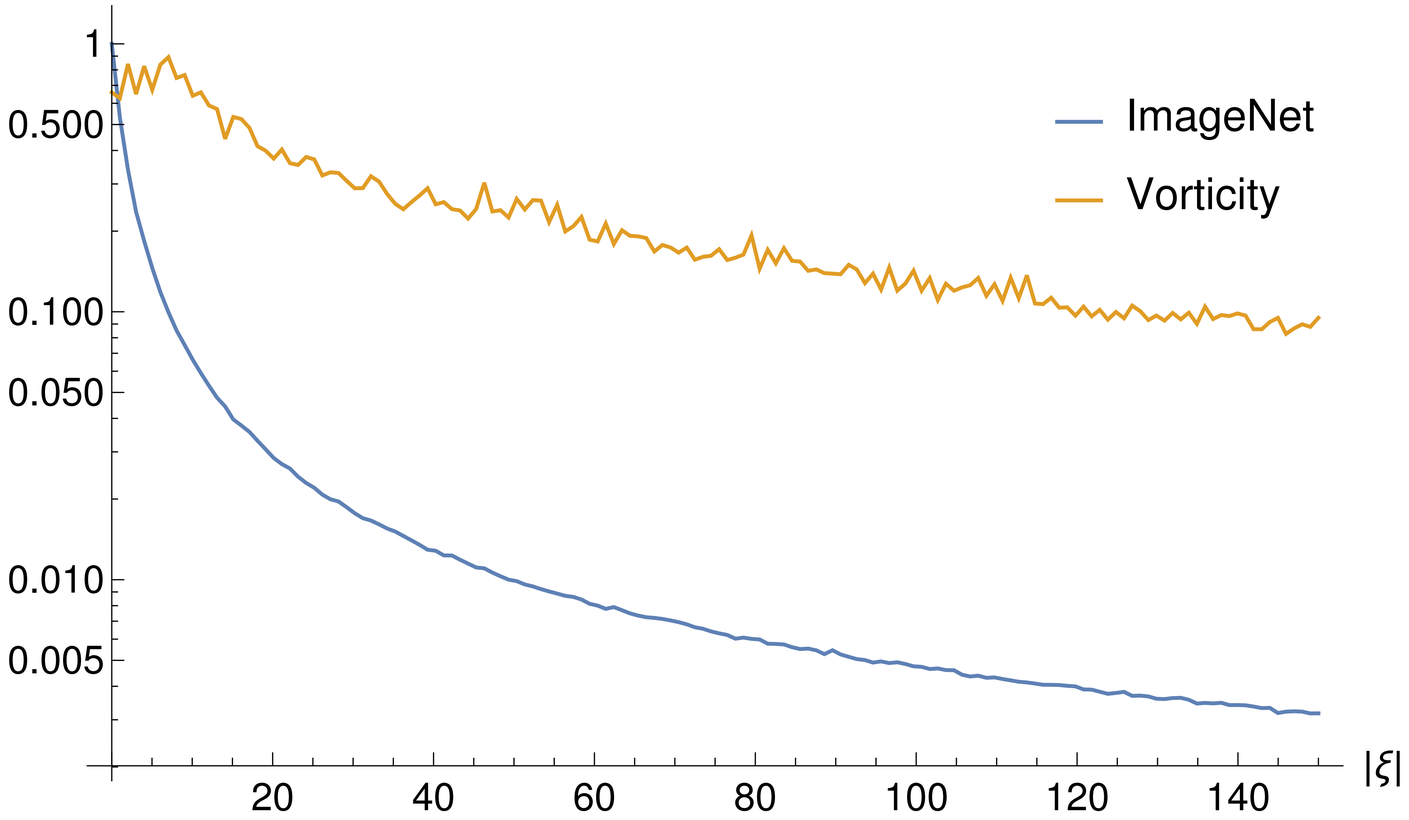
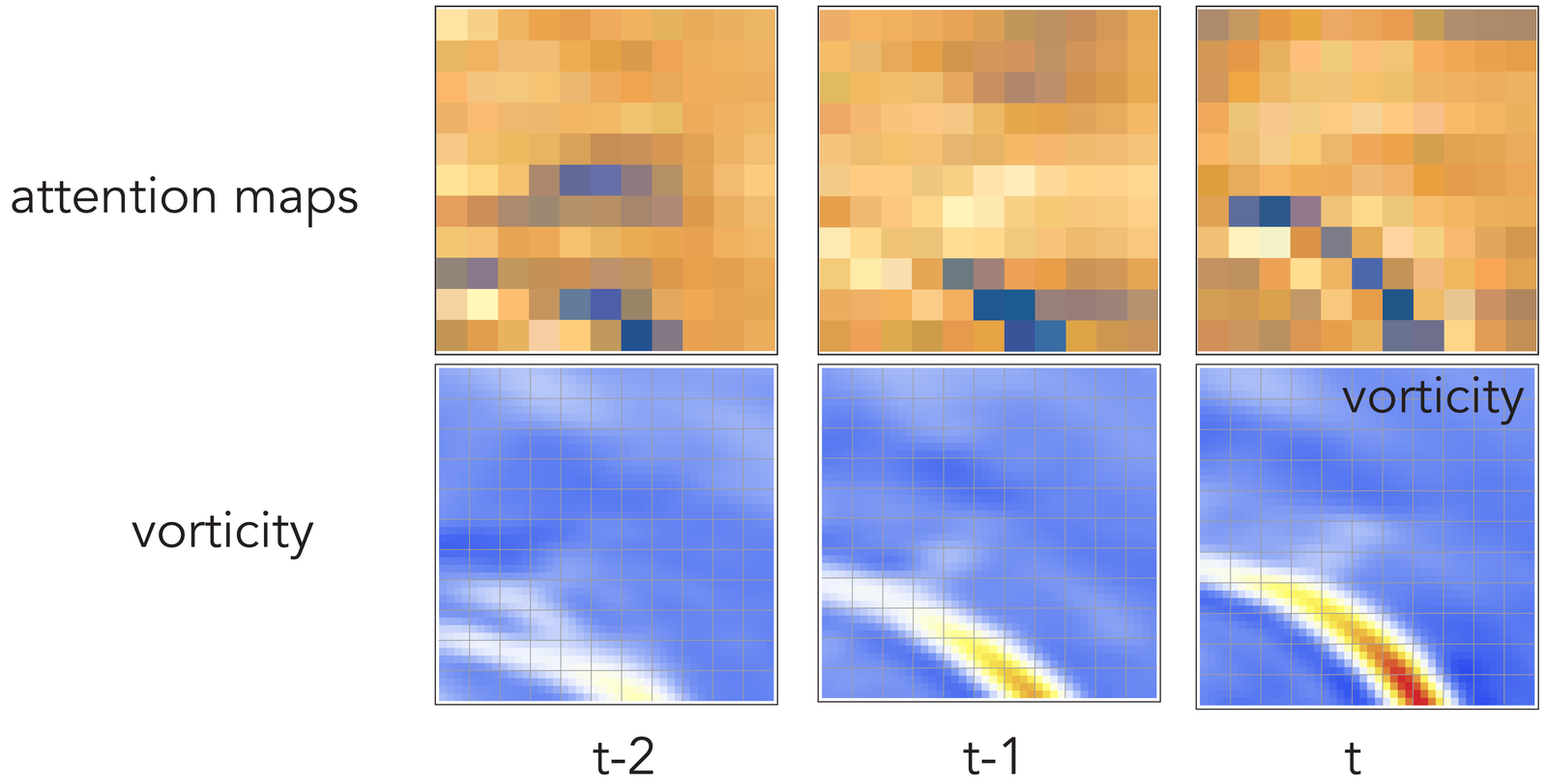


Statistical loss

- Attention maps:



Statistical loss

- Statistical loss:

$$\mathcal{L}_{\text{stats}} = \left| 1 - \int_{\mathrm{R}} \delta_y(x)\, G_{\tilde{\mu},\tilde{\sigma}}(x)\, \mathrm{d}x \right|^2$$

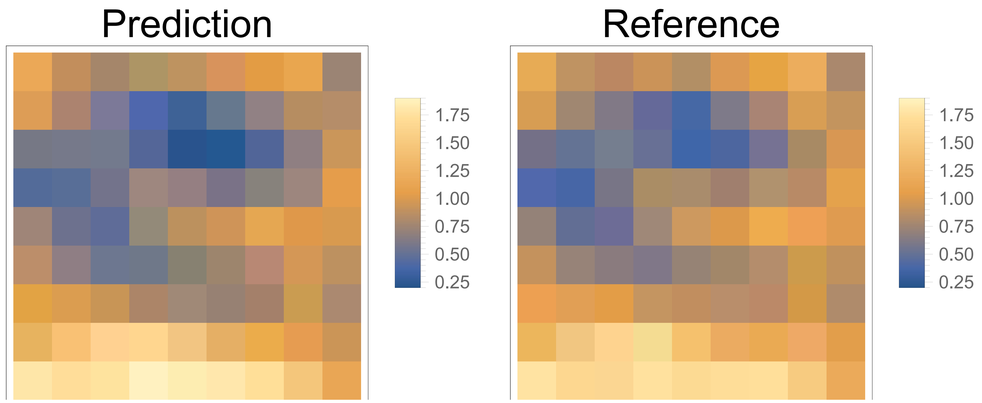
- CRPS:[1]

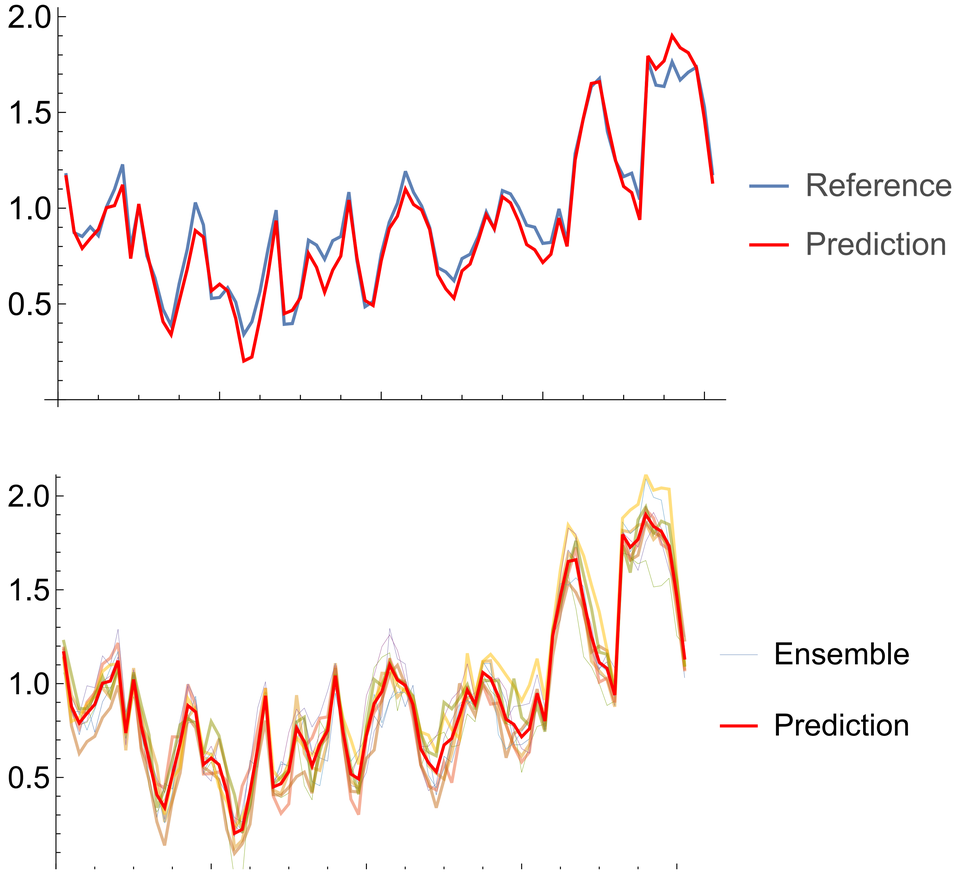
$$\mathcal{L}_{\text{CRPS}} = \int_{\mathrm{R}} \left| H_y(x)\, \mathrm{erf}_{\tilde{\mu},\tilde{\sigma}}(x) \right|^2 \mathrm{d}x$$

[1] S. Rasp and S. Lerch. Neural networks for postprocessing ensemble weather forecasts. Monthly Weather Review, 146(11):3885 – 3900, 2018.

Statistical loss

- Predictions:





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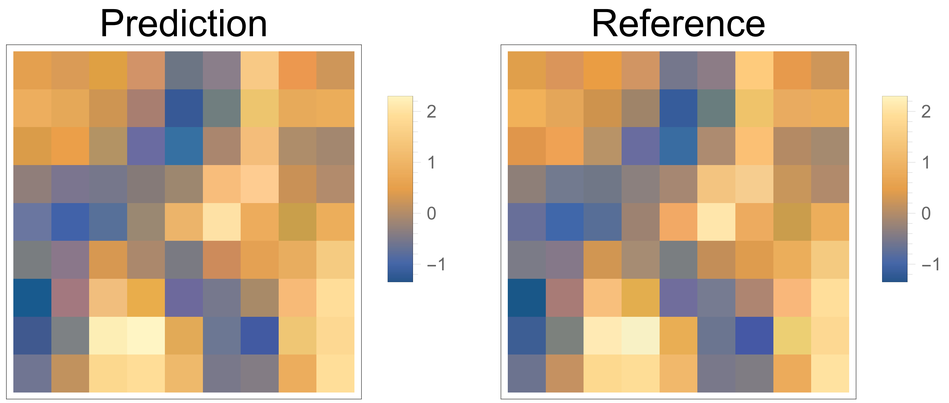

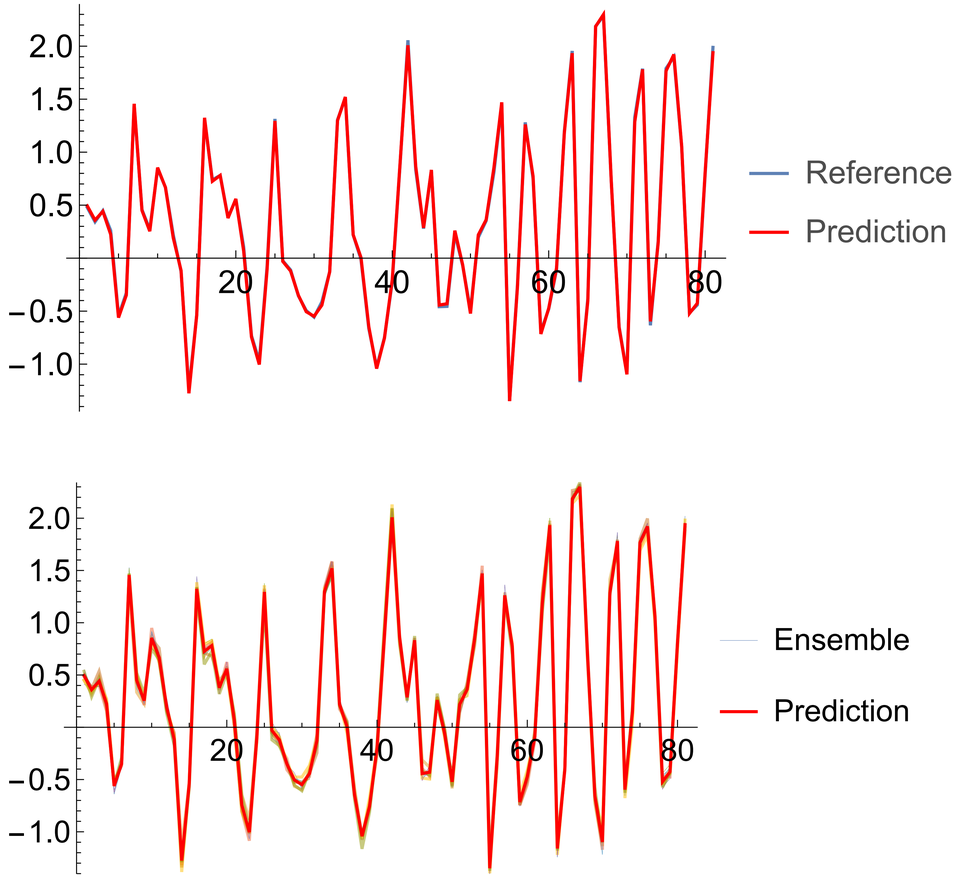

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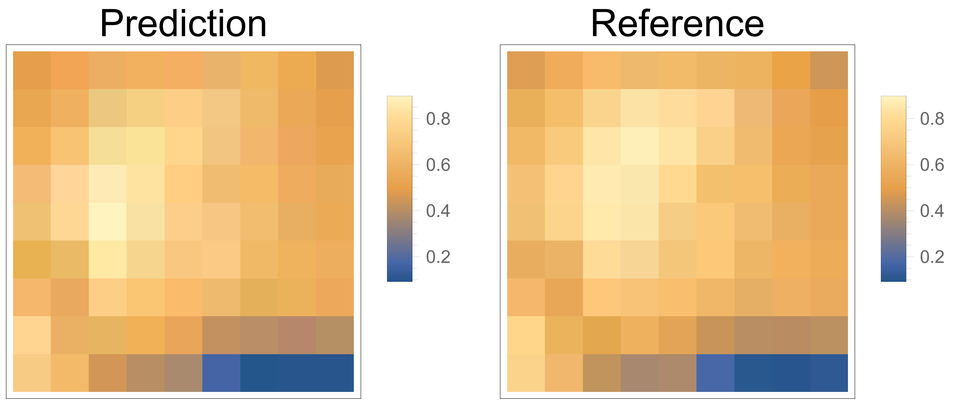
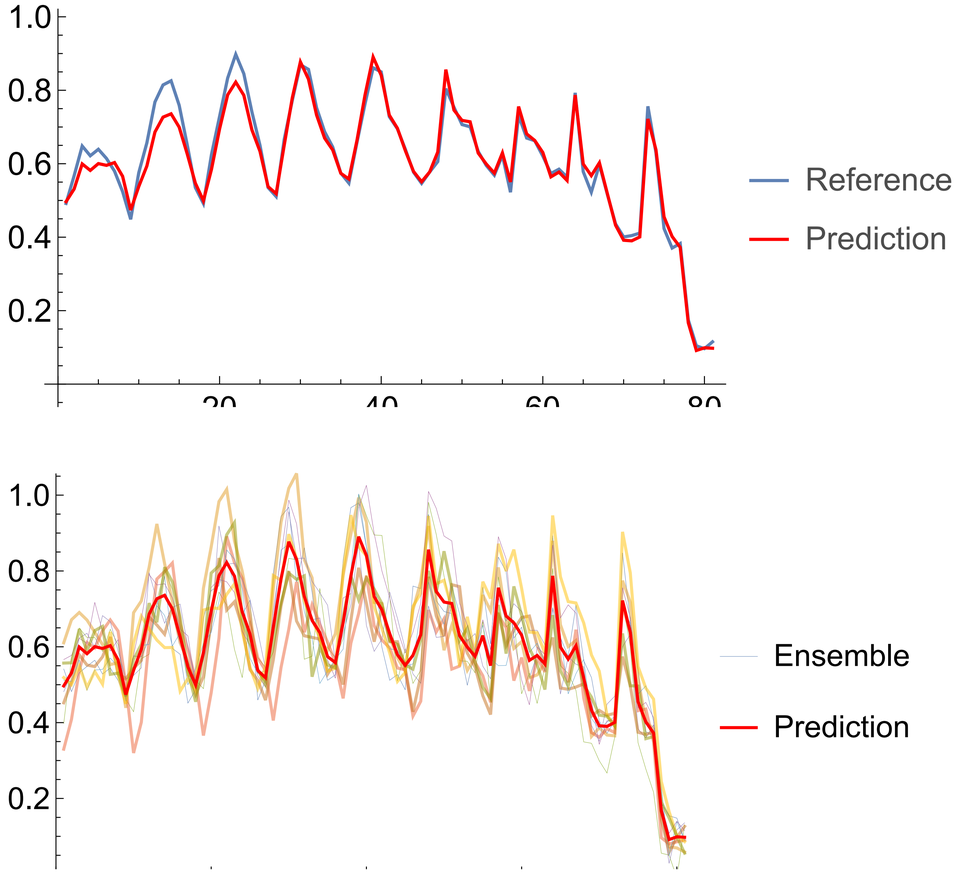
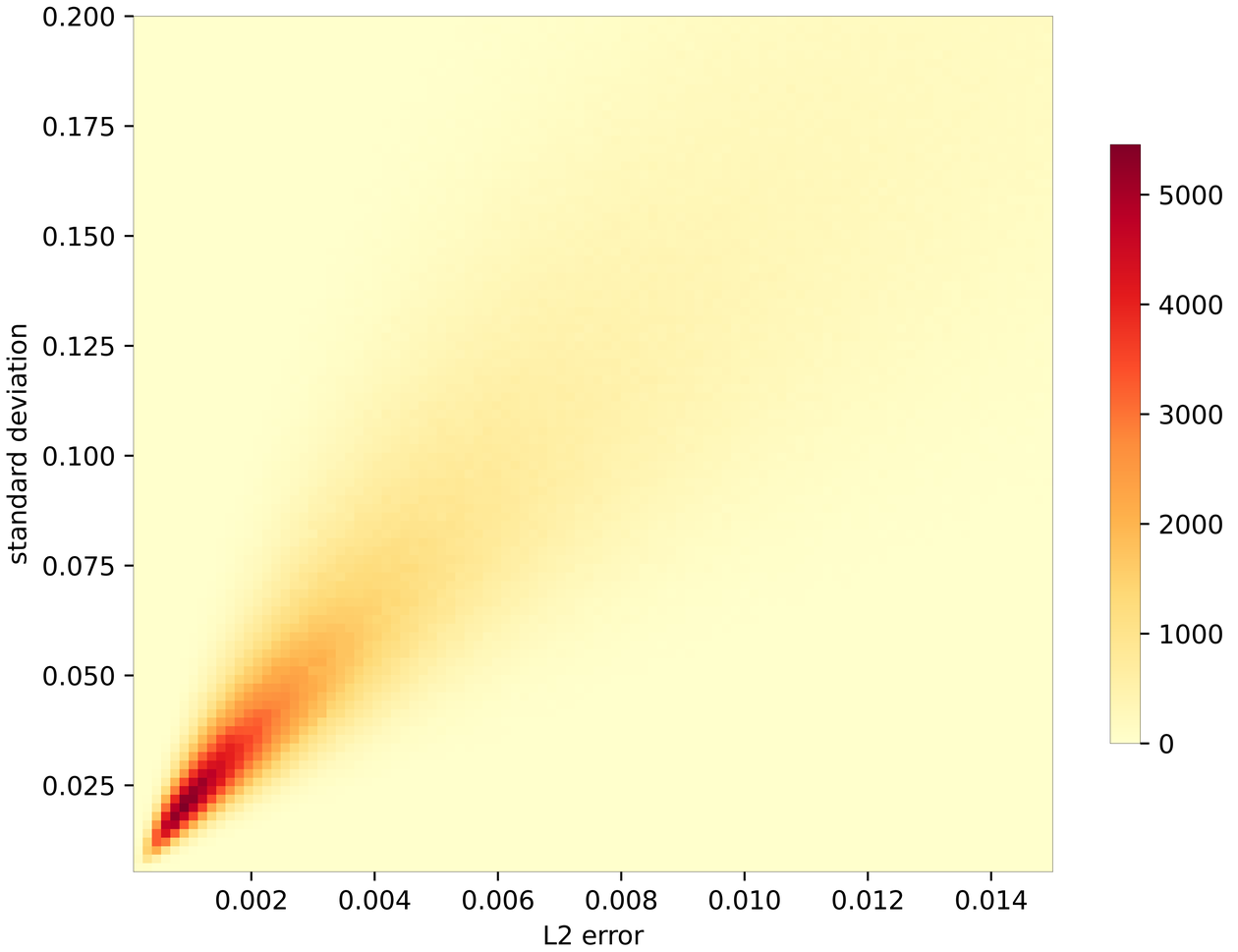


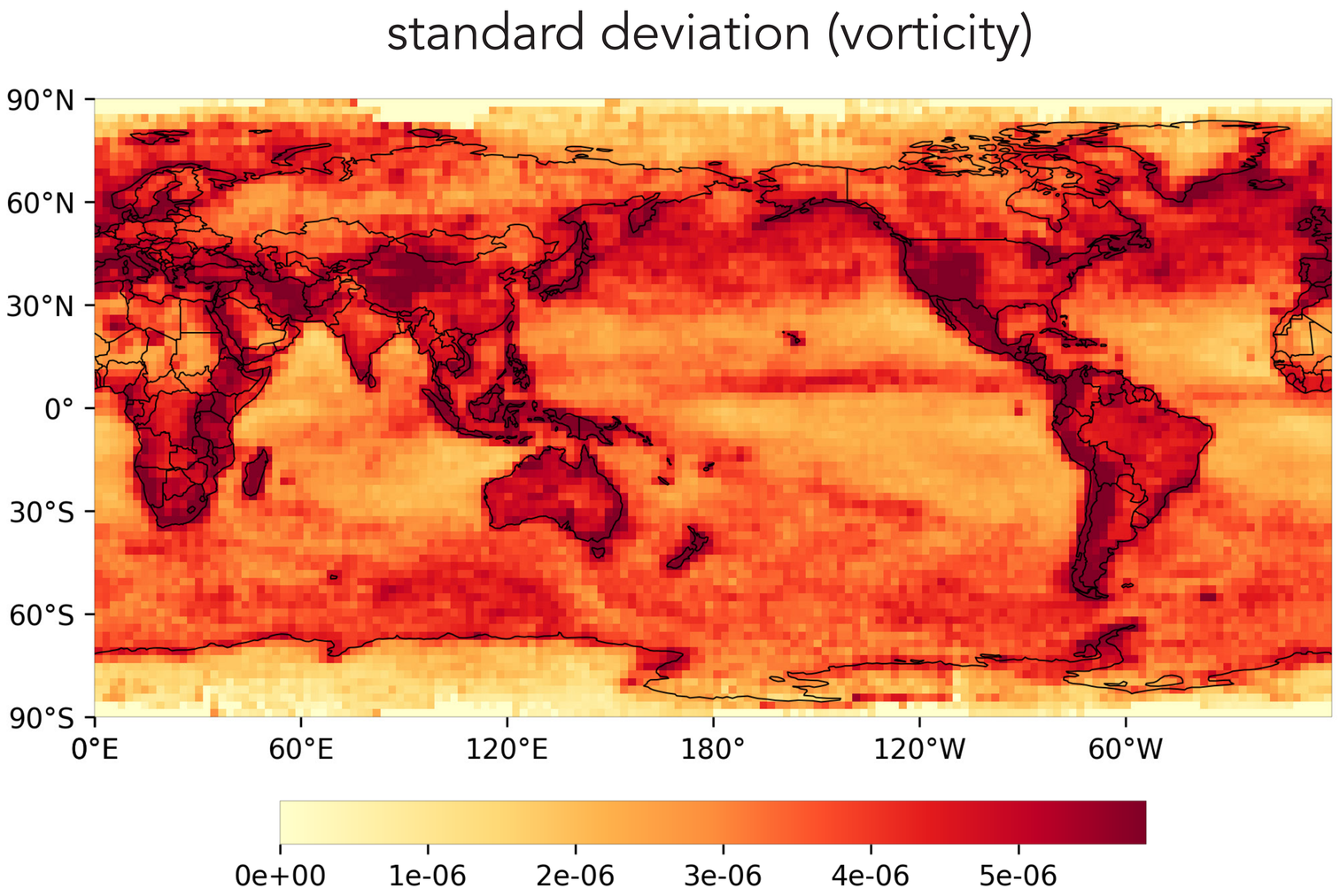


Statistical loss



2D Histogram of L_2 error vs. std. dev. (temperature)

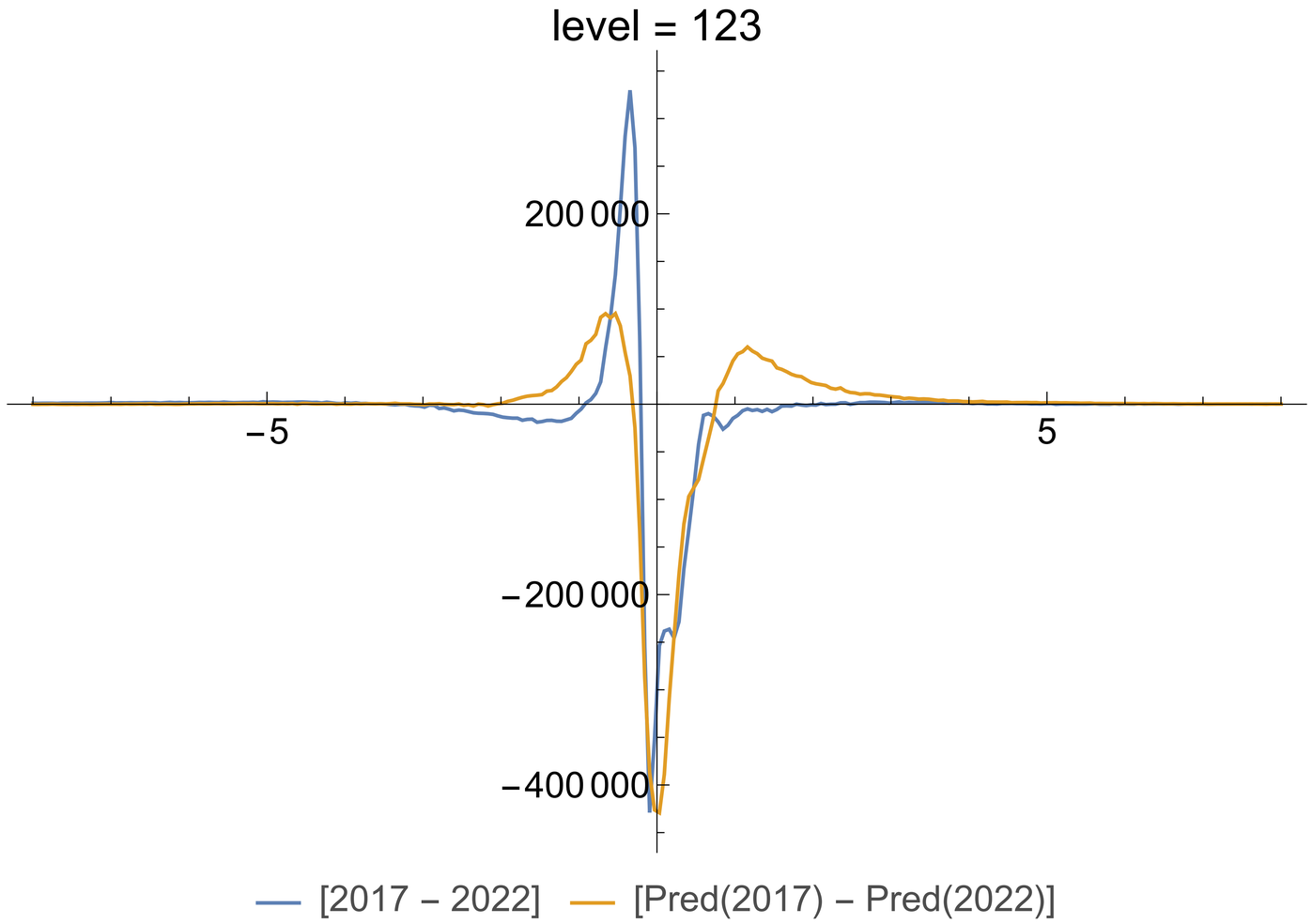
Statistical loss



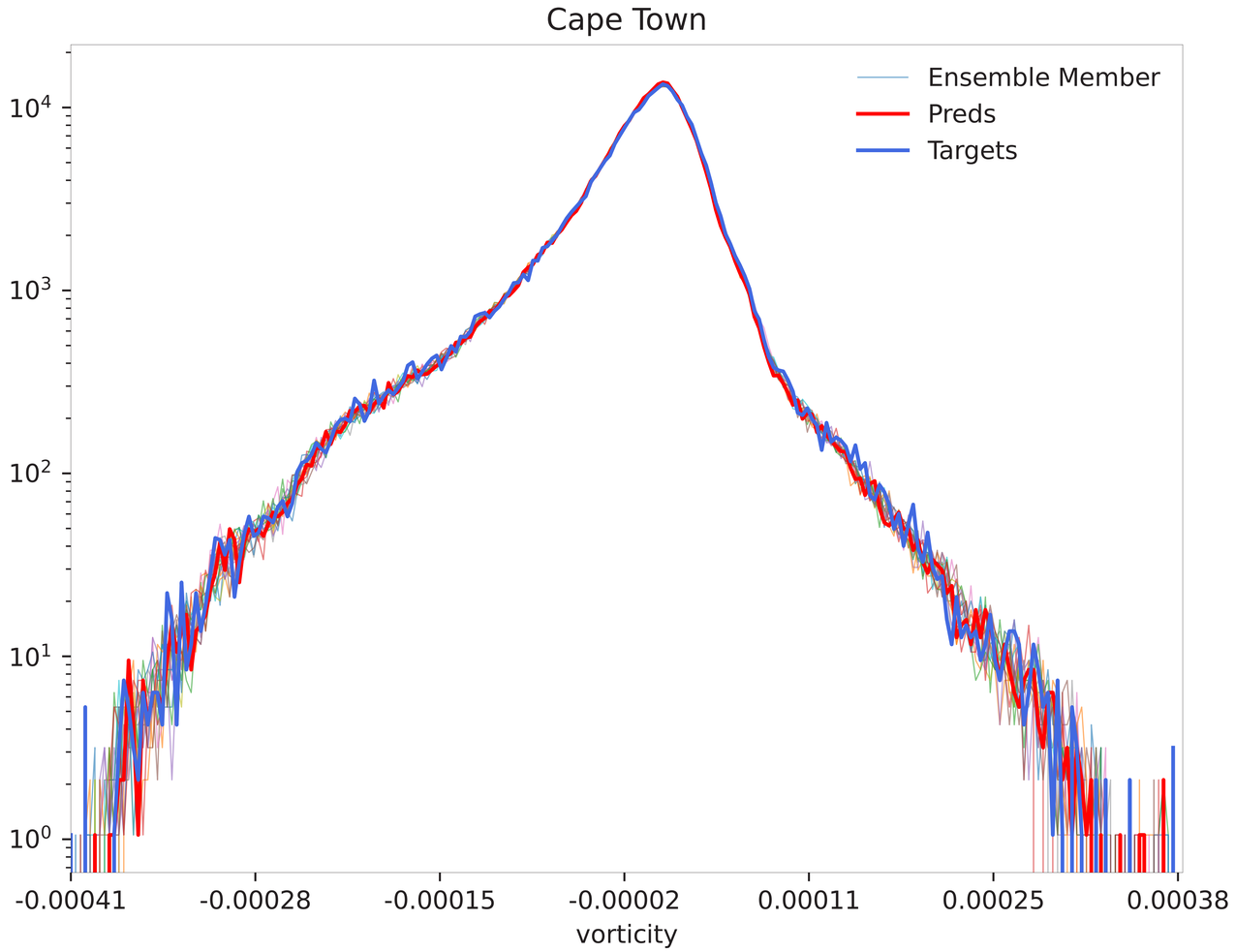
Some observations on training

- No overfitting
  - No difference between train and test set even with few months and limited spatial domain
- Different fields behave rather differently
  - Masking ratios have to be chosen differently
  - Statistical loss performs differently
- MSE loss accross fields not comparable and misleading

Counterfactuals: extrapolation



Pre-training results



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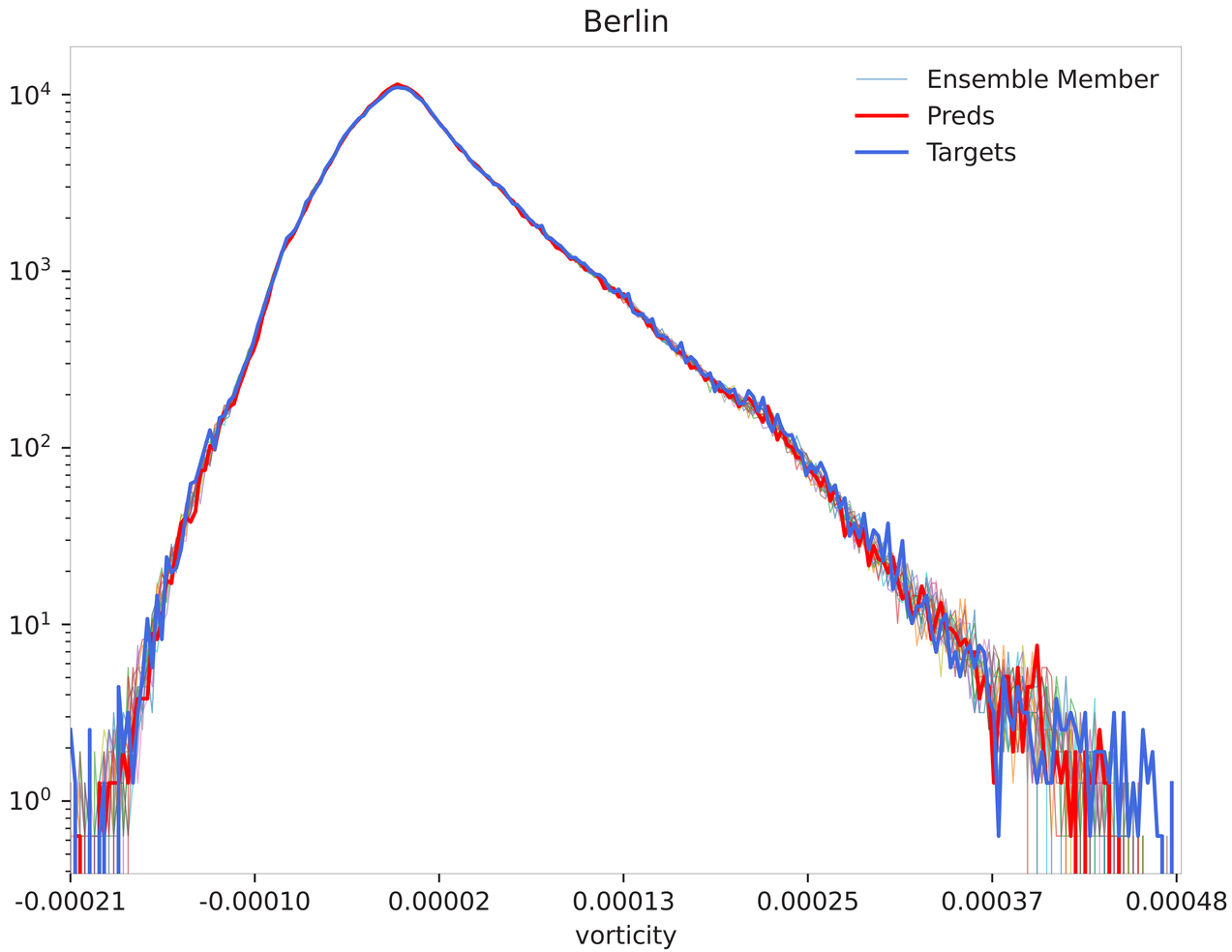


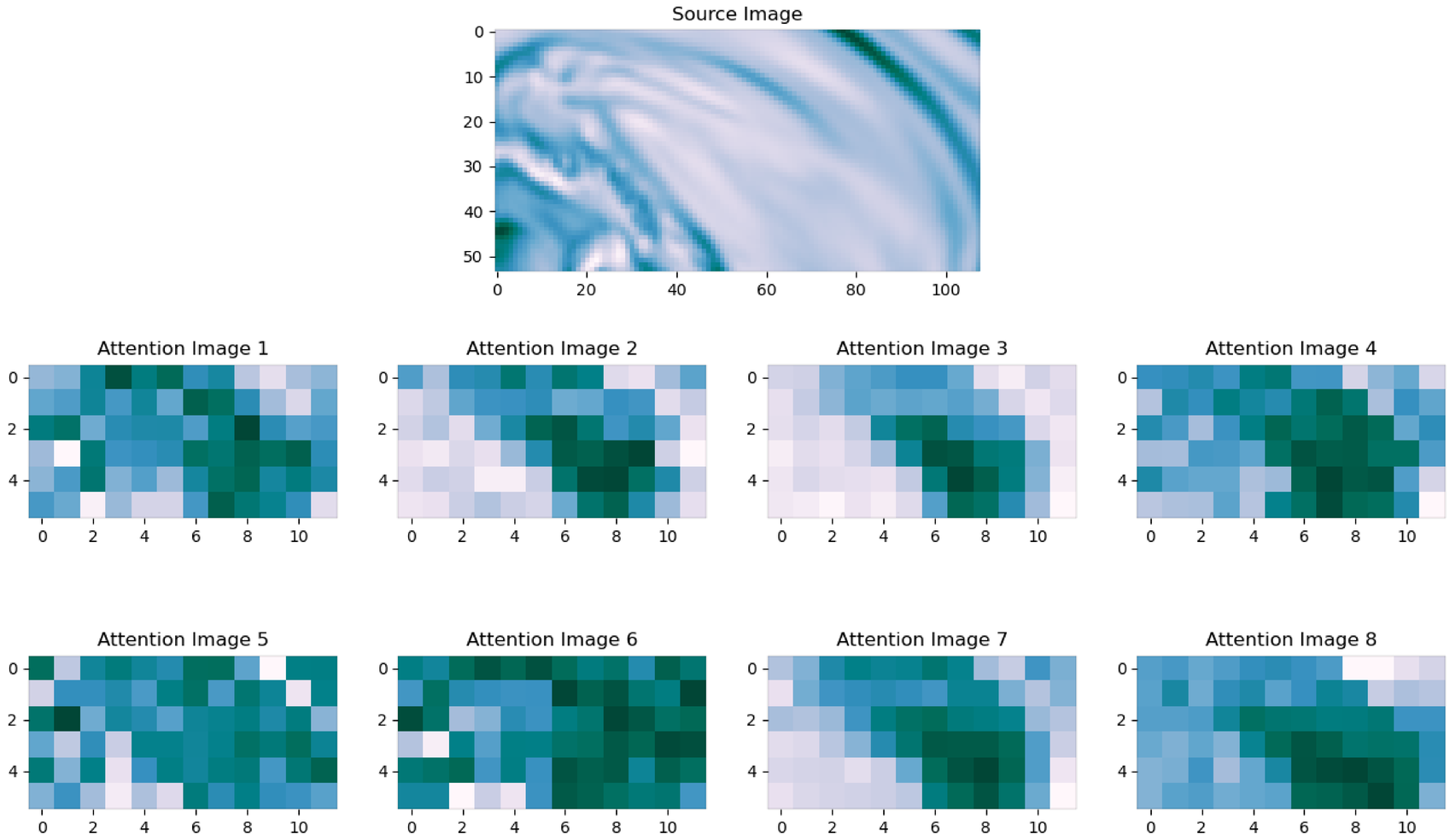
Training on observations

- Neural networks are models that work well on heterogenous and noisy data
- Fine-tune/bias correct a pre-trained model with observations (instead of training from scratch)

Can one continuous update a model with observations?

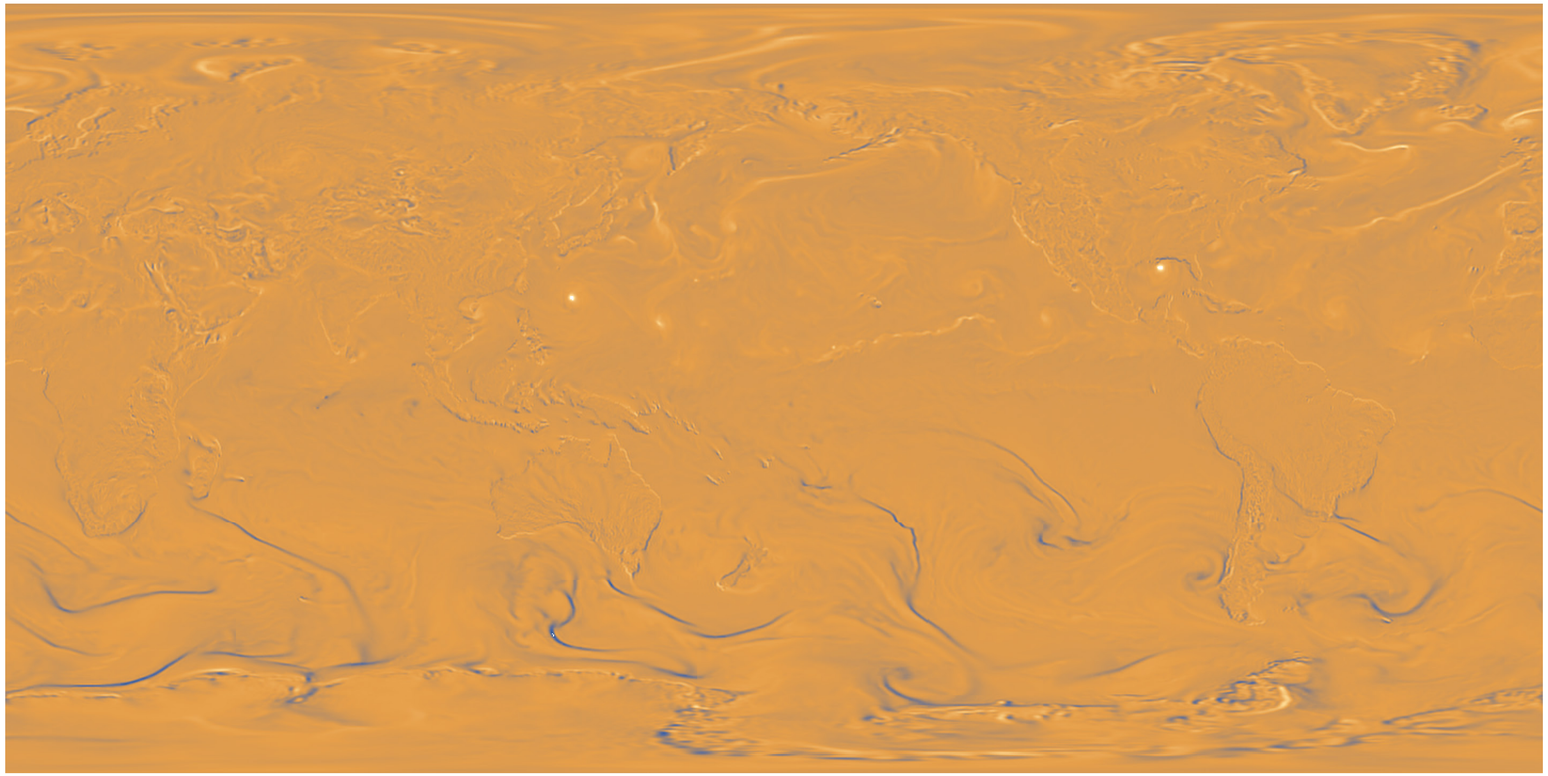
How to handle and propagate uncertainties?

Physics of trained network



Medium range forecasting

- How to do global forecasts with a local model?



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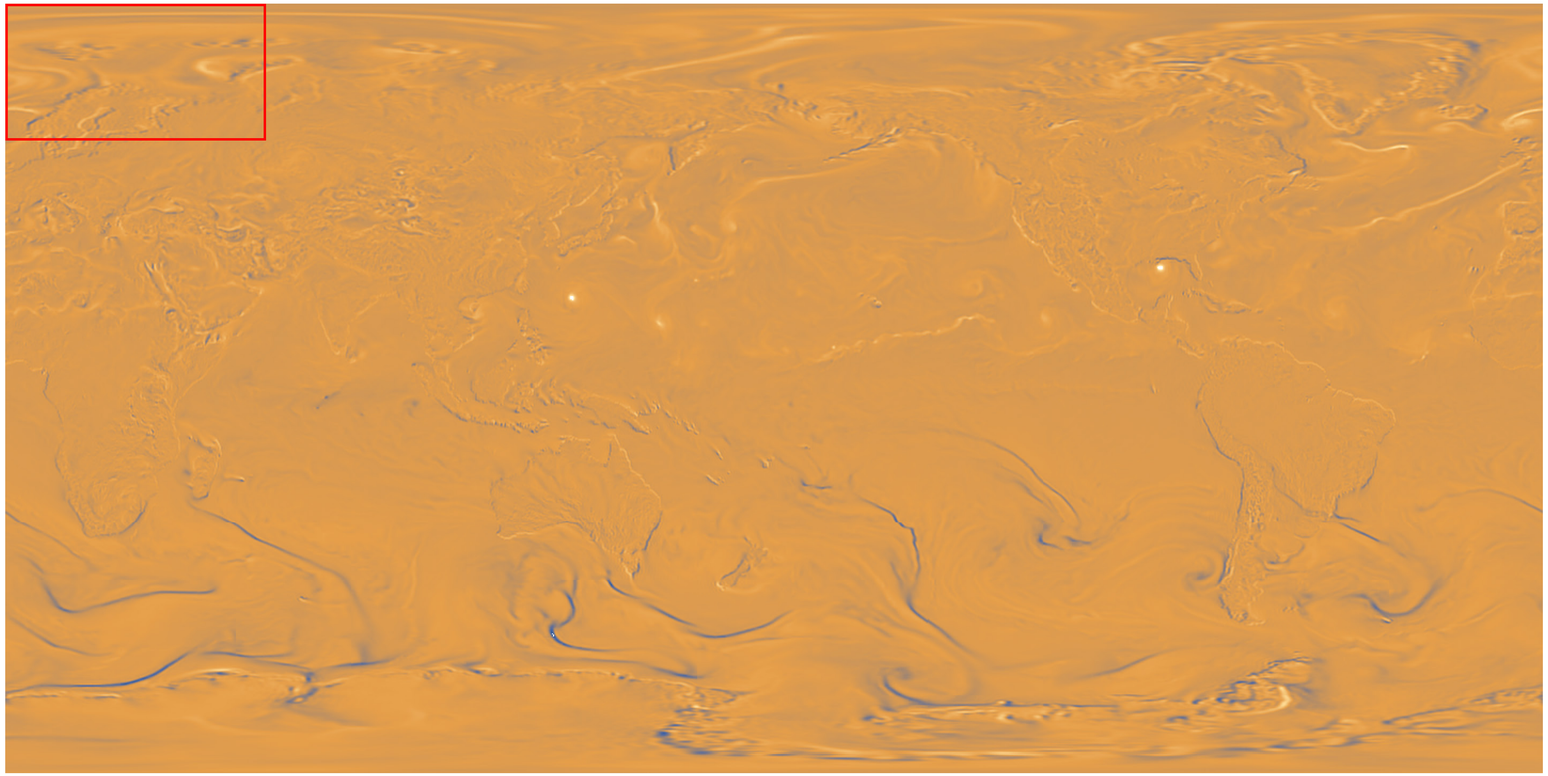

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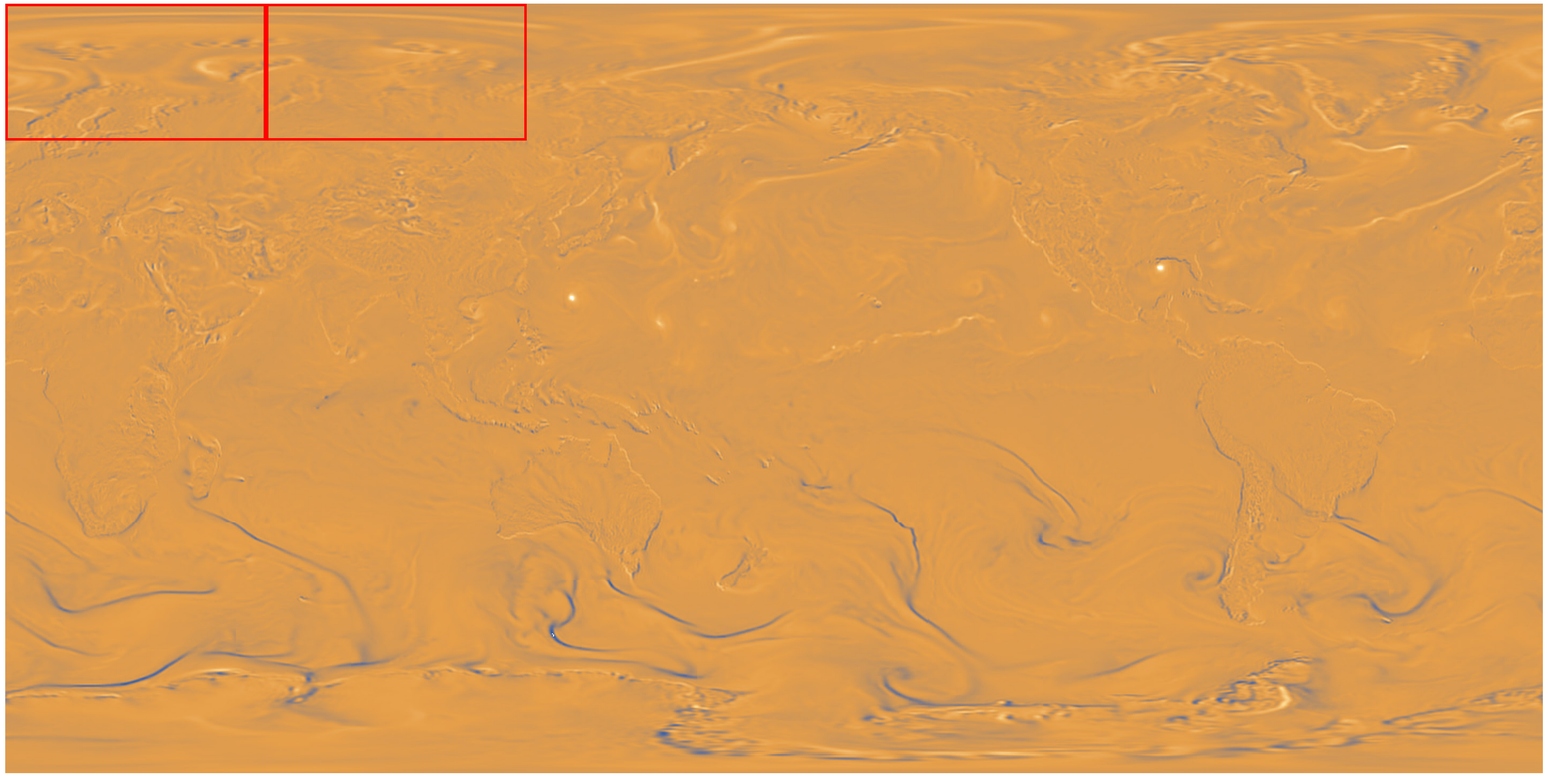

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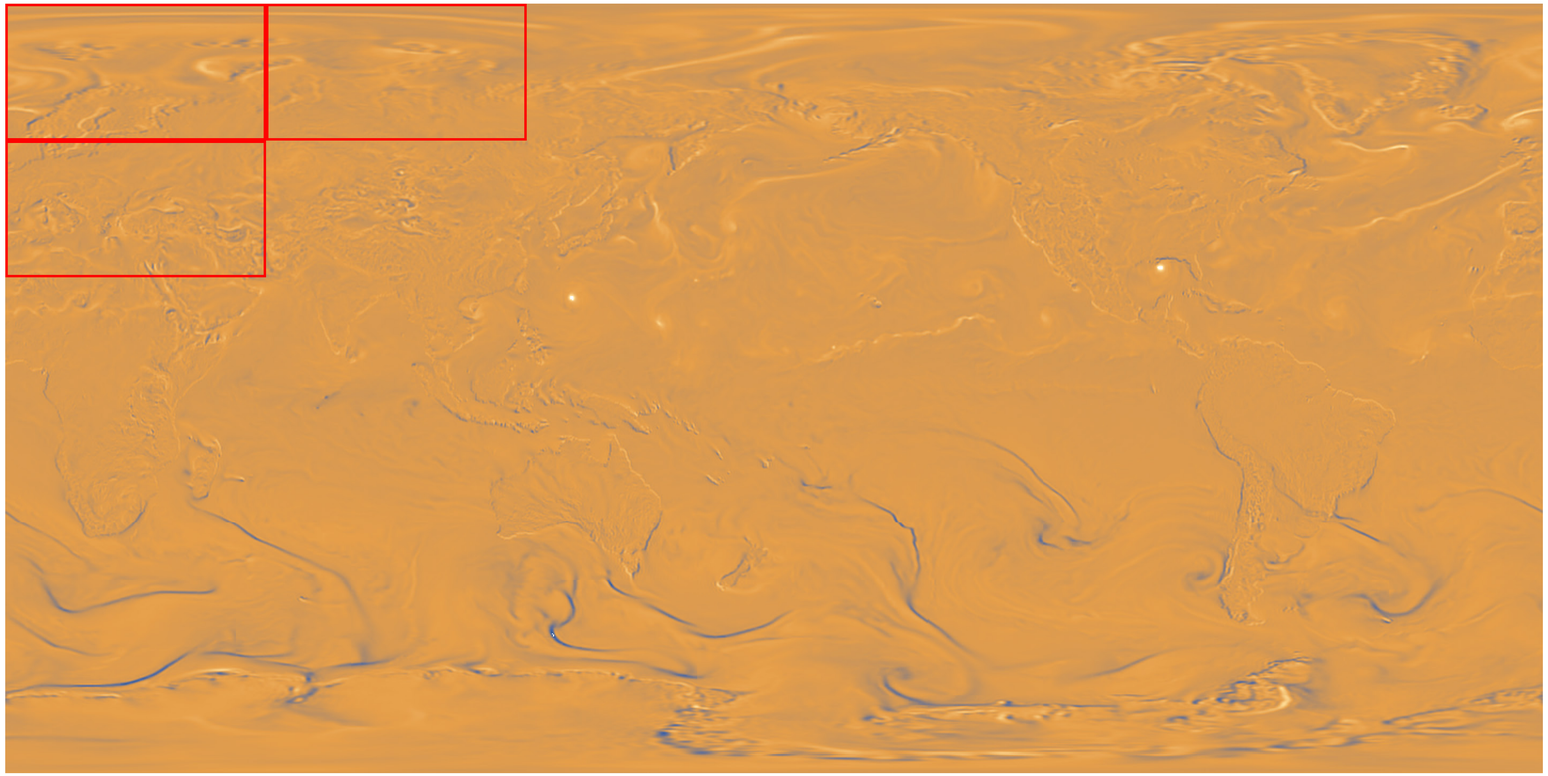

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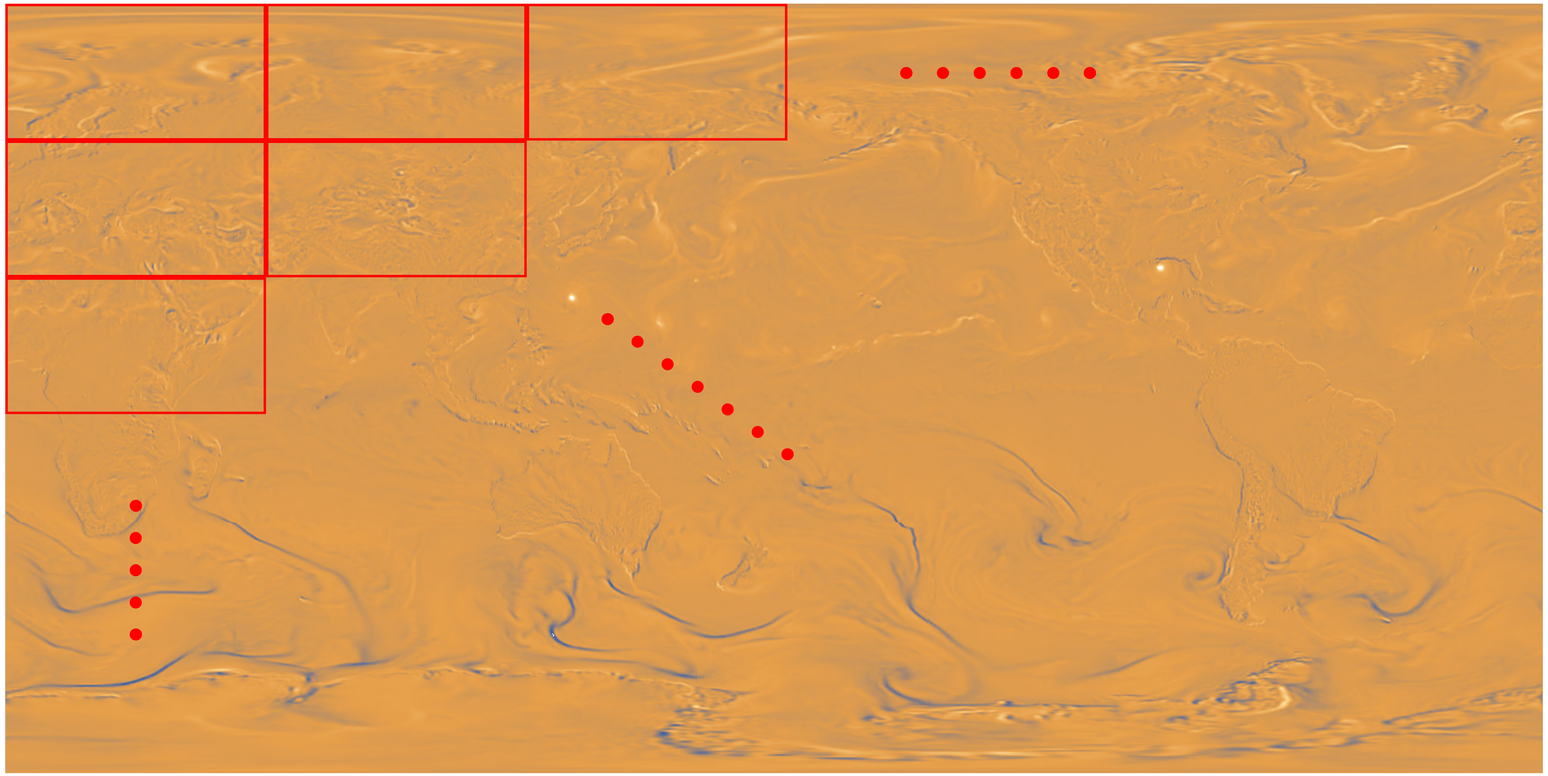

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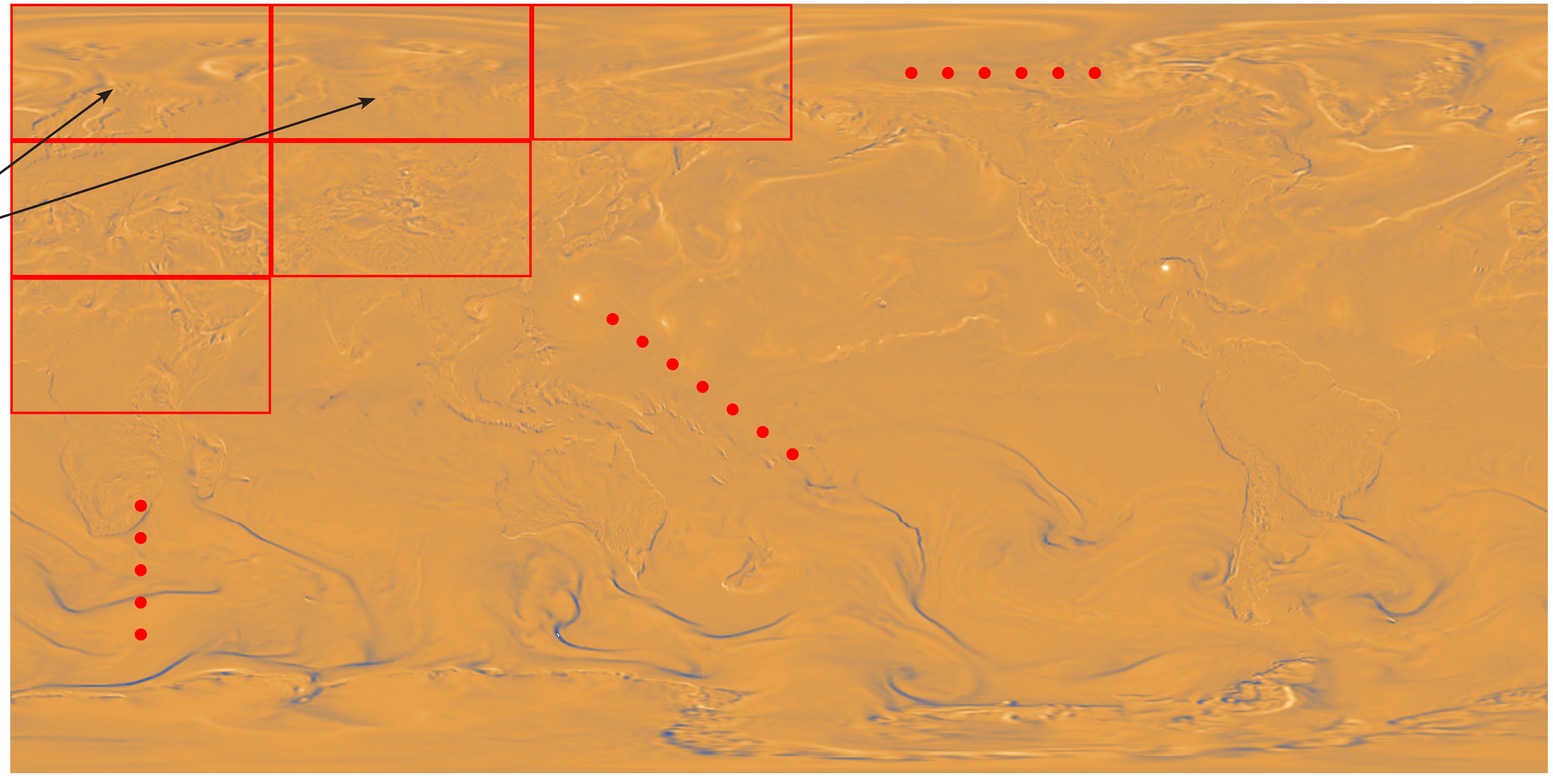

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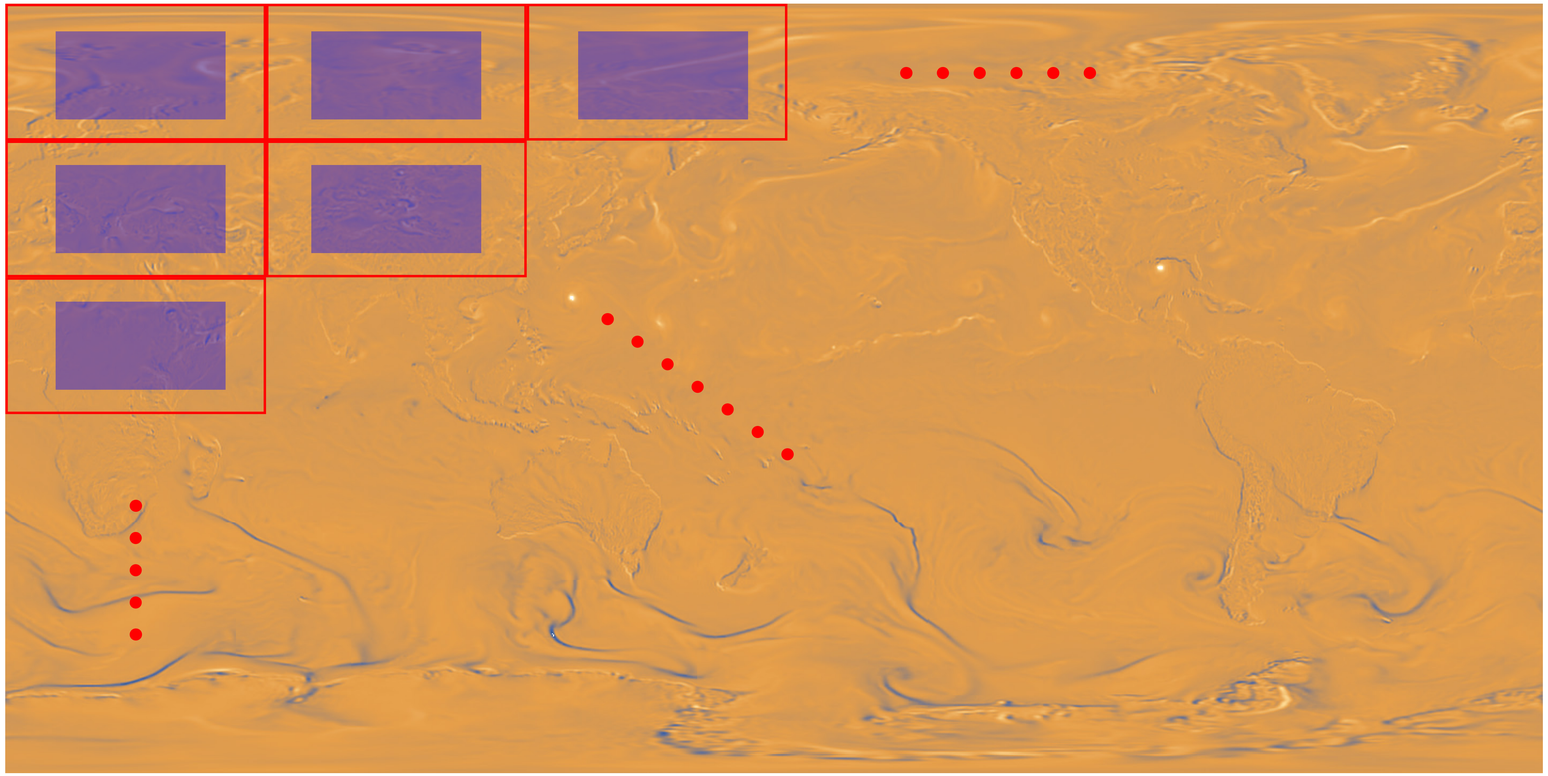

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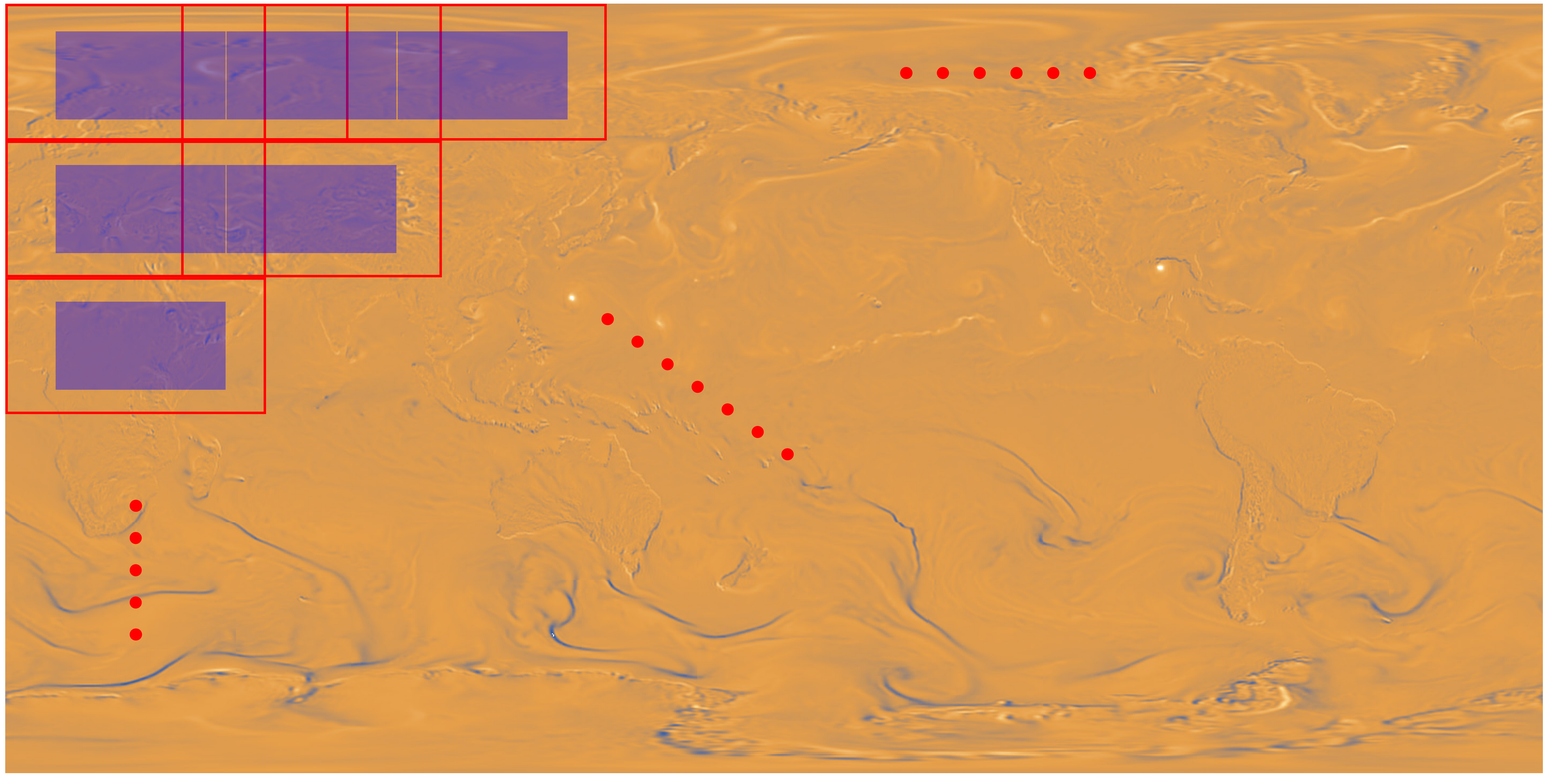

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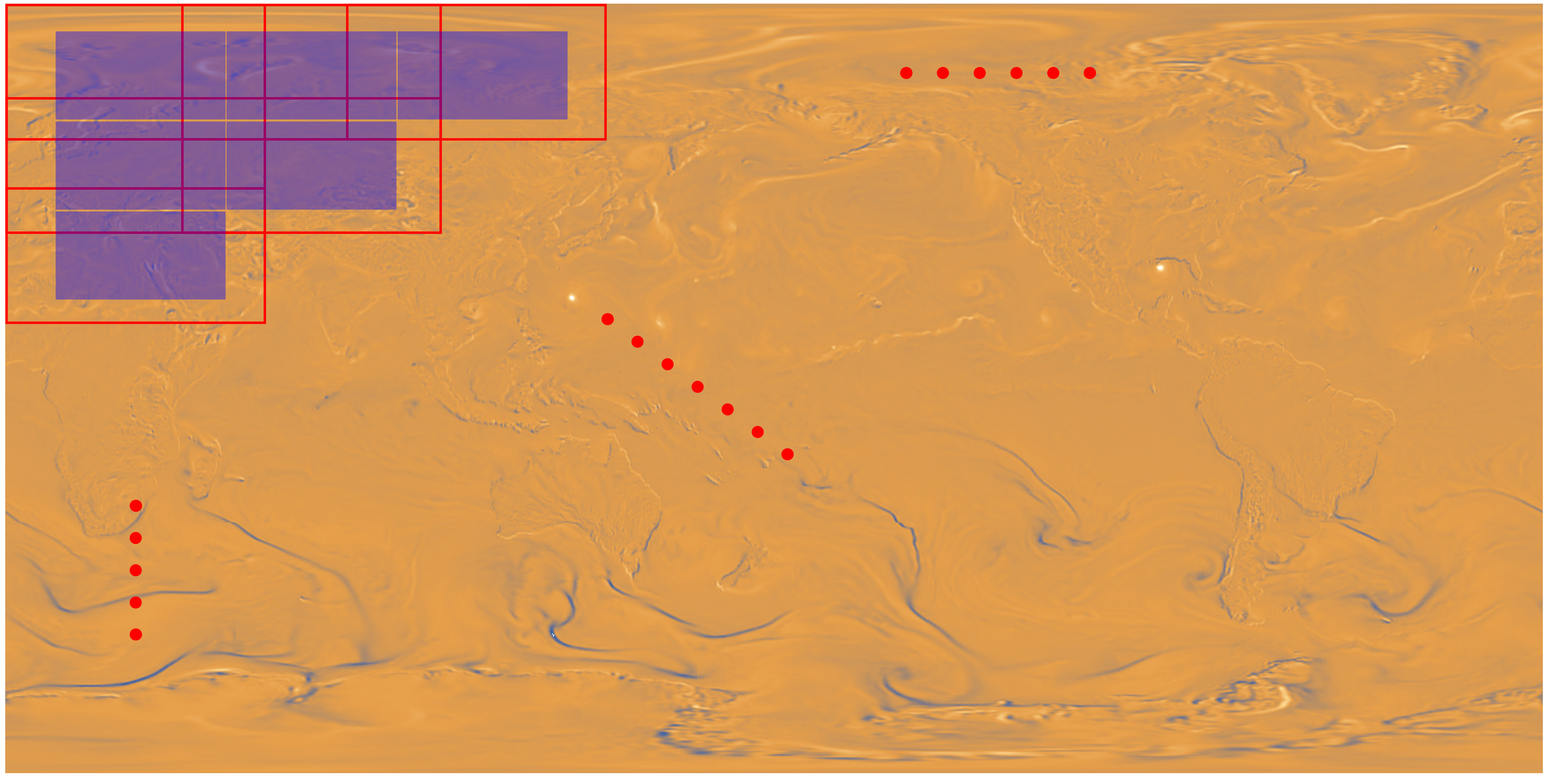

Multiformer: standard configuration

- Per token: $\alpha = \left(\mathrm{year}, \mathrm{day}, \mathrm{hour}, \mathrm{ml}, \theta, \phi, \mathrm{res}\right)$

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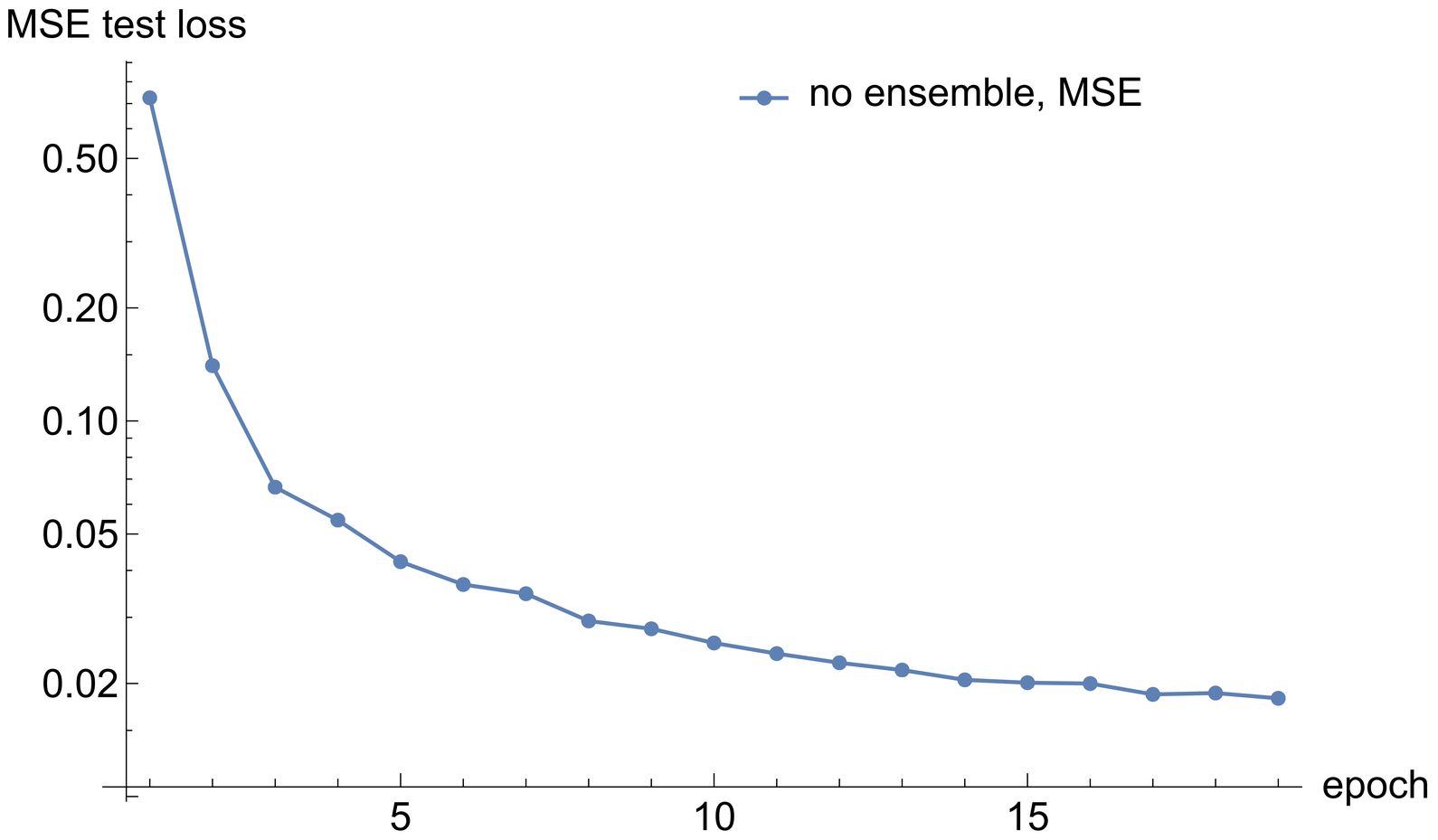
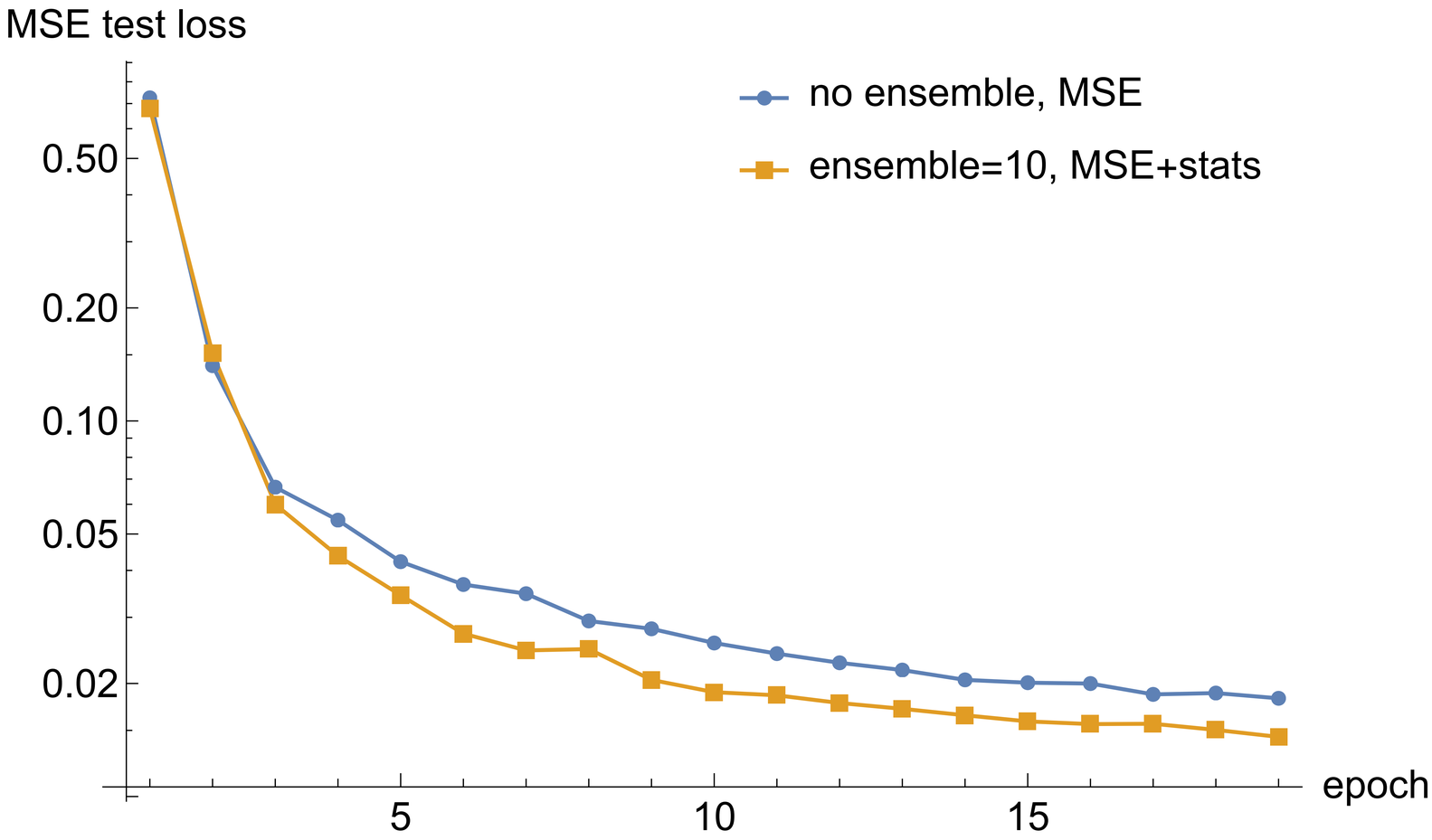
- Total number of parameters: 3.5 billion

Statistical loss



vorticity,
ml=137

Statistical loss



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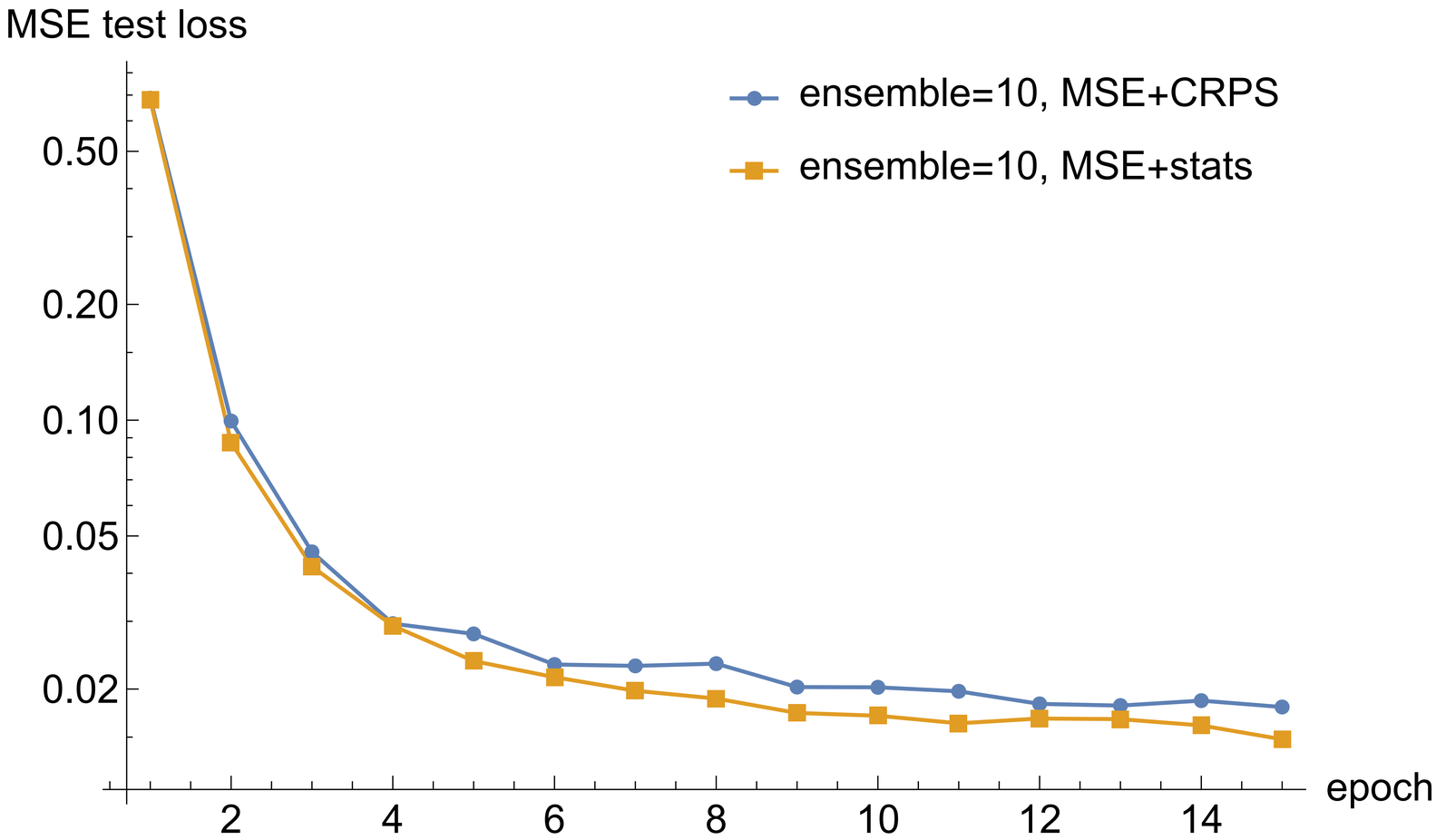
Statistical loss



vorticity,
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Zero-shot capabilities

Large language model: $p_\theta\left(y|x\right)$

The three settings we explore for in-context learning

Zero-shot

The model predicts the answer given only a natural language description of the task. No gradient updates are performed.

```
1  Translate English to French:        ← task description
2  cheese =>                           ← prompt
```

Traditional fine-tuning (not used for GPT-3)

Fine-tuning

The model is trained via repeated gradient updates using a large corpus of example tasks.

```
1  sea otter => loutre de mer          ← example #1
```

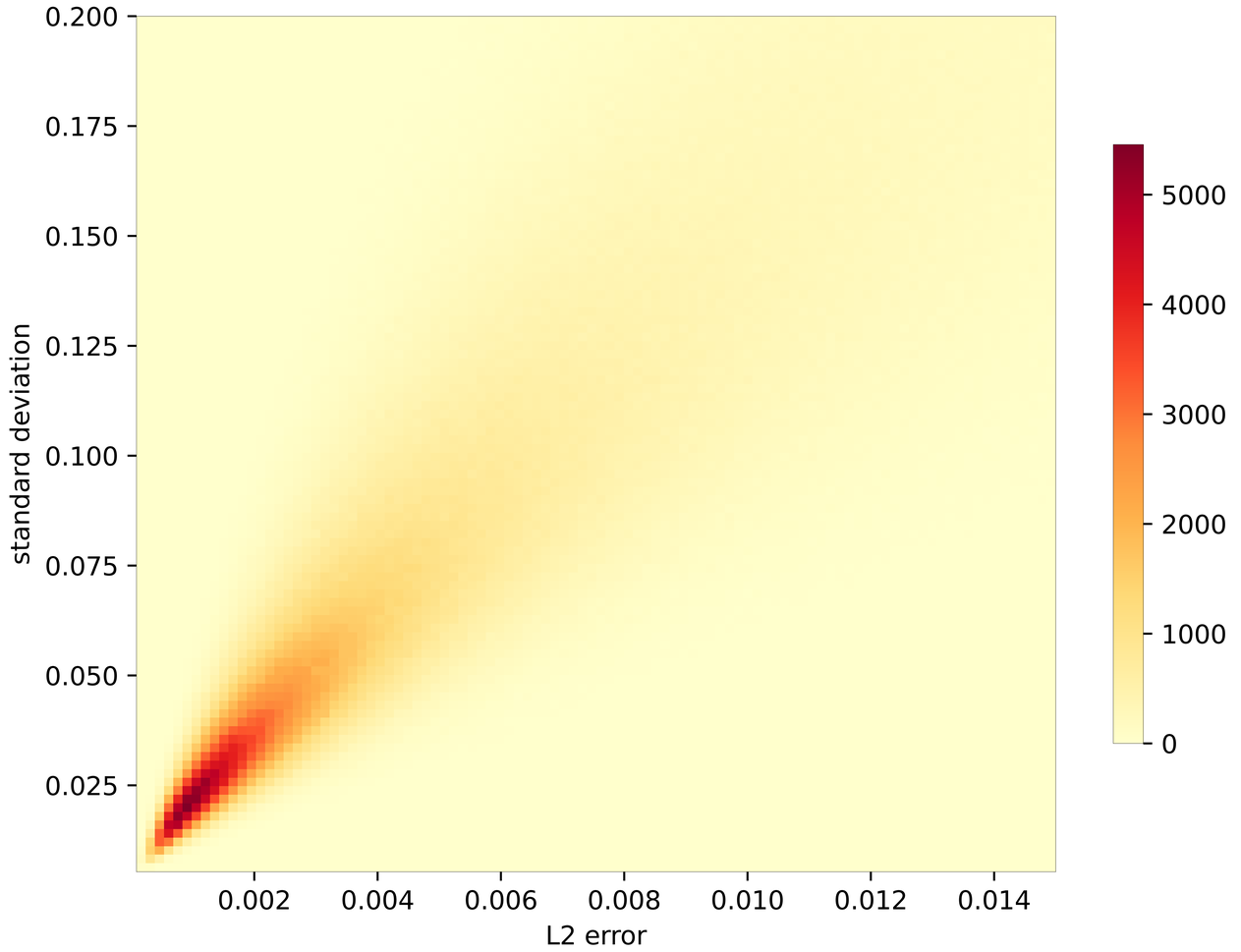
↓

gradient update

↓

T. Brown, B. Mann, N. Ryder, M. Subbiah, J. D. Kaplan, P. Dhariwal, A. Neelakantan, P. Shyam, G. Sastry, A. Askell, S. Agarwal, A. Herbert-Voss, G. Krueger, T. Henighan, R. Child, A. Ramesh, D. Ziegler, J. Wu, C. Winter, C. Hesse, M. Chen, E. Sigler, M. Litwin, S. Gray, B. Chess, J. Clark, C. Berner, S. McCandlish, A. Radford, I. Sutskever, and D. Amodei. *Language models are few-shot learners*. In Advances in Neural Information Processing Systems, volume 33, pages 1877–1901. Curran Associates, Inc., 2020.

Statistical loss



2D Histogram of L_2 error vs. std.-dev. (temperature)

Pre-training results

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  - More compute-efficient

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- Pre-training of individual fields
  - More compute-efficient
- Assembly of multiformer from pre-trained fields
  - Fields can be assembled as needed for application
  - Very little training time needed to “synchronize” pre-trained fields in assembled multiformer

Pre-training results