Representation learning for the Earth Sciences

Christian Lessig, Otto-von-Guericke-Universität Magdeburg

Motivation

- Large amounts of data available in the Earth sciences and growing fast:
  - ERA5: ≈6 PB
  - CMIP6: ≈100 PB
  - MetOp-SG: 8 x 864 GB/day (80 Mbit/s)
  - OCEAN5: ≈4 PB

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  - OCEAN5: ≈4 PB
- Observational or quasi-observational data with effects and phenomena not captured in, e.g., analytic models

Motivation

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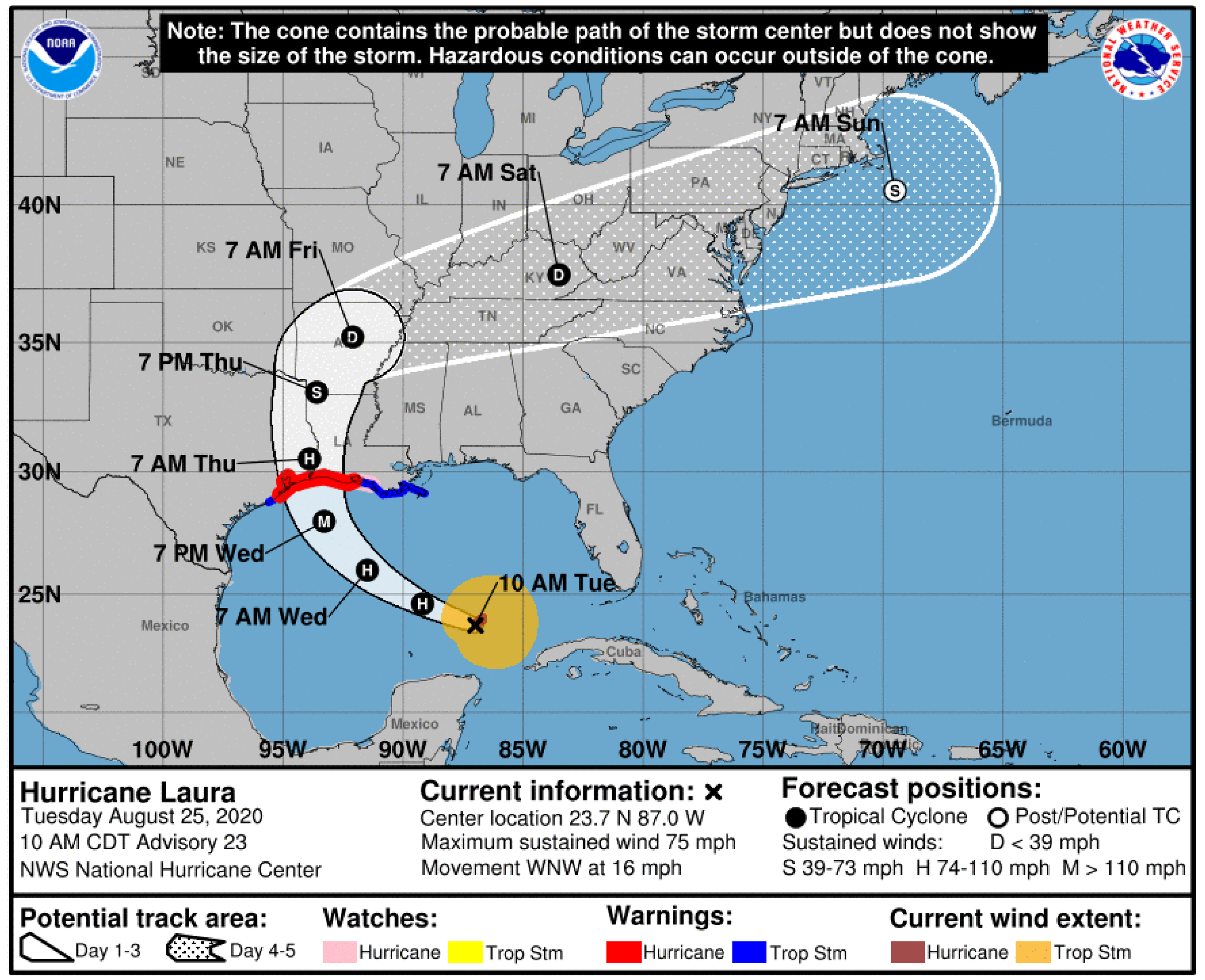
- How to use this data for machine learning in the Earth sciences?
  - Most data is unlabeled for most purposes
  - Super-computing infrastructure required for storing and processing
  - How to obtained learned models that are physically consistent?

Motivation

- Example: hurricane tracking
  - Large importance for immediate effects and climate projections



https://www.nhc.noaa.gov/aboutnhcgraphics.shtml

Motivation

- Example: hurricane tracking
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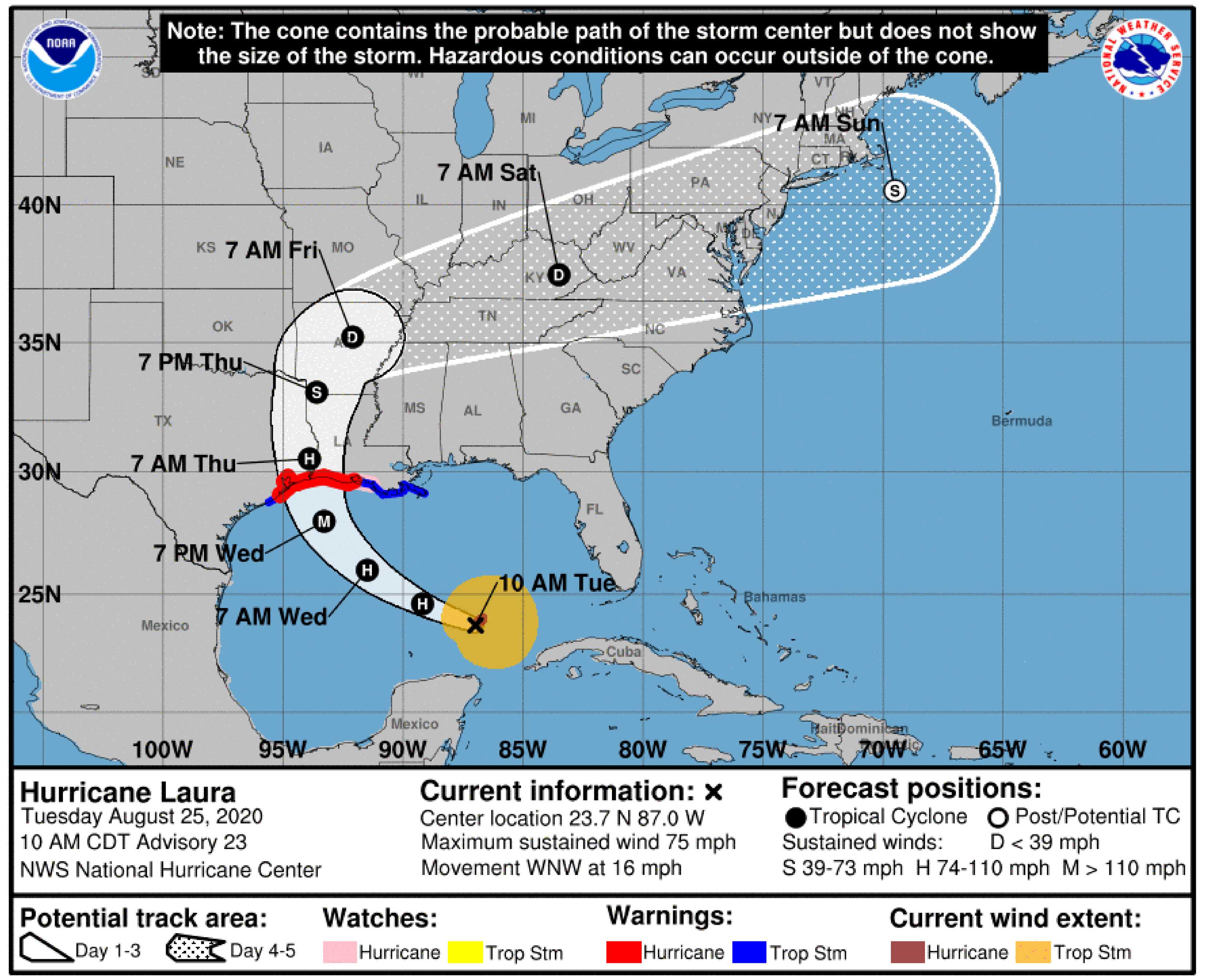

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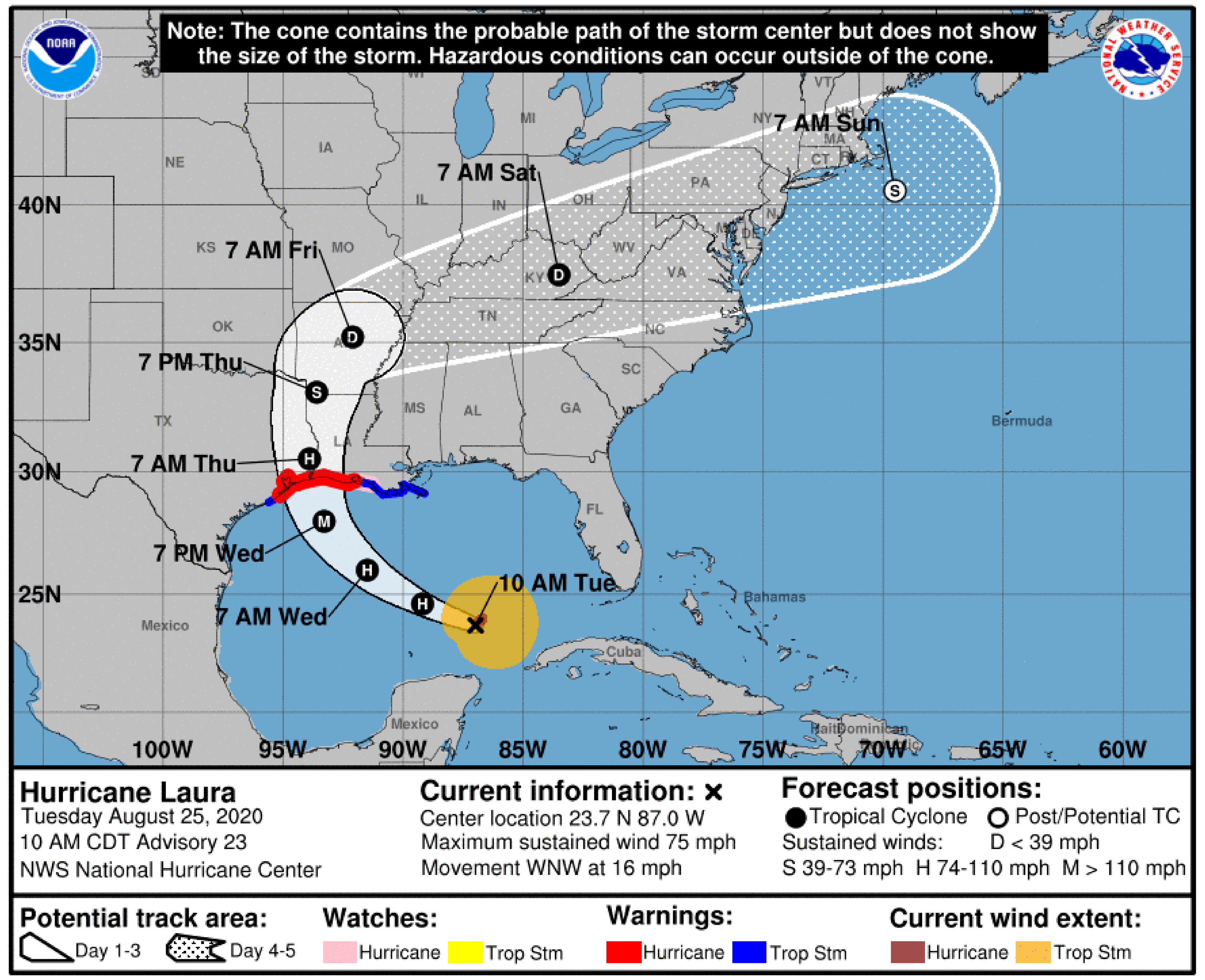

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$\Rightarrow$ Can we train a machine learning model using, e.g. ERA5, to learn overall atmospheric dynamics and then adapt to hurricane tracking with little labeled training data?

Motivation

- Similar situation for other applications:
  - Ozone and air pollution prediction
  - Observations with missing data
  - Classification of extreme events
  - Prediction of extreme events
  - …

Self-supervised representation learning

Self-supervised representation learning

- Yoshua Bengio: “Humans develop representations and abstractions to enable problem-solving and reasoning; our computers should do the same.”[1]

- Yann LeCun: “Self-supervised learning: The dark matter of intelligence“[2]

[1] http://www.iro.umontreal.ca/~bengioy/talks/icml2012-YB-tutorial.pdf
[2] https://ai.facebook.com/blog/self-supervised-learning-the-dark-matter-of-intelligence/

Self-supervised representation learning

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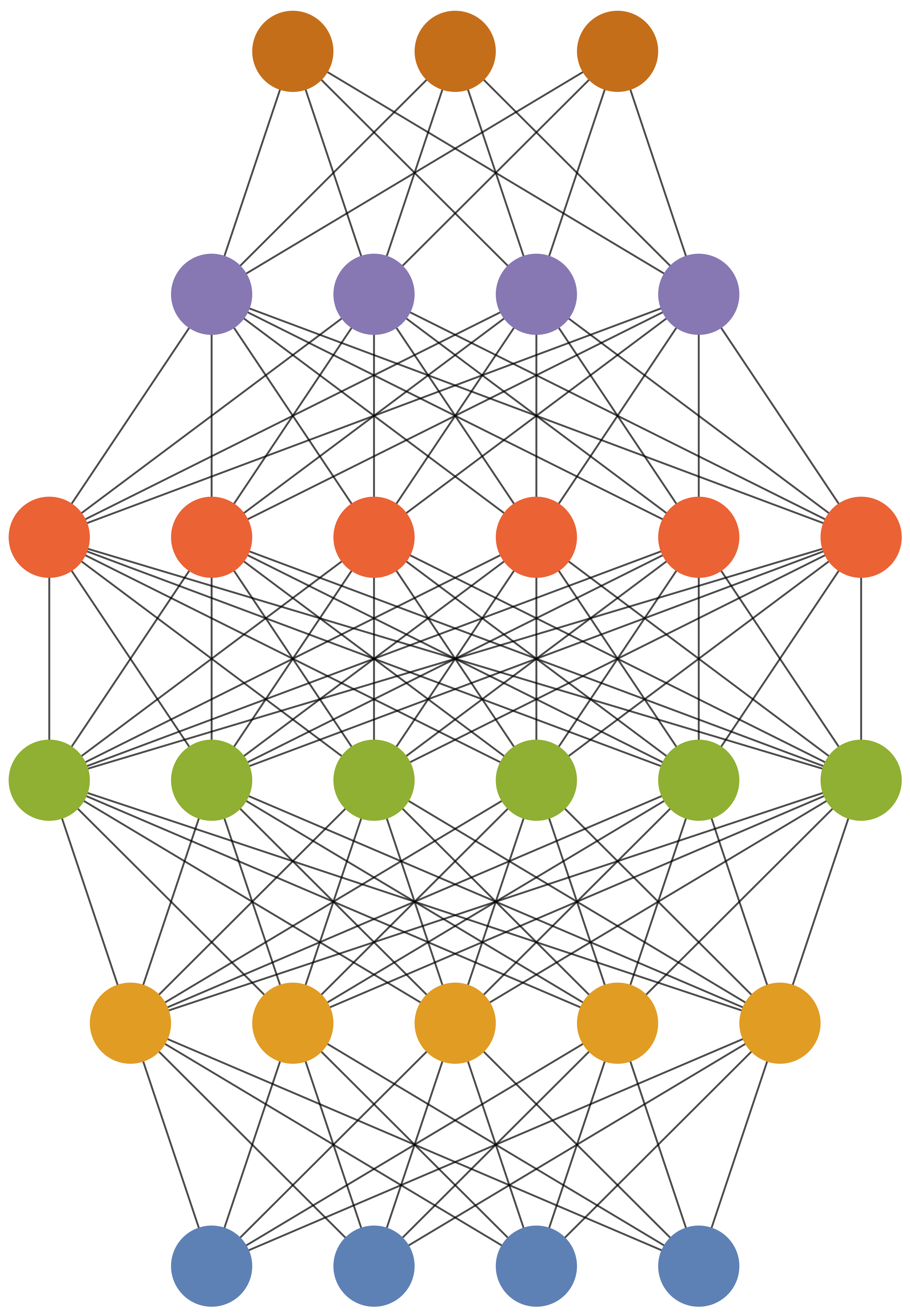
  - Learn a task-independent representation of the data in the feature space of the neural network

Self-supervised representation learning



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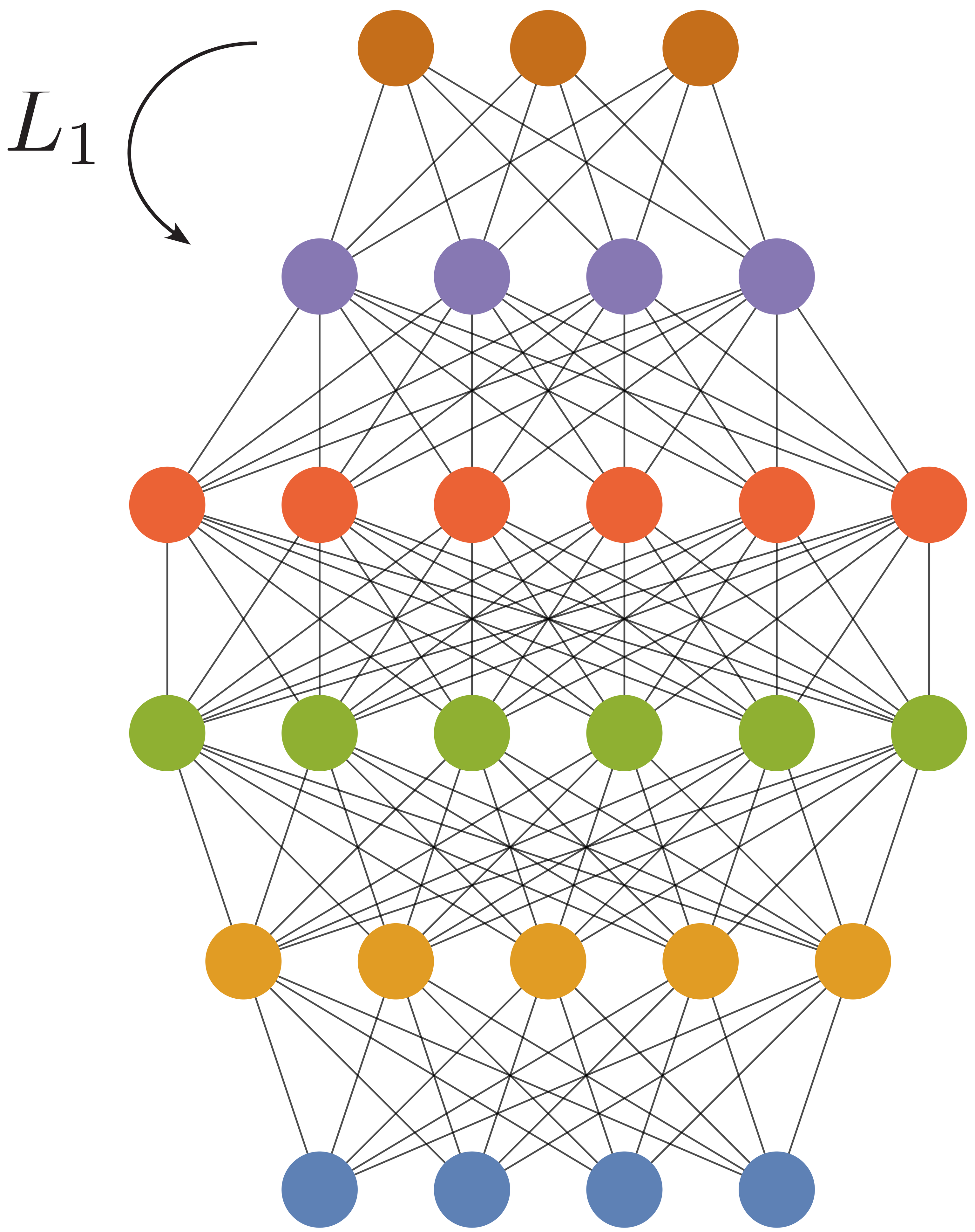

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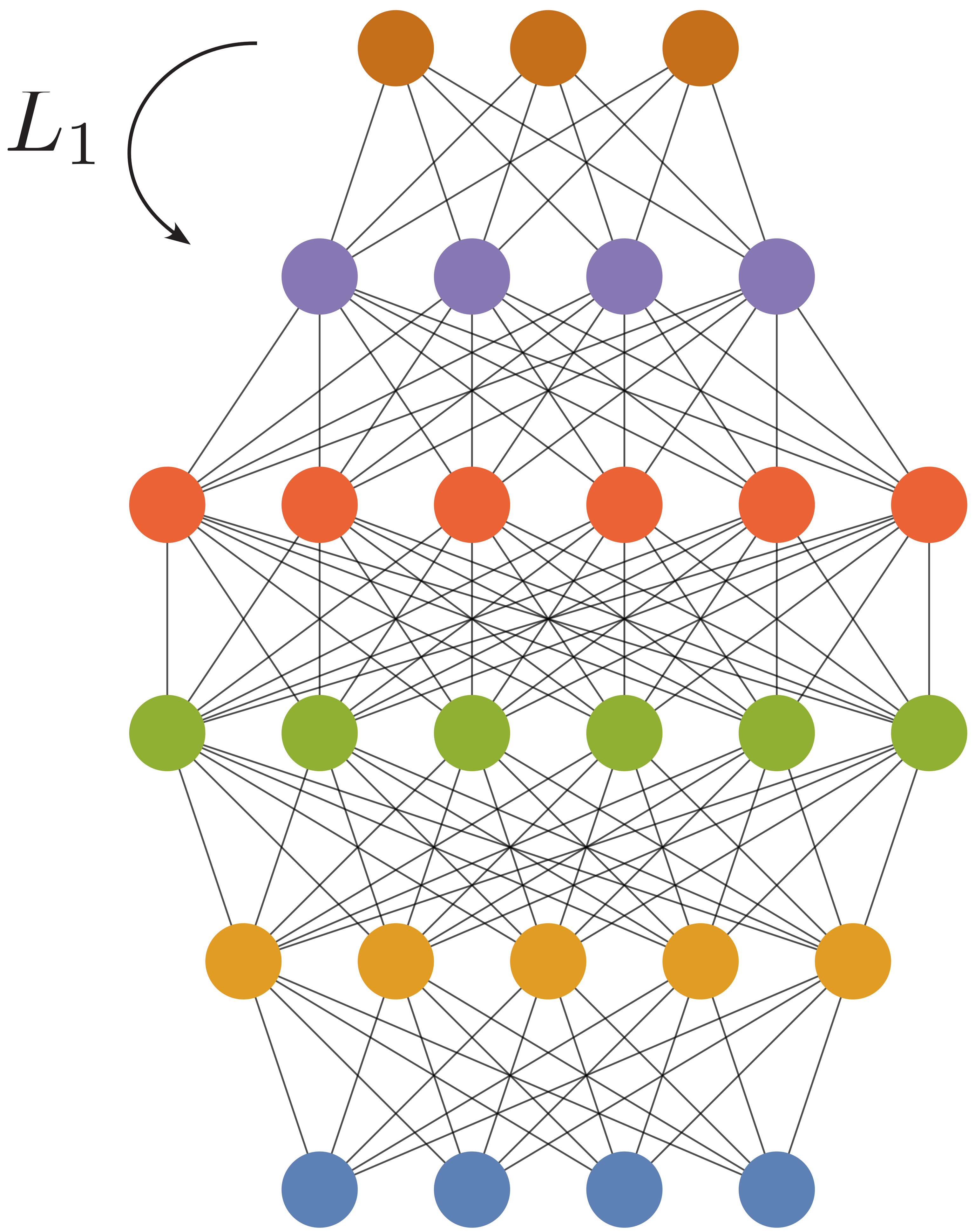
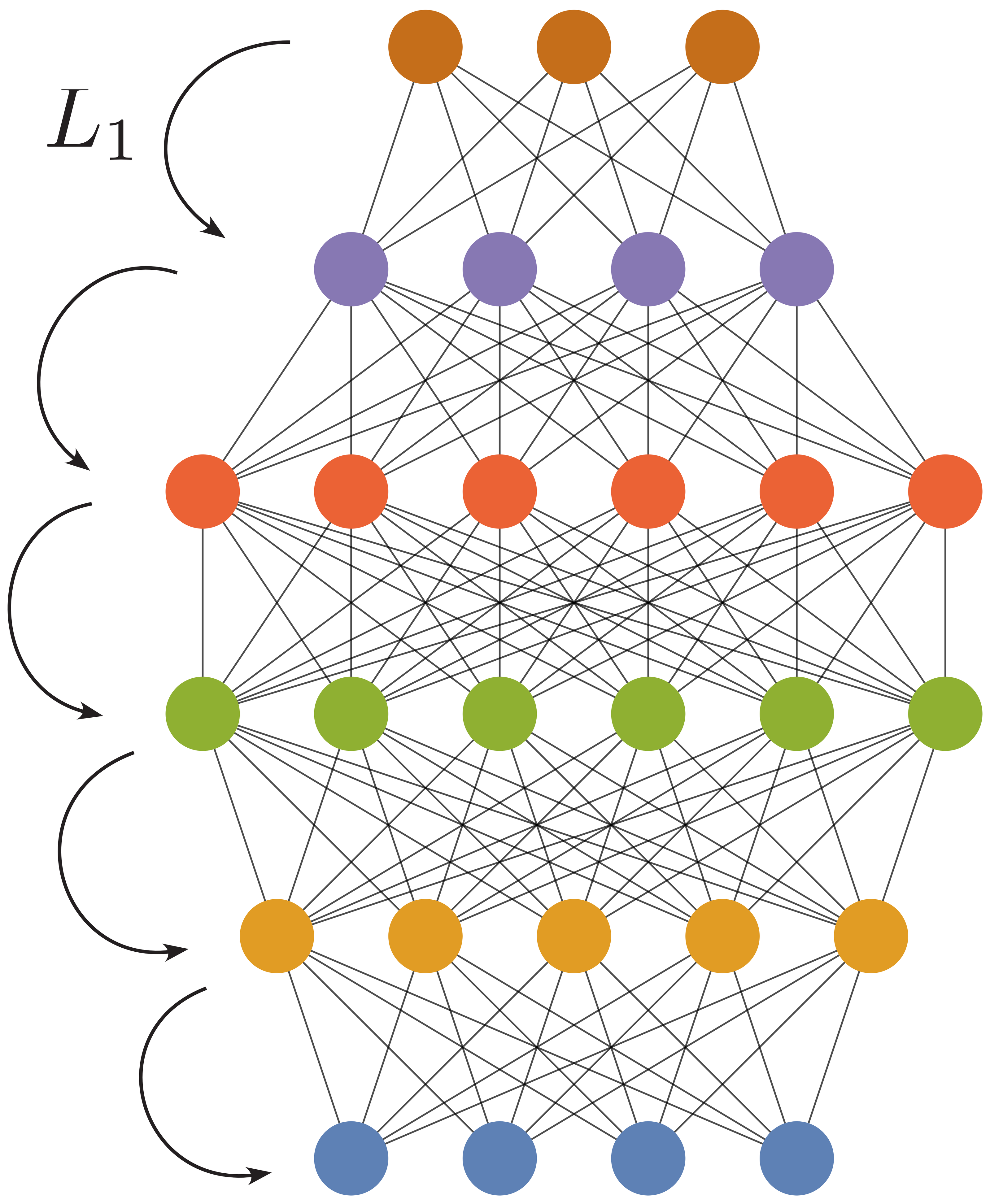


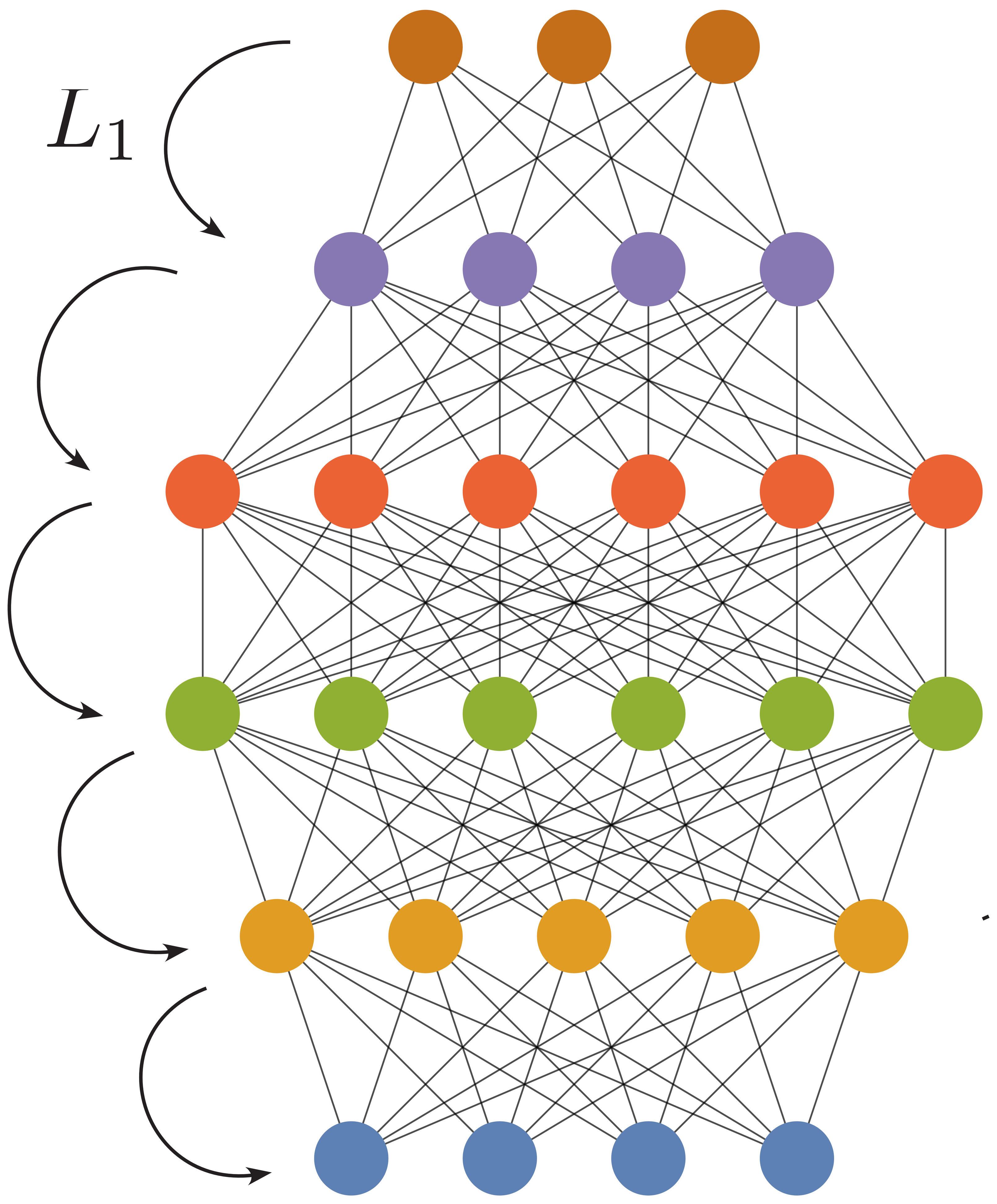
$$L_1 : \mathbb{R}^n \to \mathbb{R}^m$$

Self-supervised representation learning



$$L_j : \mathbb{R}^n \to \mathbb{R}^m$$

Self-supervised representation learning



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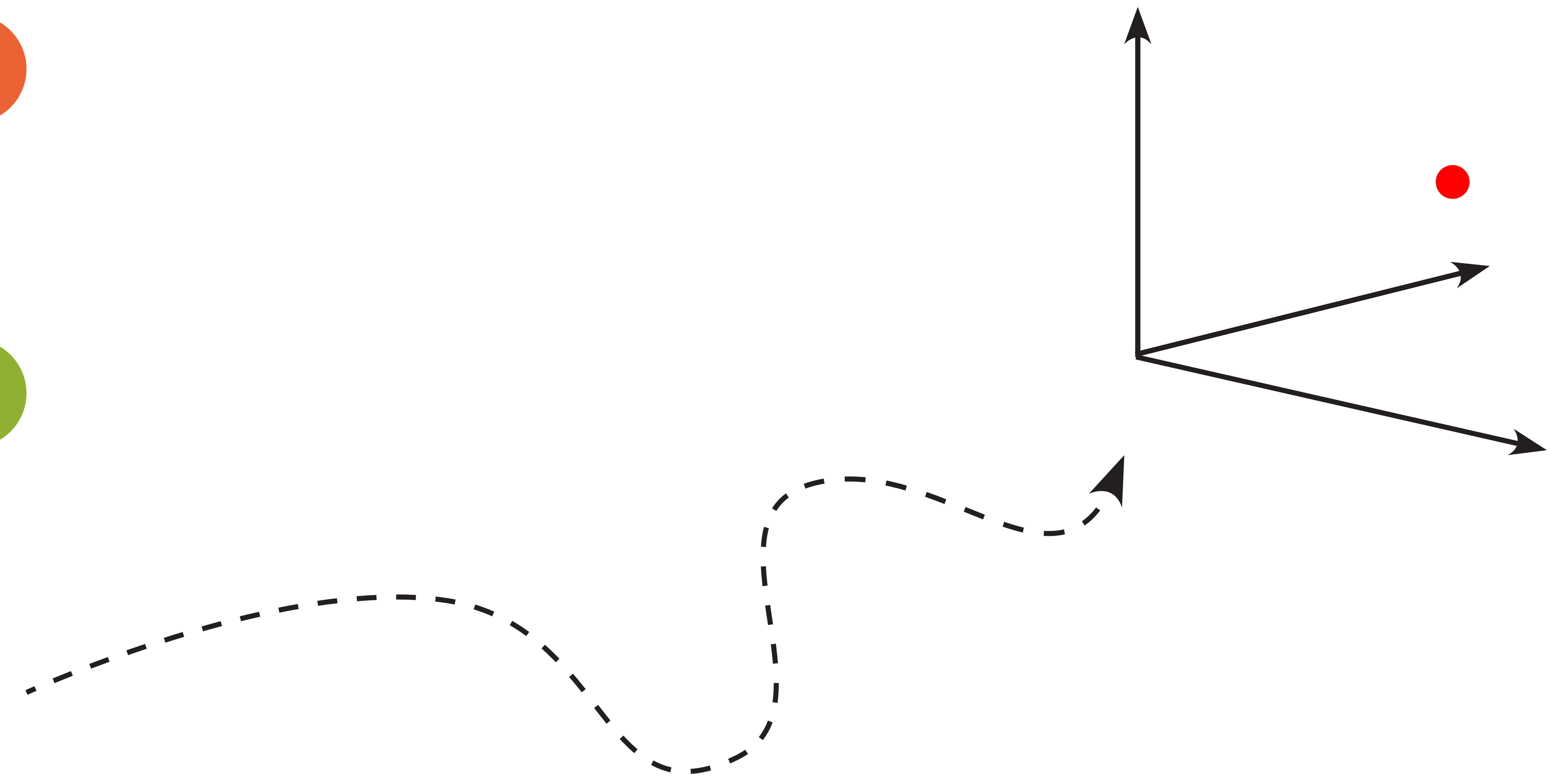

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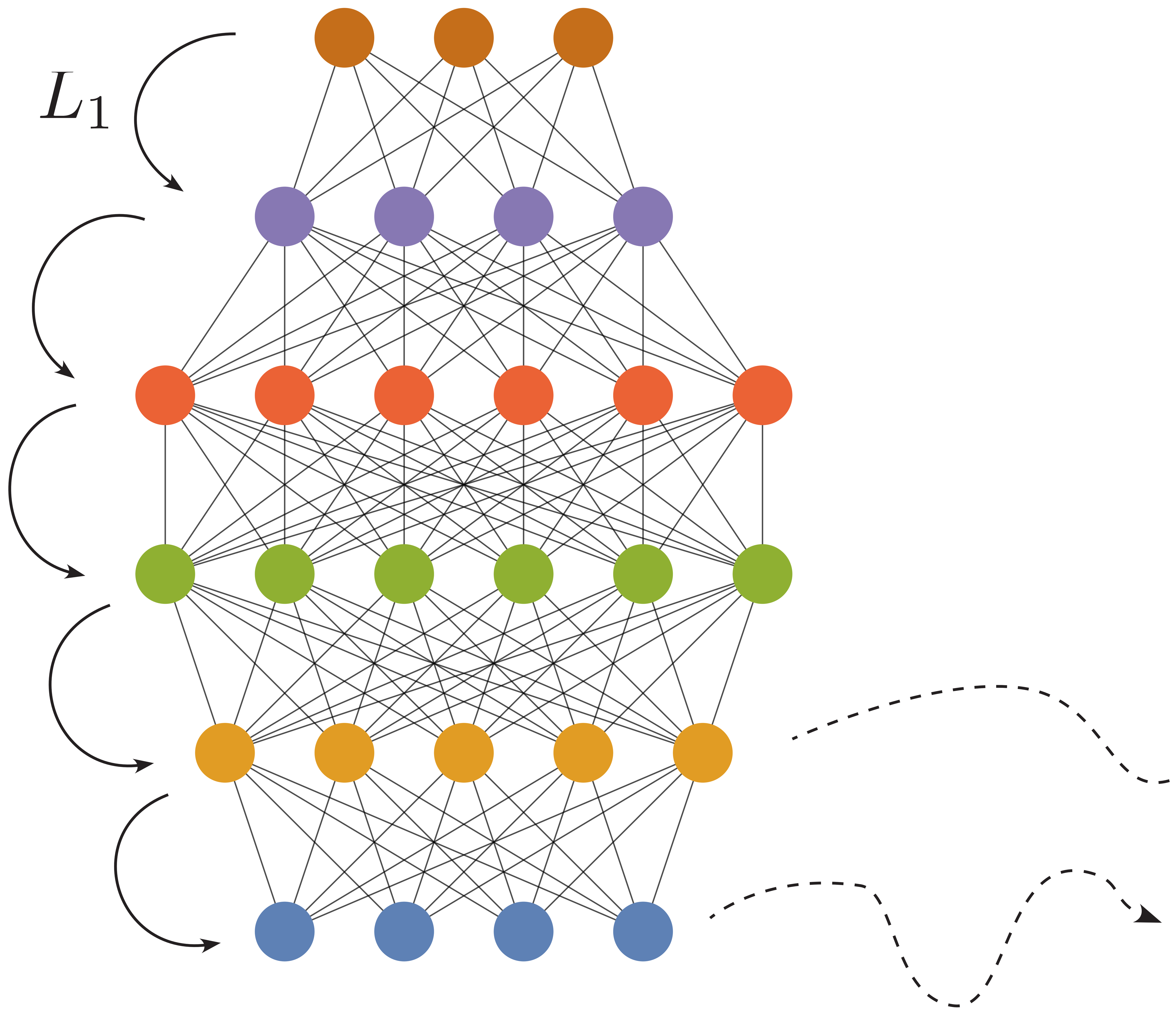

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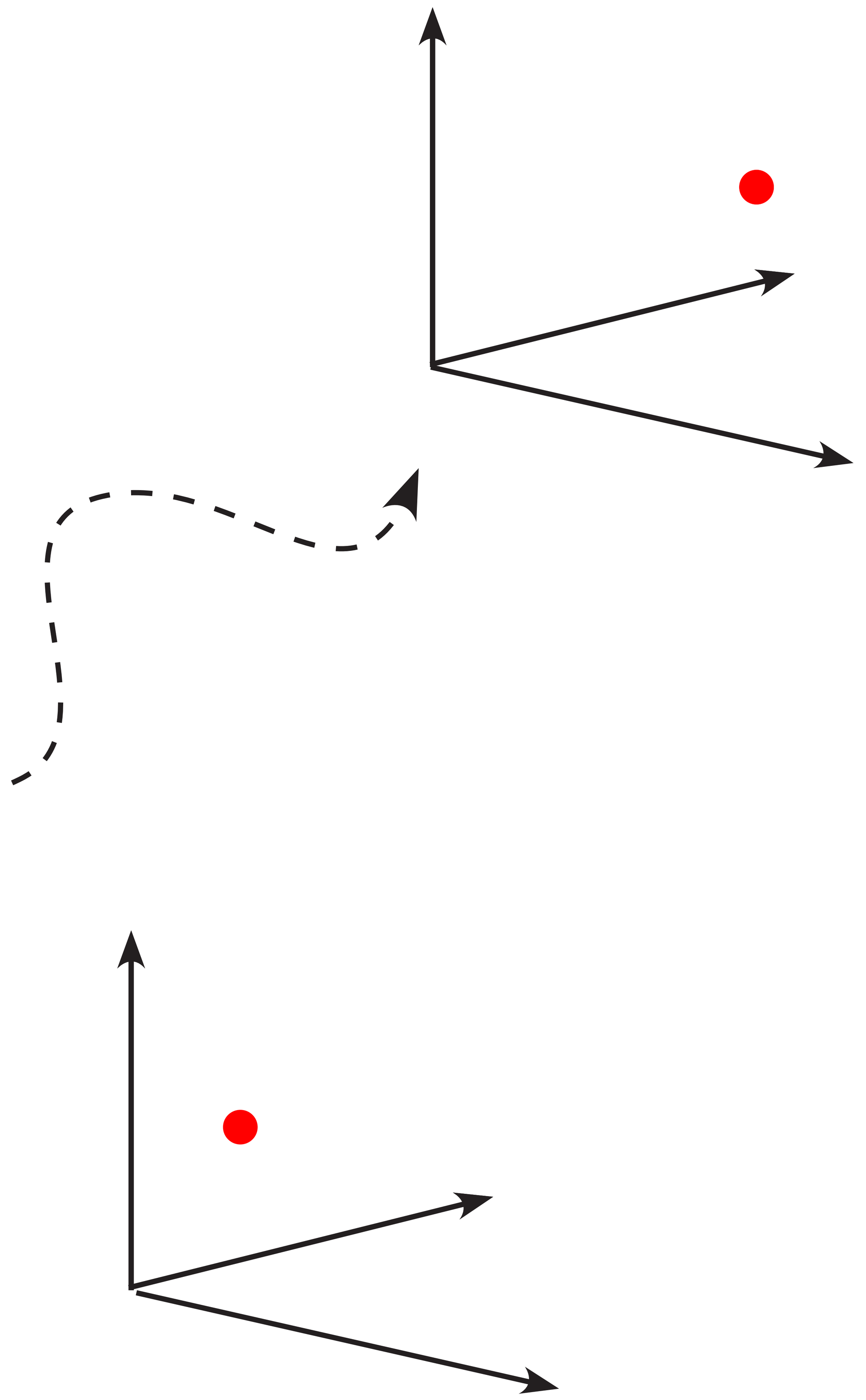

Self-supervised representation learning

- Representation learning
  - Learn a task-independent representation of the data in the *feature space* of the neural network

$$\mathcal{N} : \mathbb{R}^n \to \mathbb{R}^{m_1} \to \cdots \to \mathbb{R}^{m_{j-1}} \to \mathbb{R}^m$$

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feature spaces

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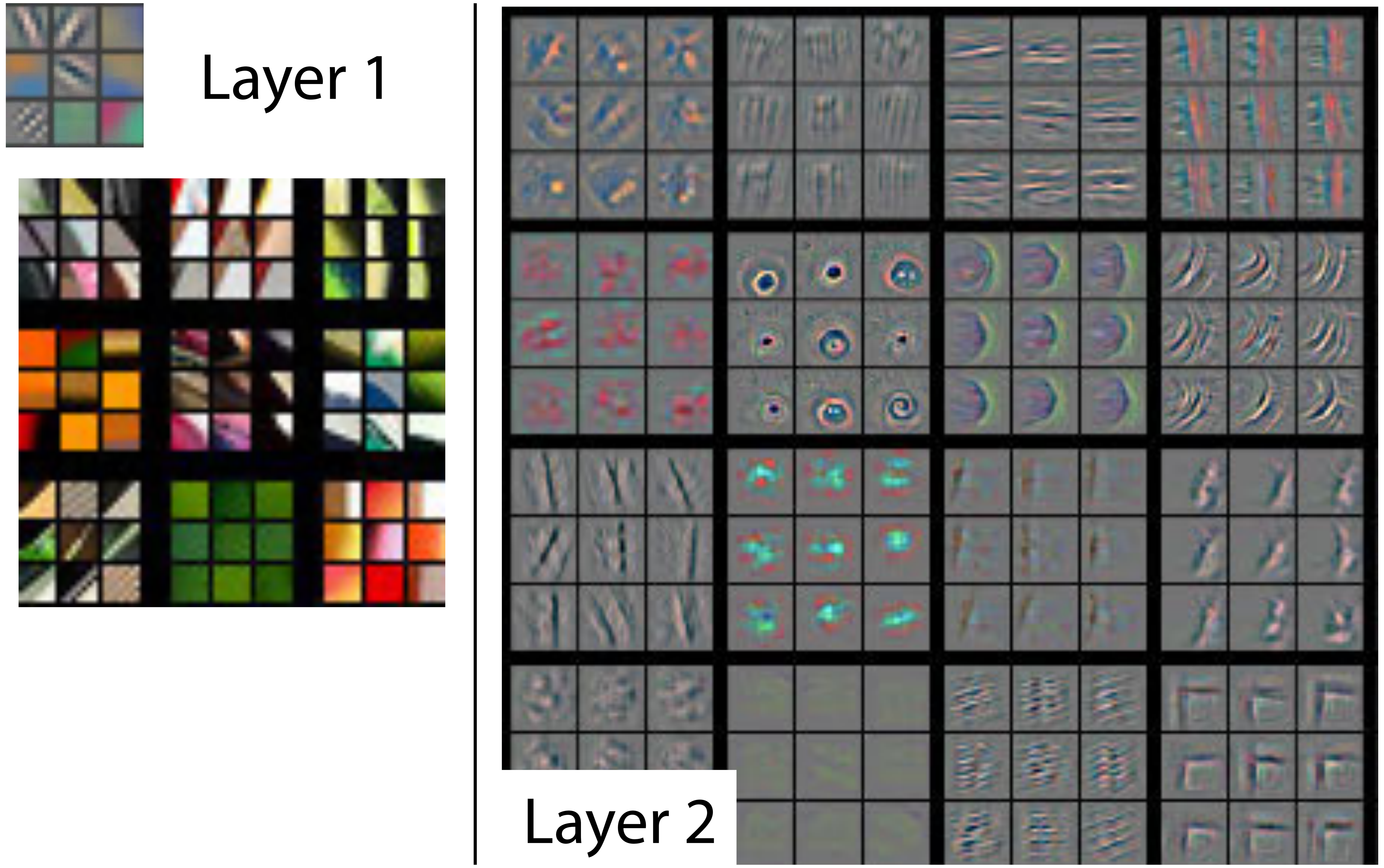
- Self-supervised training
  - Train with “labels” or information intrinsic to the data

Self-supervised representation learning



From M. D. Zeiler and R. Fergus. Visualizing and understanding convolutional networks. In D. Fleet, T. Pajdla, B. Schiele, and T. Tuytelaars, editors, Computer Vision – ECCV 2014, pages 818–833, Cham, 2014. Springer International Publishing.

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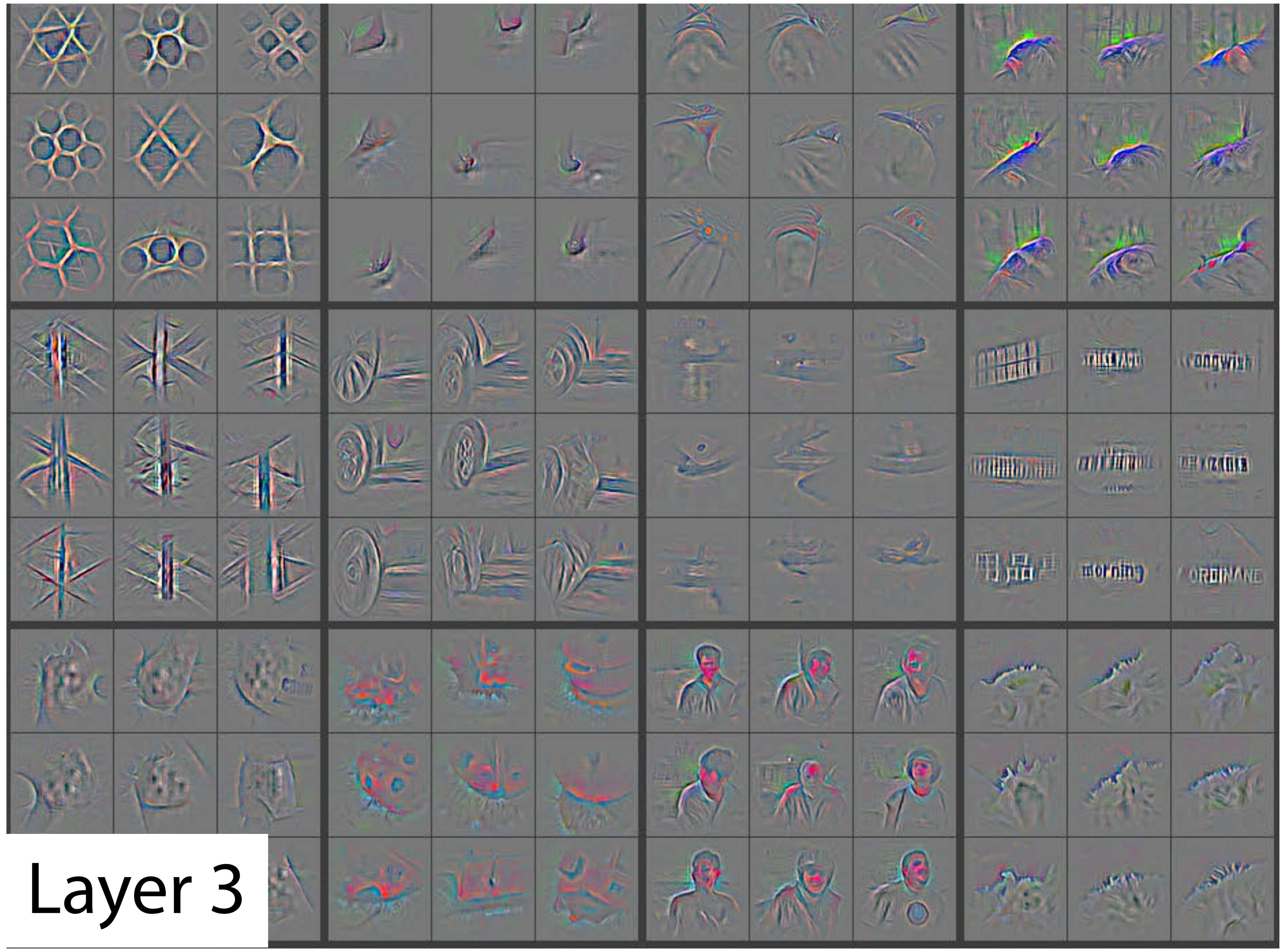

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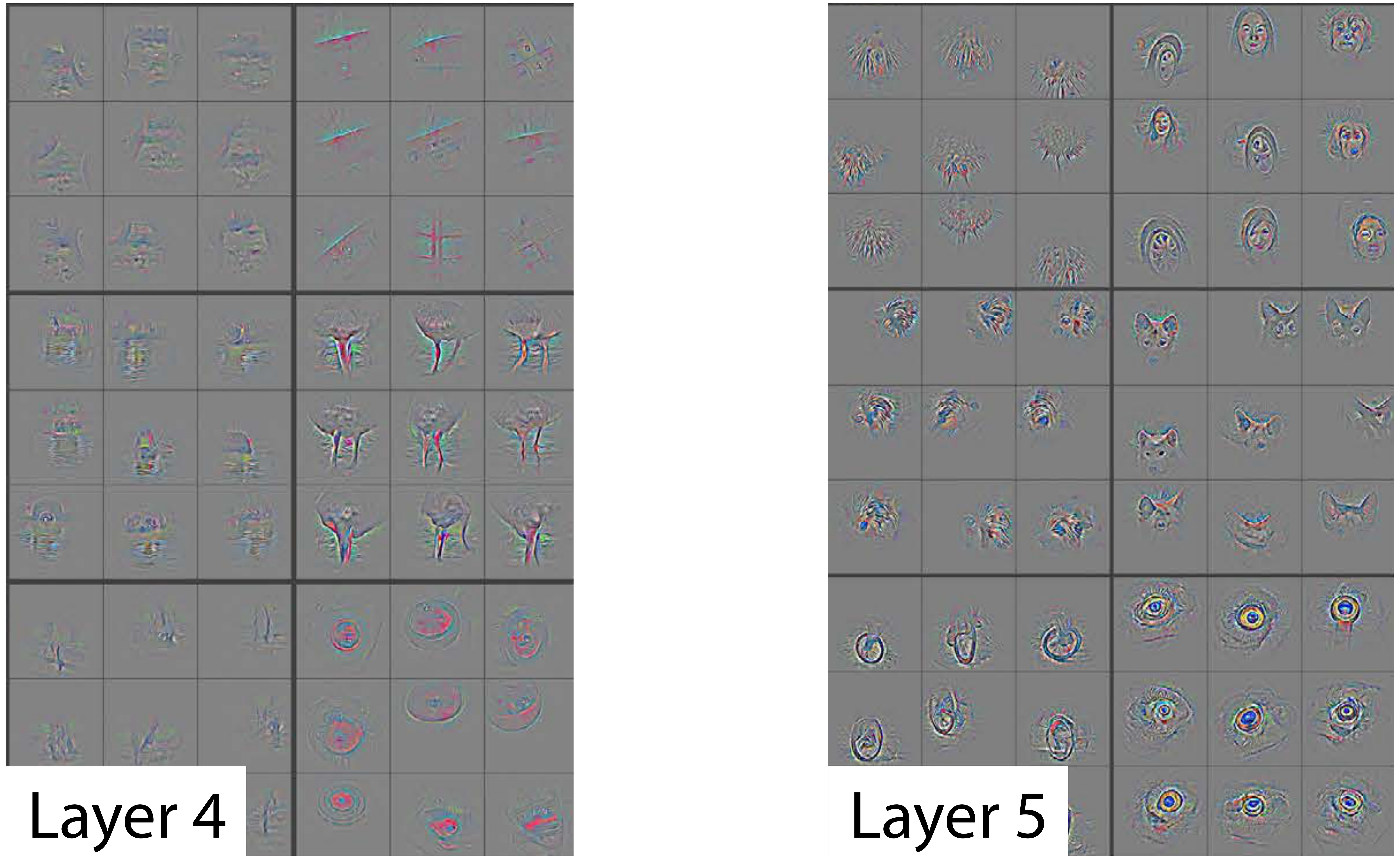

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Self-supervised representation learning

- Self-supervised pretext task:

Self-supervised representation learning

- Self-supervised pretext task: inpainting of randomly deleted image parts[1]

[1] D. Pathak, P. Krahenbuhl, J. Donahue, T. Darrell, and A. A. Efros. Context encoders: Feature learning by inpainting. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (CVPR), June 2016.

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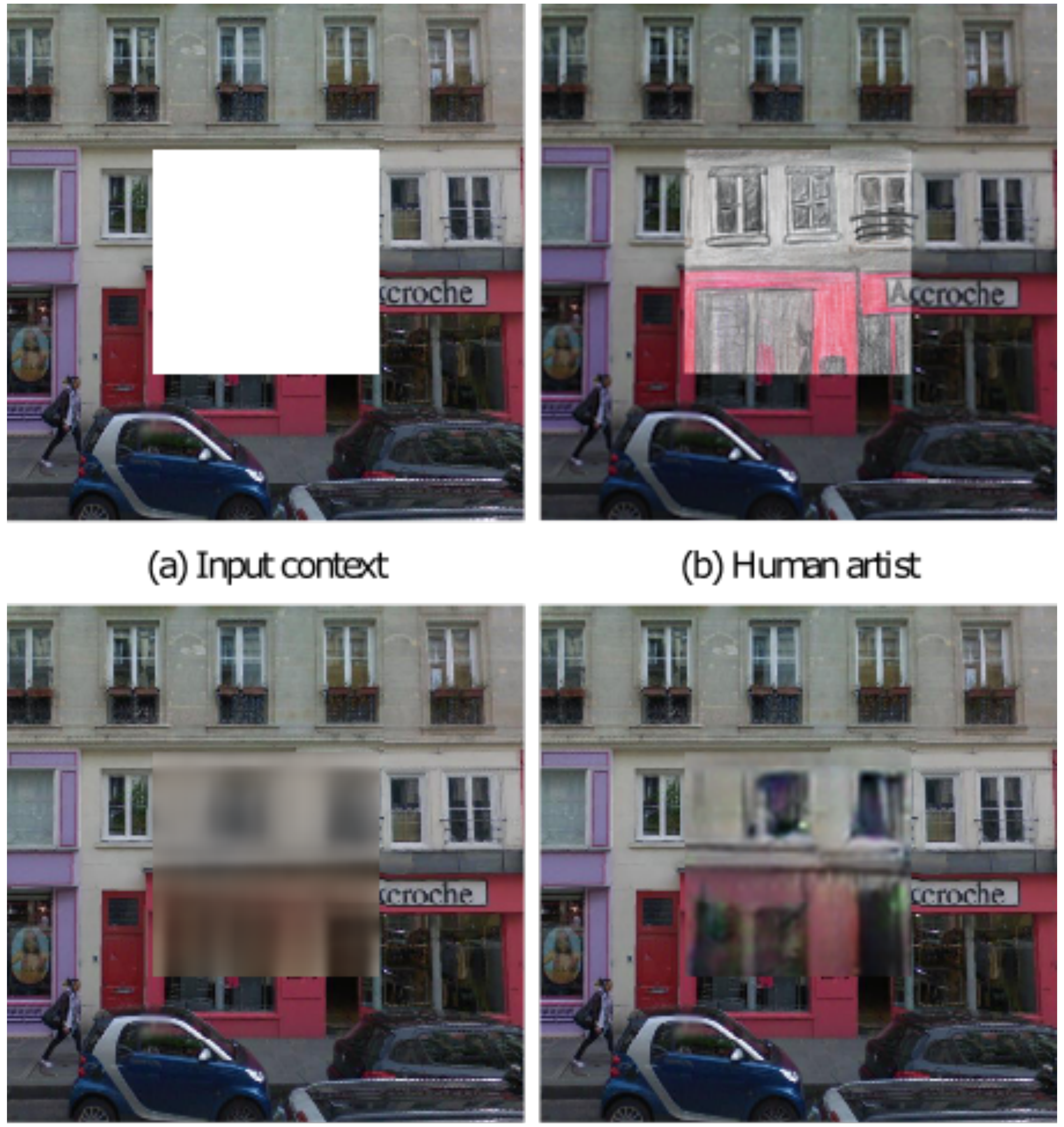

(a) Input context (b) Human artist
(c) Context Encoder (L 2 loss) (d) Context Encoder (L 2 + Adversarial loss)

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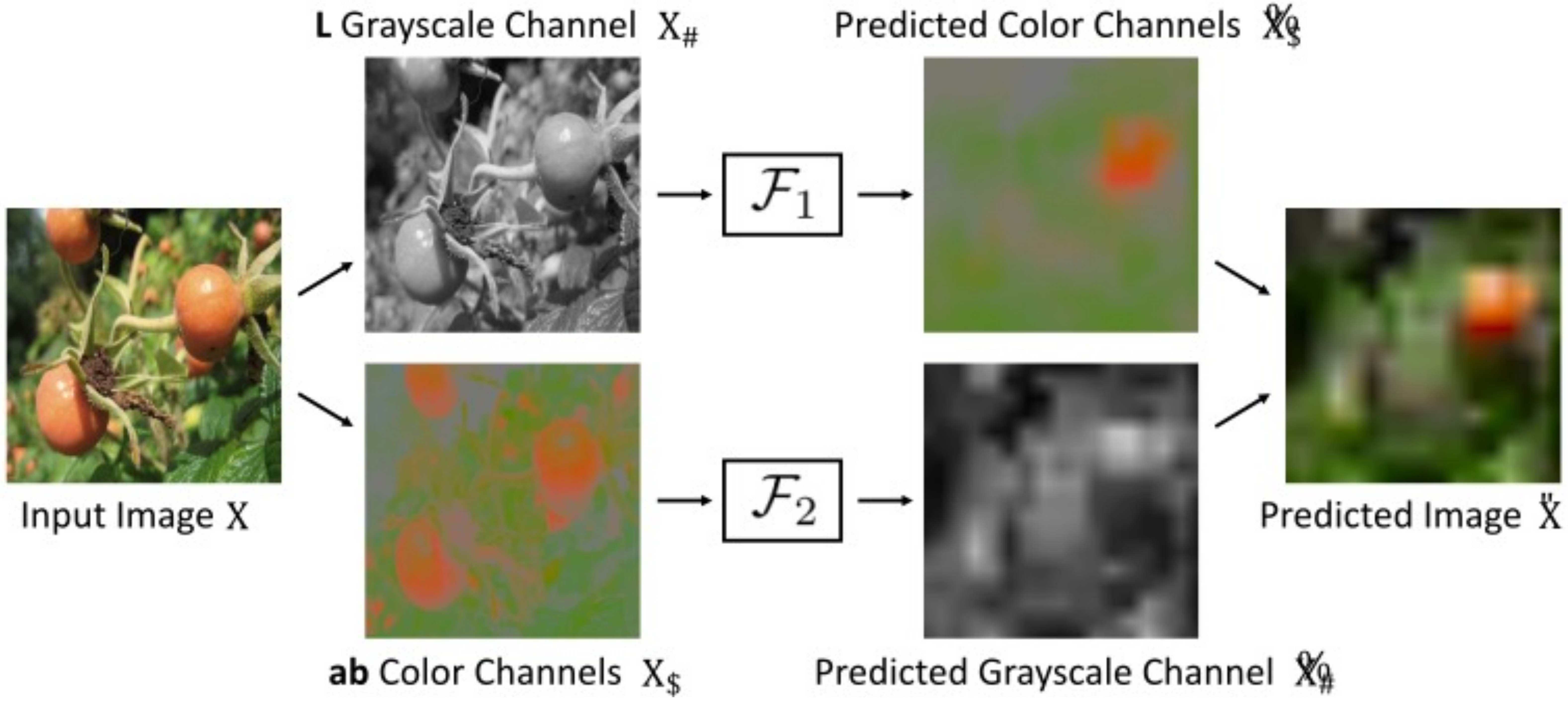
Motivation

- Self-supervised pretext task: predicting deleted color and gray scale channels[1]



[1] R. Zhang, P. Isola, and A. A. Efros. Split-brain autoencoders: Unsupervised learning by cross-channel prediction. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (CVPR), July 2017.

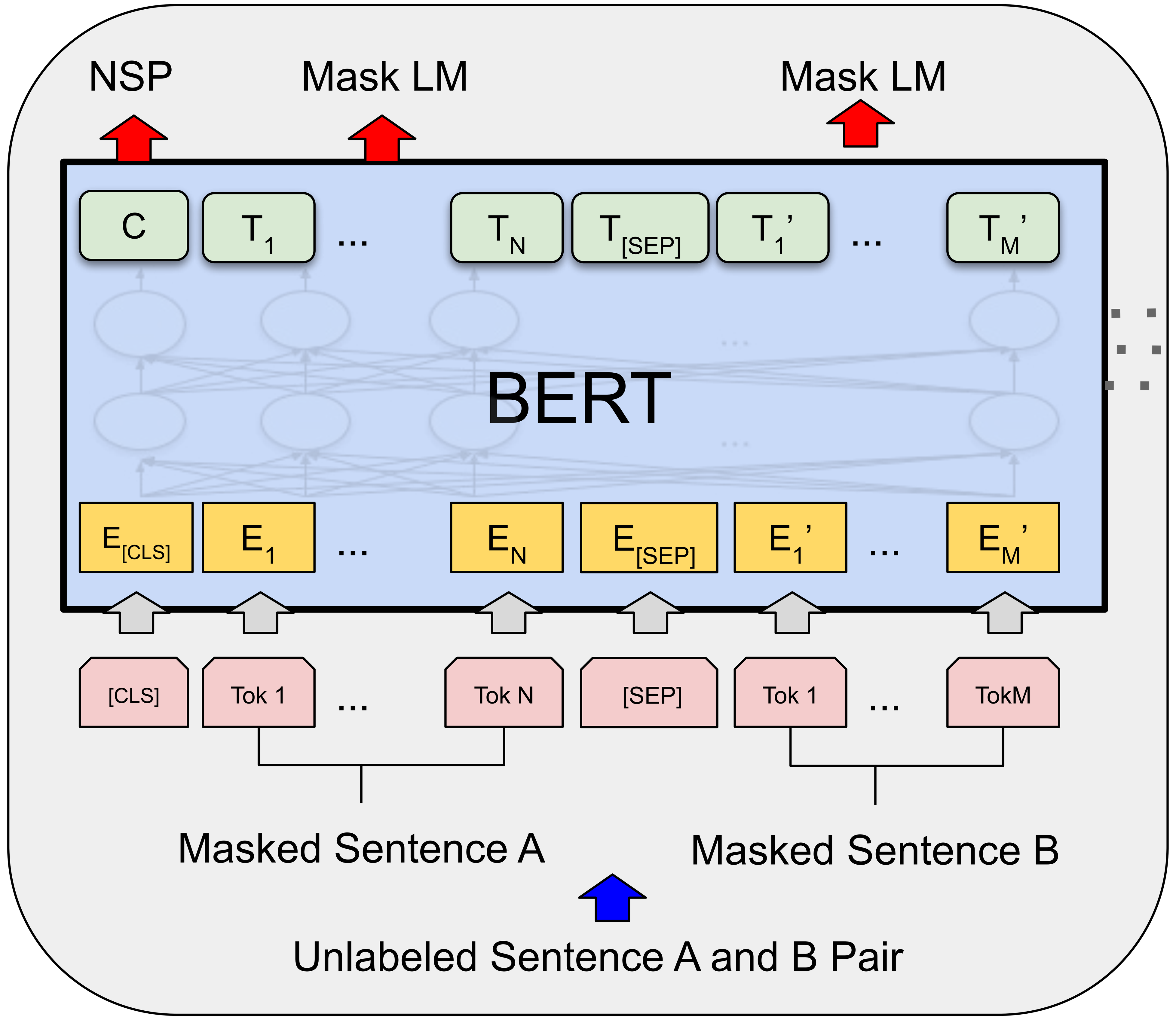
Self-supervised representation learning

- BERT[1]
  - Self-supervised representation learning for natural language processing (NLP)
  - Very large transformer neural network with billions of parameters
  - Self-supervised training essentially only feasible option at this scale

[1] J. Devlin, M.-W. Chang, K. Lee, and K. Toutanova. BERT: Pre-training of deep bidirectional transformers for language understanding, 2019.

Self-supervised representation learning

- BERT[1]



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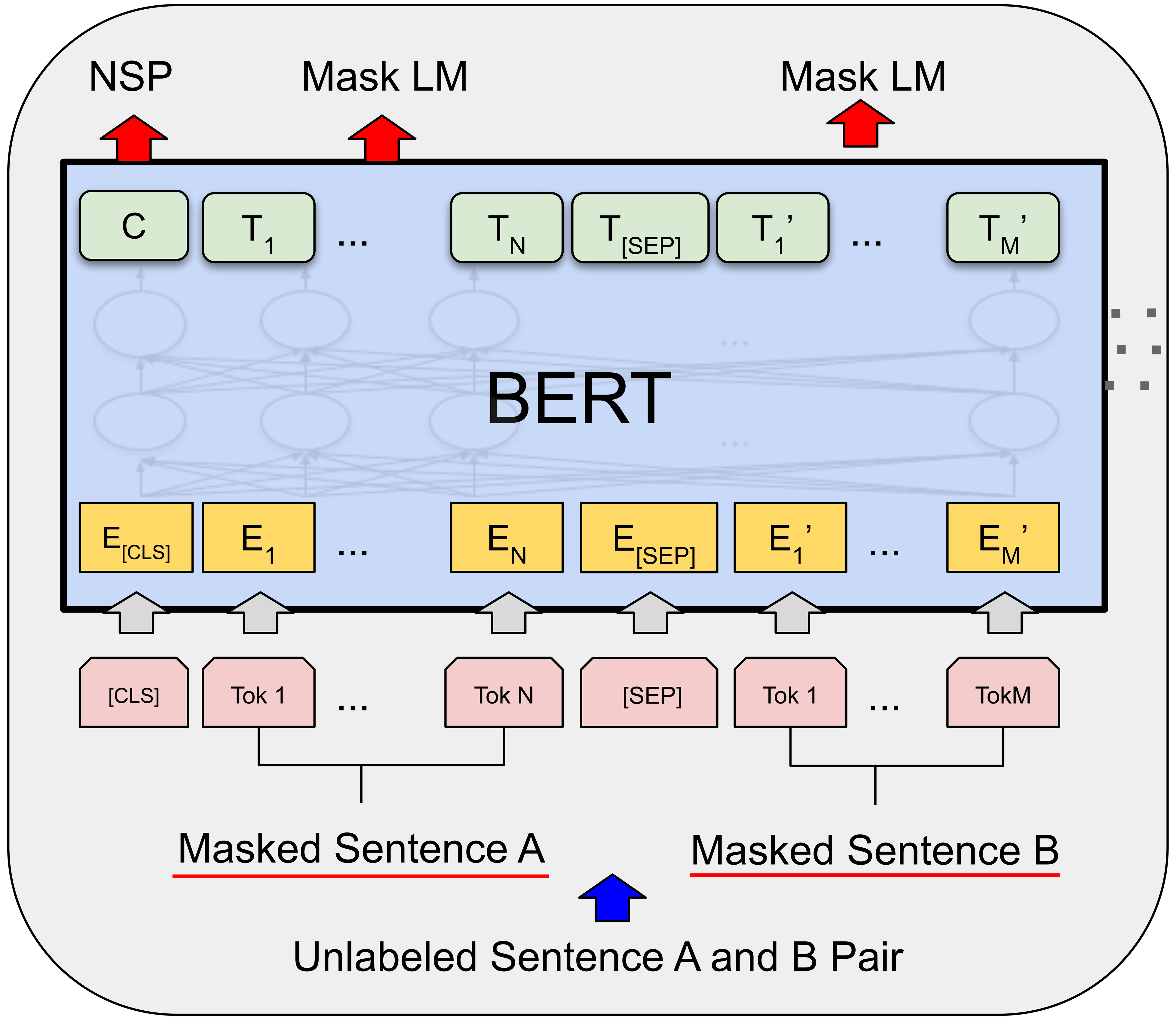

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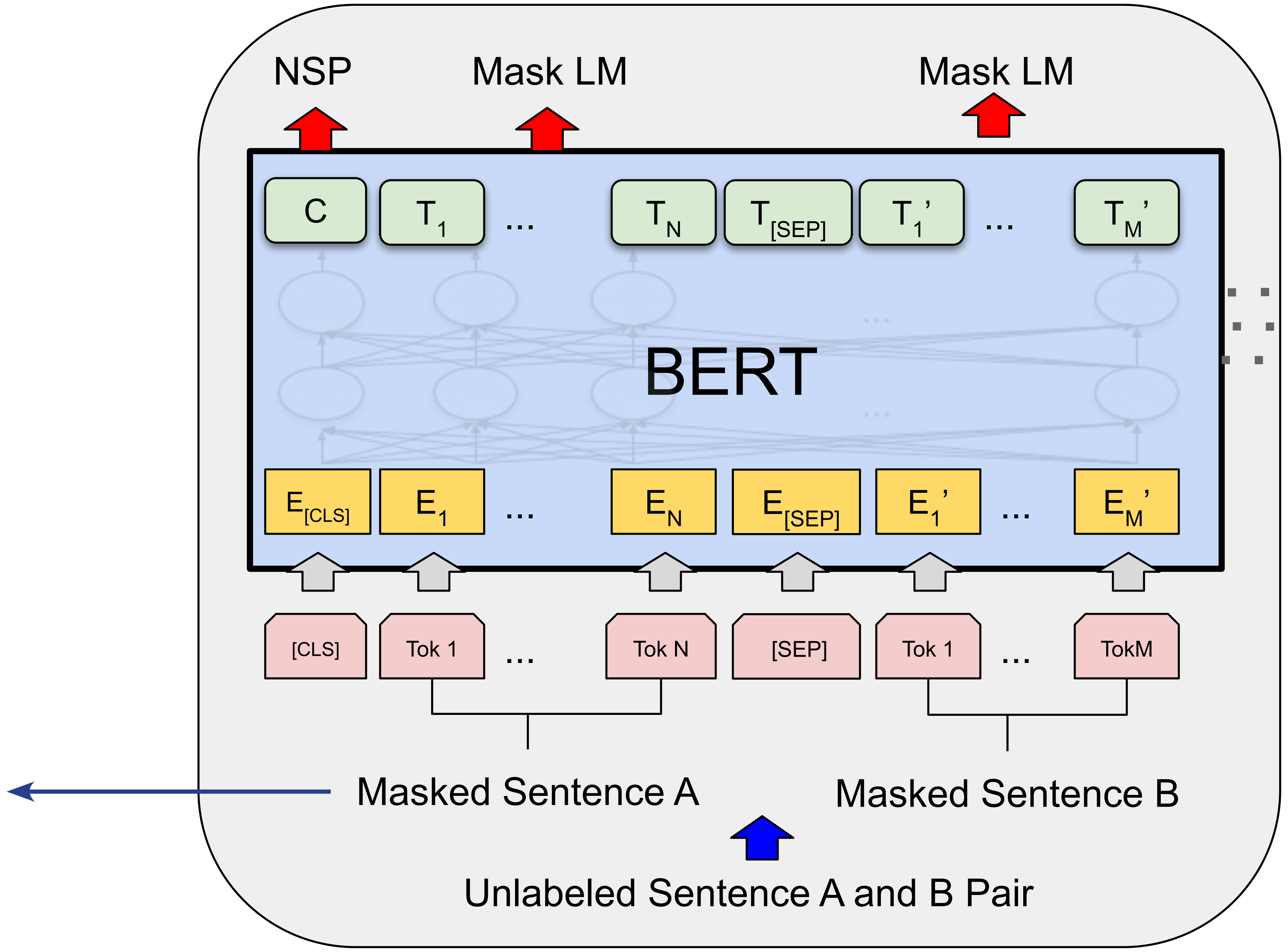
Self-supervised representation learning

- BERT[1]

The sun was
shining bright.



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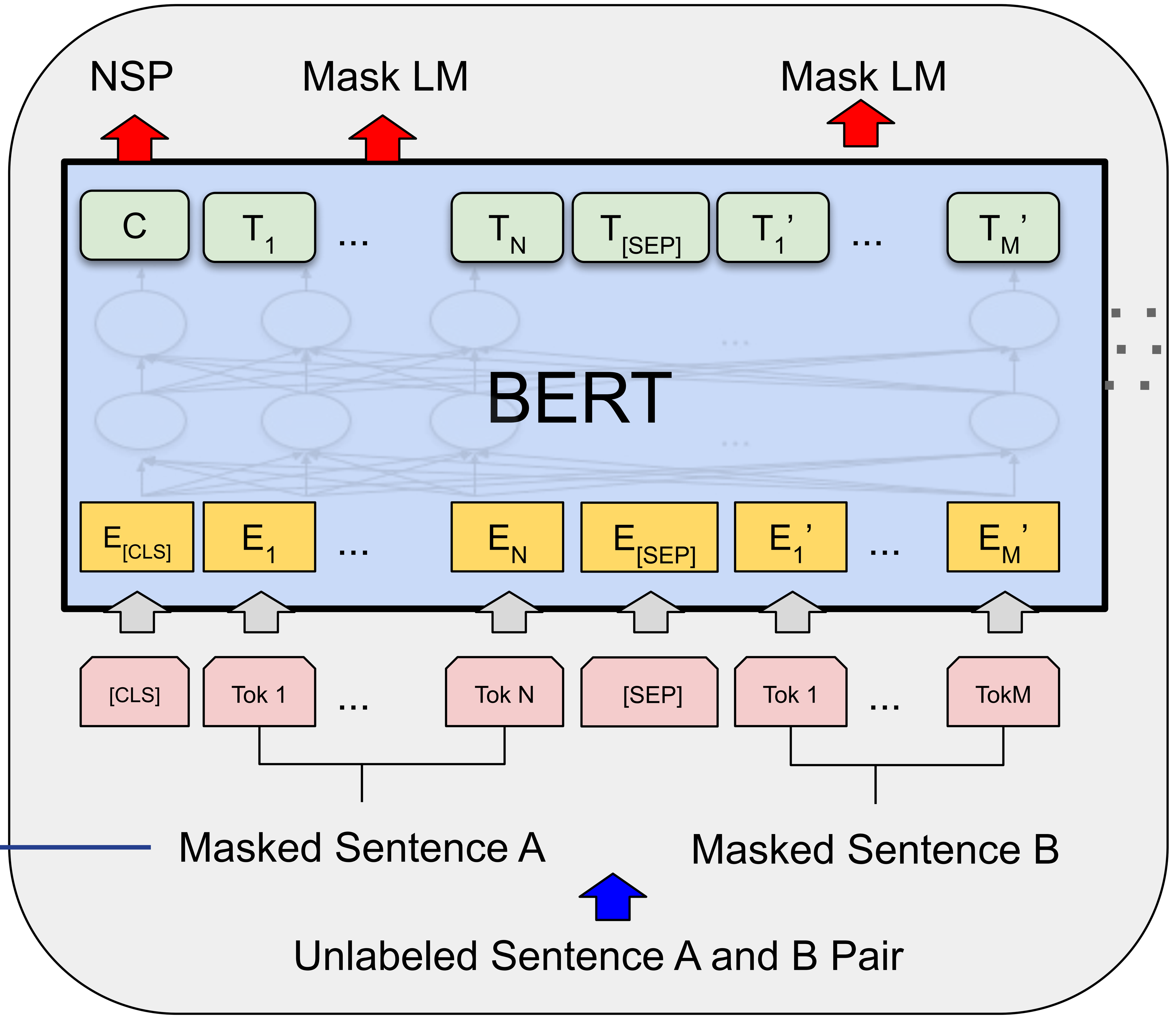

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Self-supervised representation learning

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Network predicts deleted word

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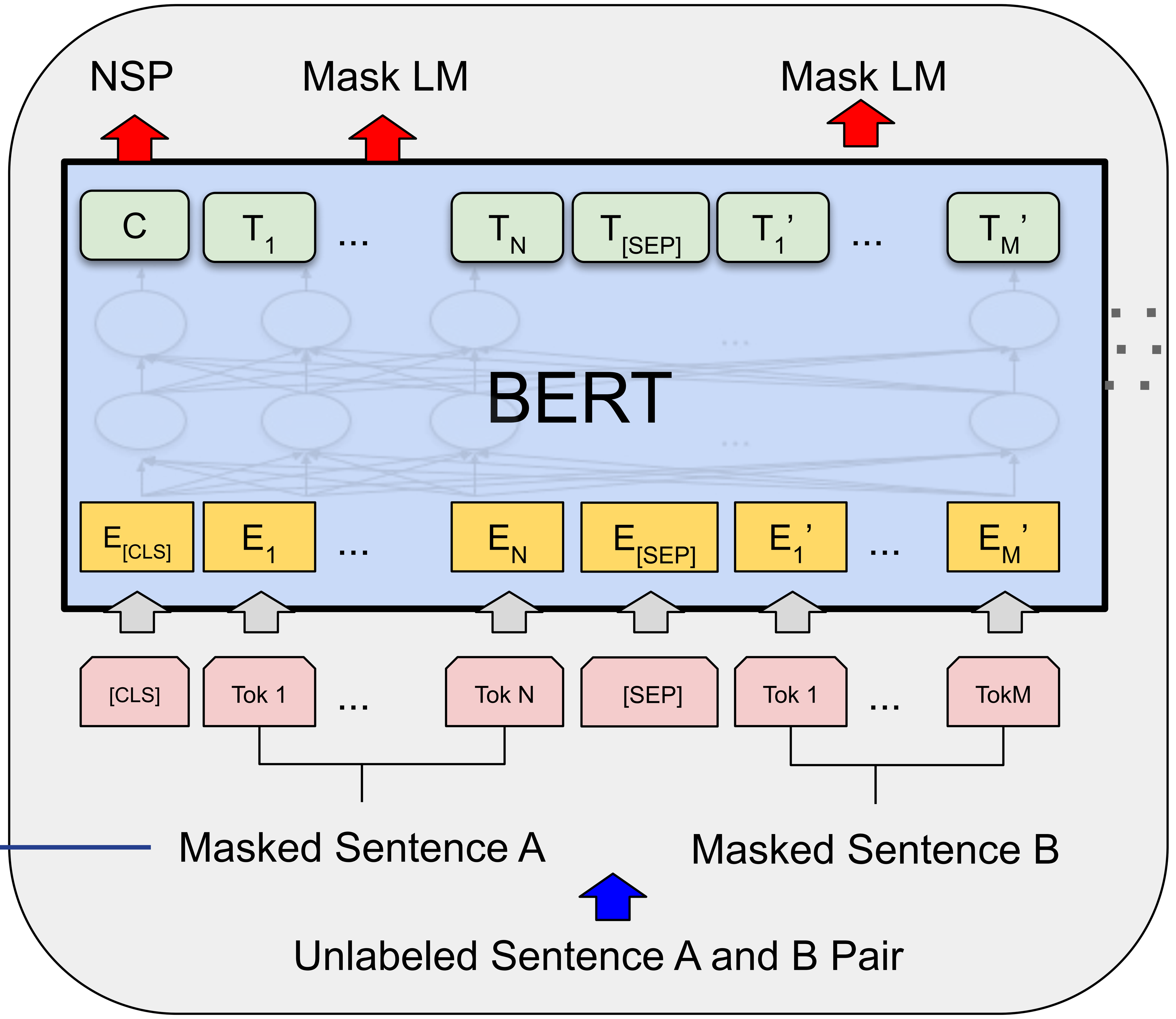

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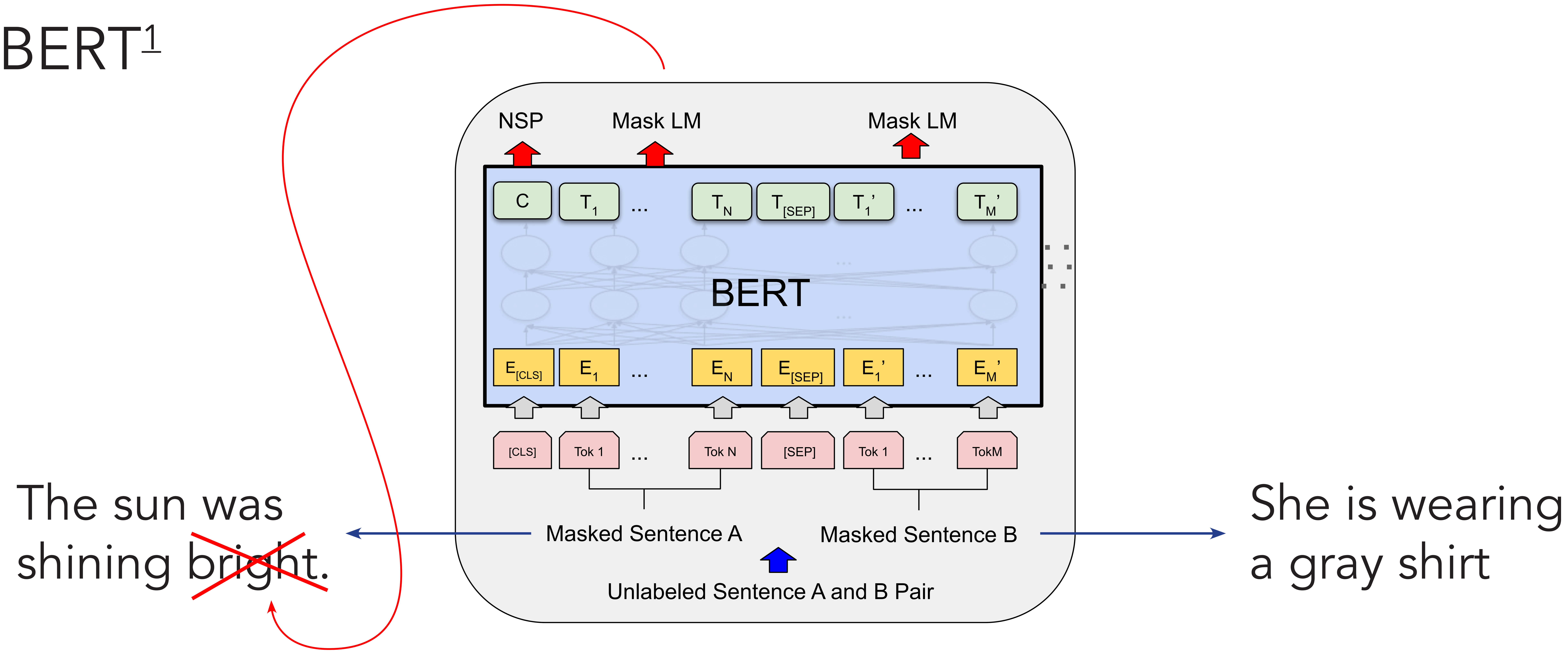

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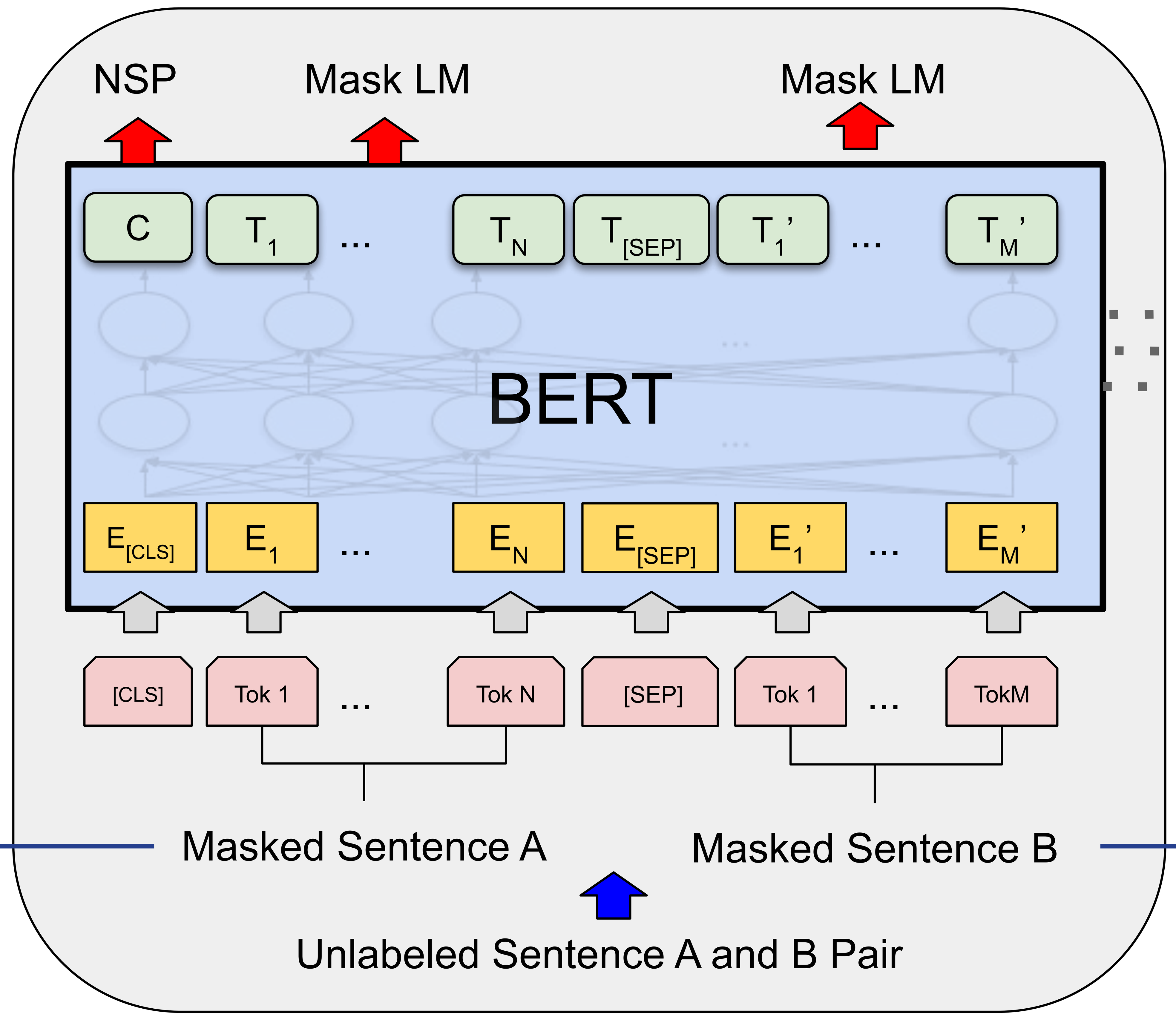

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Self-supervised representation learning

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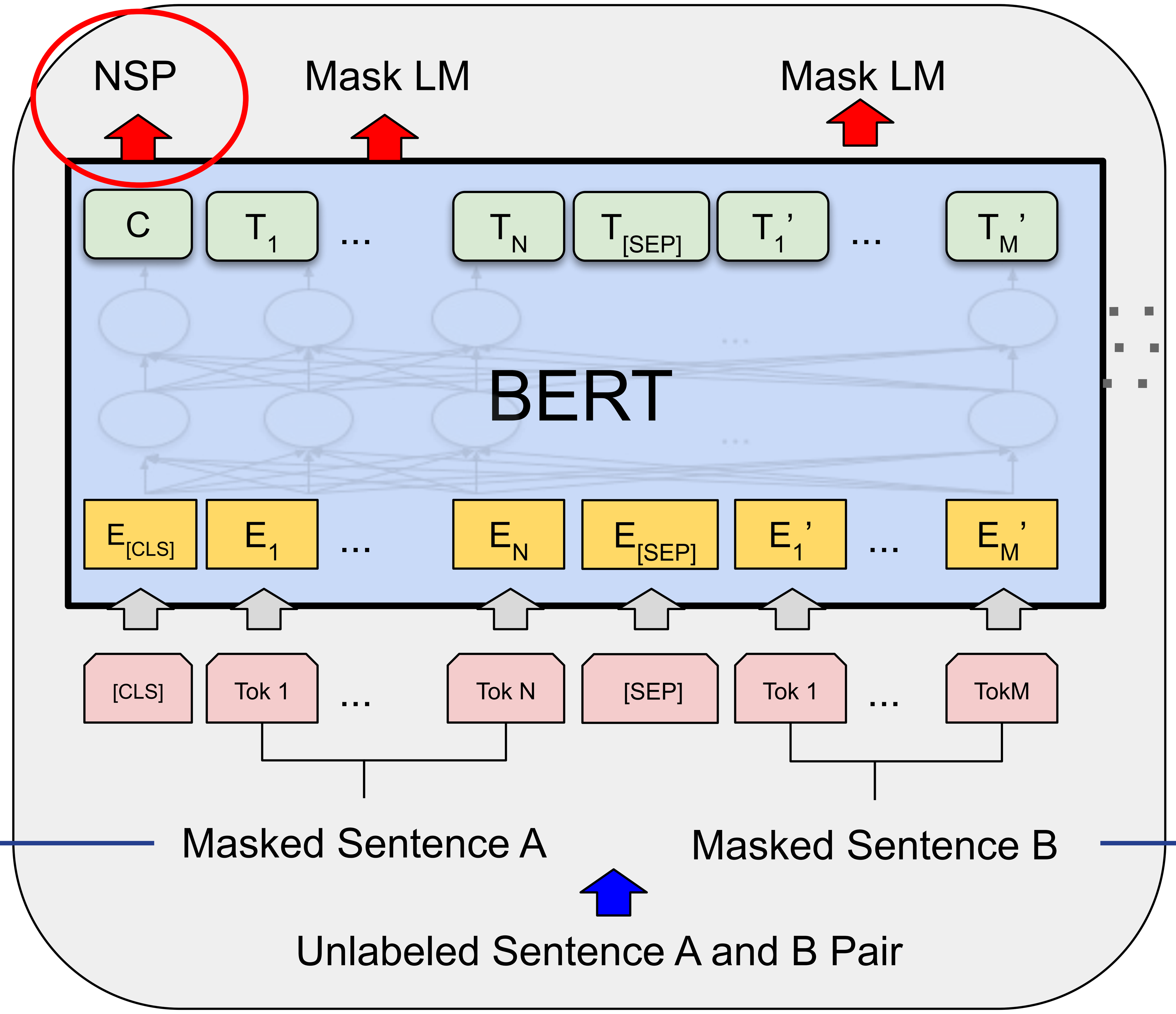
binary next sentence prediction



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Self-supervised representation learning

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Top Leaderboard Systems (Dec 10th, 2018)				
Human	-	-	82.3	91.2
#1 Ensemble - nlnet	-	-	86.0	91.7
#2 Ensemble - QANet	-	-	84.5	90.5
Published				
BiDAF+ELMo (Single)	-	85.6	-	85.8
R.M. Reader (Ensemble)	81.2	87.9	82.3	88.5
Ours				
$\text{BERT}_{\text{BASE}}$ (Single)	80.8	88.5	-	-
$\text{BERT}_{\text{LARGE}}$ (Single)	84.1	90.9	-	-
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$\text{BERT}_{\text{LARGE}}$ (Sgl.+TriviaQA)	**84.2**	**91.1**	**85.1**	**91.8**
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Table 2: SQuAD 1.1 results. The BERT ensemble is 7x systems which use different pre-training checkpoints and fine-tuning seeds.

Performance of fine-tuned model on question-answer benchmark

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Self-supervised representation learning

- DINO[1]
  - Self-supervised representation learning for computer vision tasks
  - Vision transformer as neural network
  - Training with unlabeled ImageNet dataset
  - Student-teacher training with virtual prediction task

[1] M. Caron, H. Touvron, I. Misra, H. Jegou, J. Mairal, P. Bojanowski, and A. Joulin. Emerging properties in self-supervised vision transformers. CoRR, 2021.

Self-supervised representation learning

- DINO[1]

	Cifar_{10}	Cifar_{100}	INat_{18}	INat_{19}	Flwrs	Cars	INet
ViT-S/16							
Sup. [69]	**99.0**	89.5	70.7	76.6	98.2	92.1	79.9
DINO	**99.0**	**90.5**	**72.0**	**78.2**	**98.5**	**93.0**	**81.5**
ViT-B/16							
Sup. [69]	99.0	90.8	**73.2**	77.7	98.4	92.1	81.8
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Transformer neural networks

- Scale well to highly parallel training and billions of parameters, especially for sequential data

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	Ours-JFT (ViT-H/14)	Ours-JFT (ViT-L/16)	Ours-I21k (ViT-L/16)	BiT-L (ResNet152x4)	Noisy Student (EfficientNet-L2)
ImageNet	**88.55** ± 0.04	87.76 ± 0.03	85.30 ± 0.02	87.54 ± 0.02	88.4/88.5*
ImageNet ReaL	**90.72** ± 0.05	90.54 ± 0.03	88.62 ± 0.05	90.54	90.55
CIFAR-10	**99.50** ± 0.06	99.42 ± 0.03	99.15 ± 0.03	99.37 ± 0.06	–
CIFAR-100	**94.55** ± 0.04	93.90 ± 0.05	93.25 ± 0.05	93.51 ± 0.08	–
Oxford-IIIT Pets	**97.56** ± 0.03	97.32 ± 0.11	94.67 ± 0.15	96.62 ± 0.23	–
Oxford Flowers-102	99.68 ± 0.02	**99.74** ± 0.00	99.61 ± 0.02	99.63 ± 0.03	–
VTAB (19 tasks)	**77.63** ± 0.23	76.28 ± 0.46	72.72 ± 0.21	76.29 ± 1.70	–
TPUv3-core-days	2.5k	0.68k	0.23k	9.9k	12.3k

[1] A. Dosovitskiy, L. Beyer, A. Kolesnikov, D. Weissenborn, X. Zhai, T. Unterthiner, M. Dehghani, M. Minderer, G. Heigold, S. Gelly, J. Uszkoreit, and N. Houlsby. An image is worth 16x16 words: Transformers for image recognition at scale. In International Conference on Learning Representations, 2021.

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very large transformer

convolutional network

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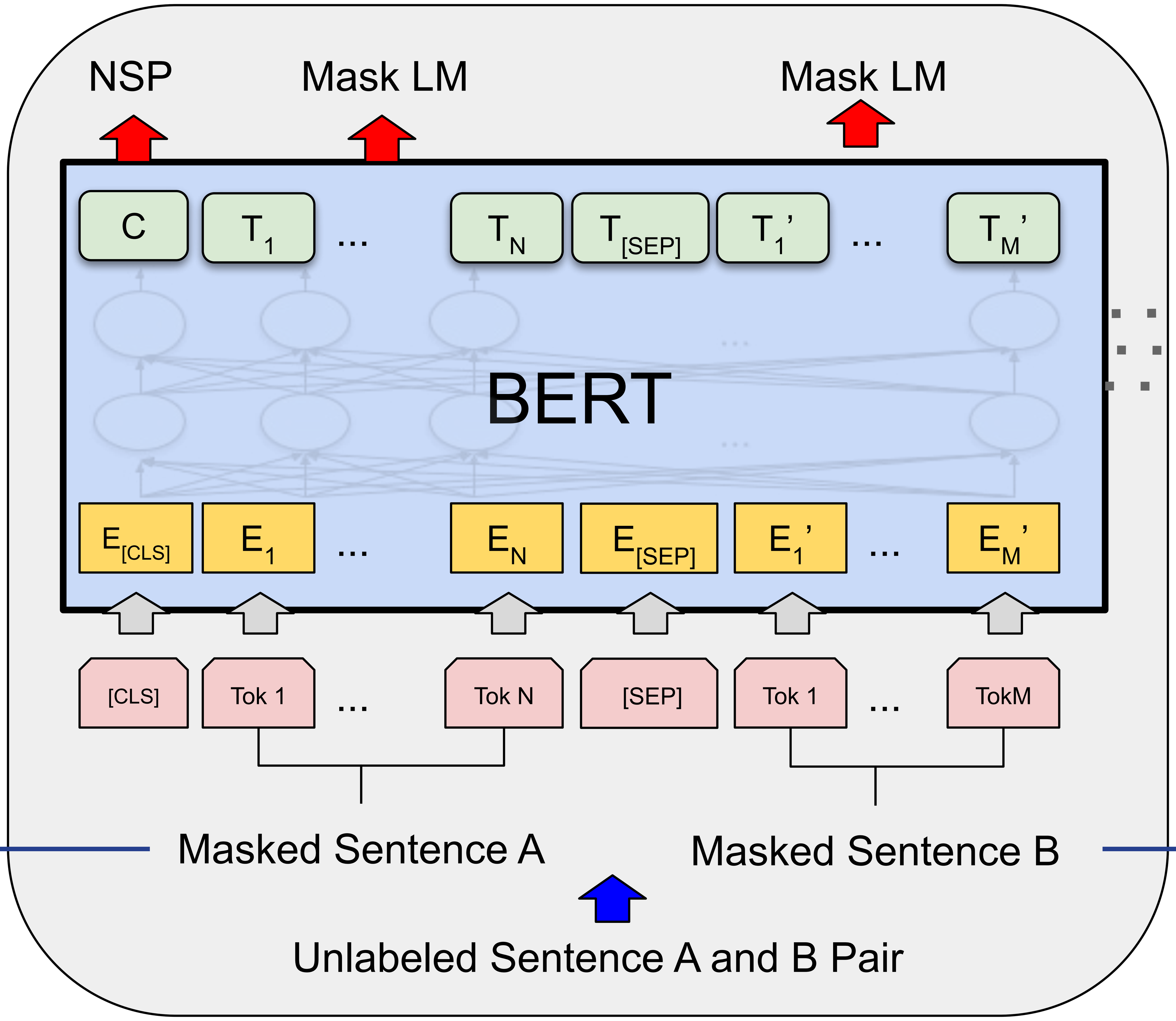
- Scale well to highly parallel training and billions of parameters, especially for sequential data
- Attention mechanism allows to model complex dependencies in data
  - Typically through learned inner product in feature space with “legs” in input domain
  - Direct interpretation of learned representations through attention maps

Transformer neural networks

- BERT:



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Transformer neural networks

- BERT-type model (natural language processing):

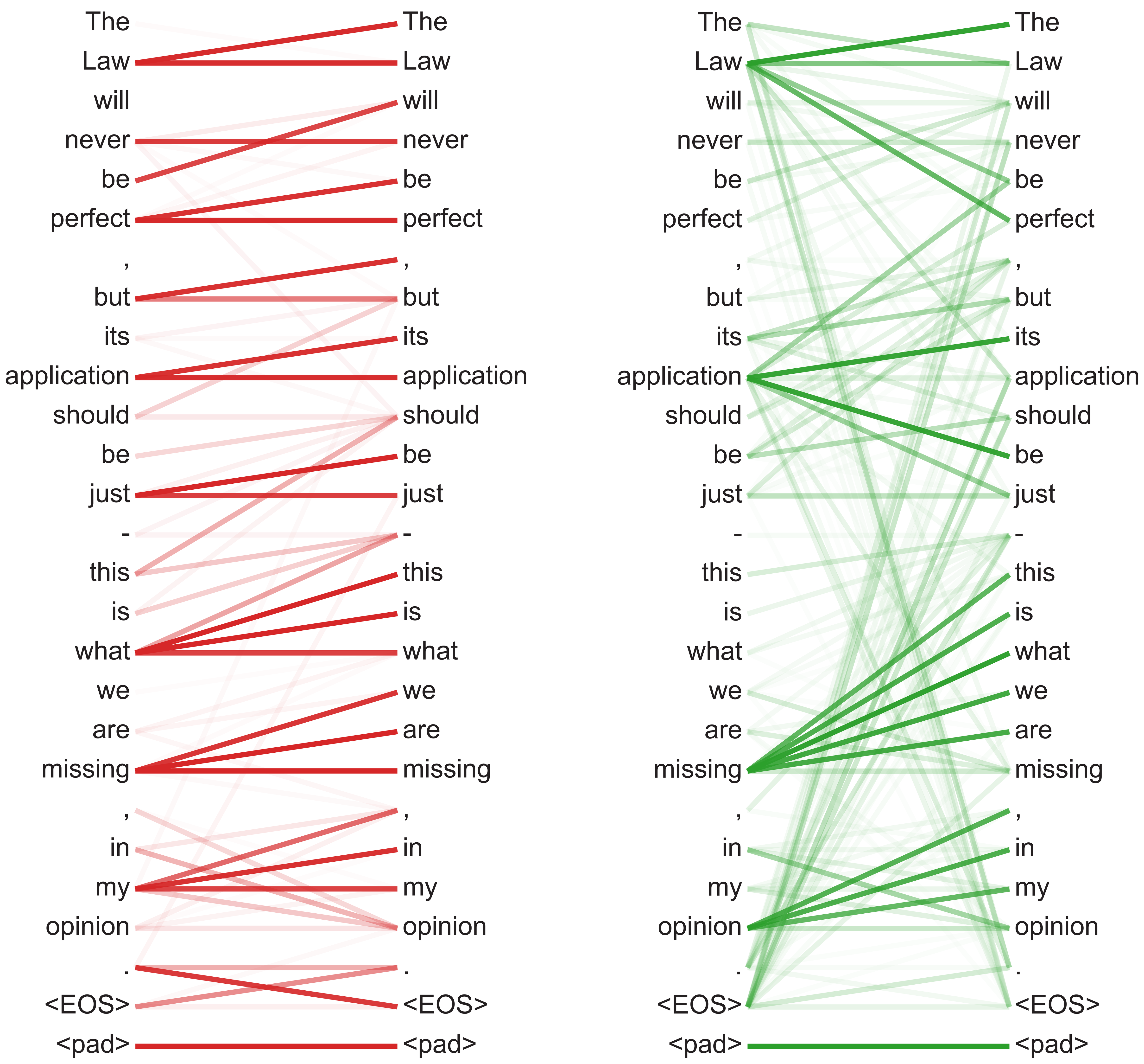
"The law will never be perfect, but its application should be just, this is what we are missing, in my opinion."

Transformer neural networks

A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. N. Gomez, L. Kaiser, and I. Polosukhin. Attention is all you need. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 30. Curran Associates, Inc., 2017.

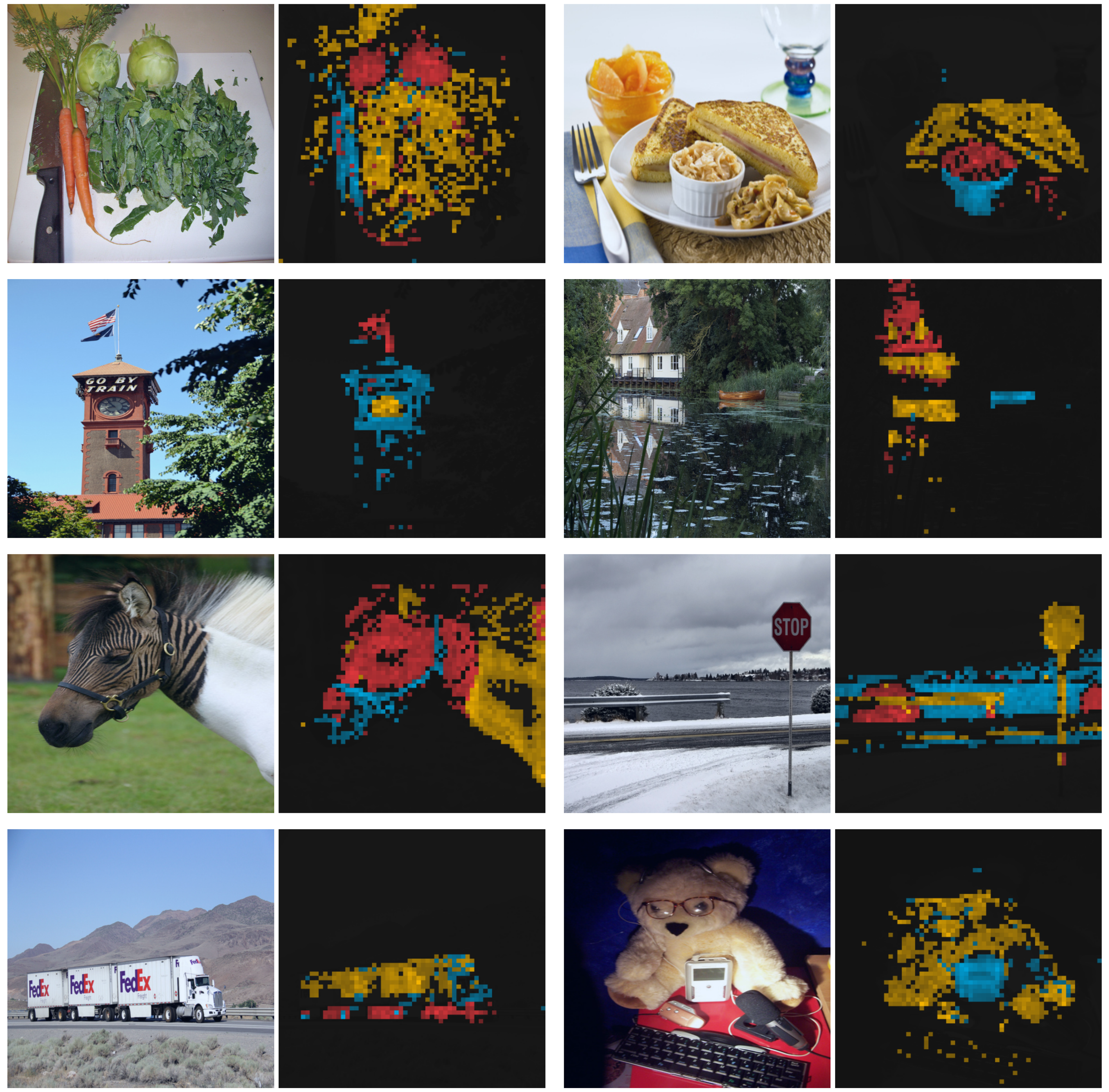
Transformer neural networks

A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. N. Gomez, L. Kaiser, and I. Polosukhin. Attention is all you need. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 30. Curran Associates, Inc., 2017.



Transformer neural networks

- DINO (computer vision):



M. Caron, H. Touvron, I. Misra, H. Jegou, J. Mairal, P. Bojanowski, and A. Joulin. Emerging properties in self-supervised vision transformers. CoRR, abs/2104.14294, 2021.

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How can we adapt these ideas to the Earth sciences?

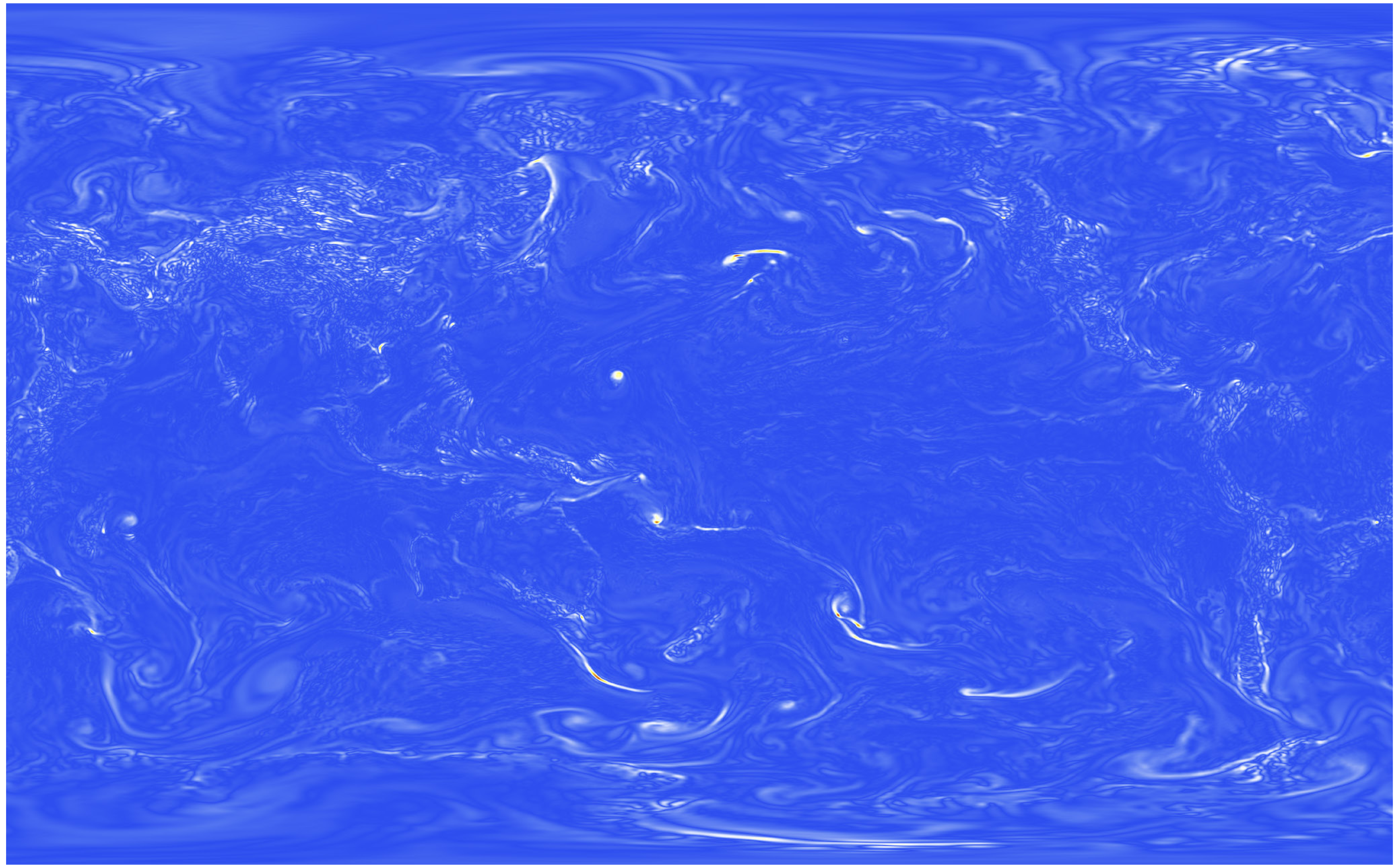
The facts

- Large amounts of data and growing fast:
  - ERA5, OCEAN5, MetOp-SG, ...
  - Unlabeled data
  - (Quasi-) observational data describing effects from the whole system
- Very limited amounts of labeled data for many appli-cations

AtmoDist

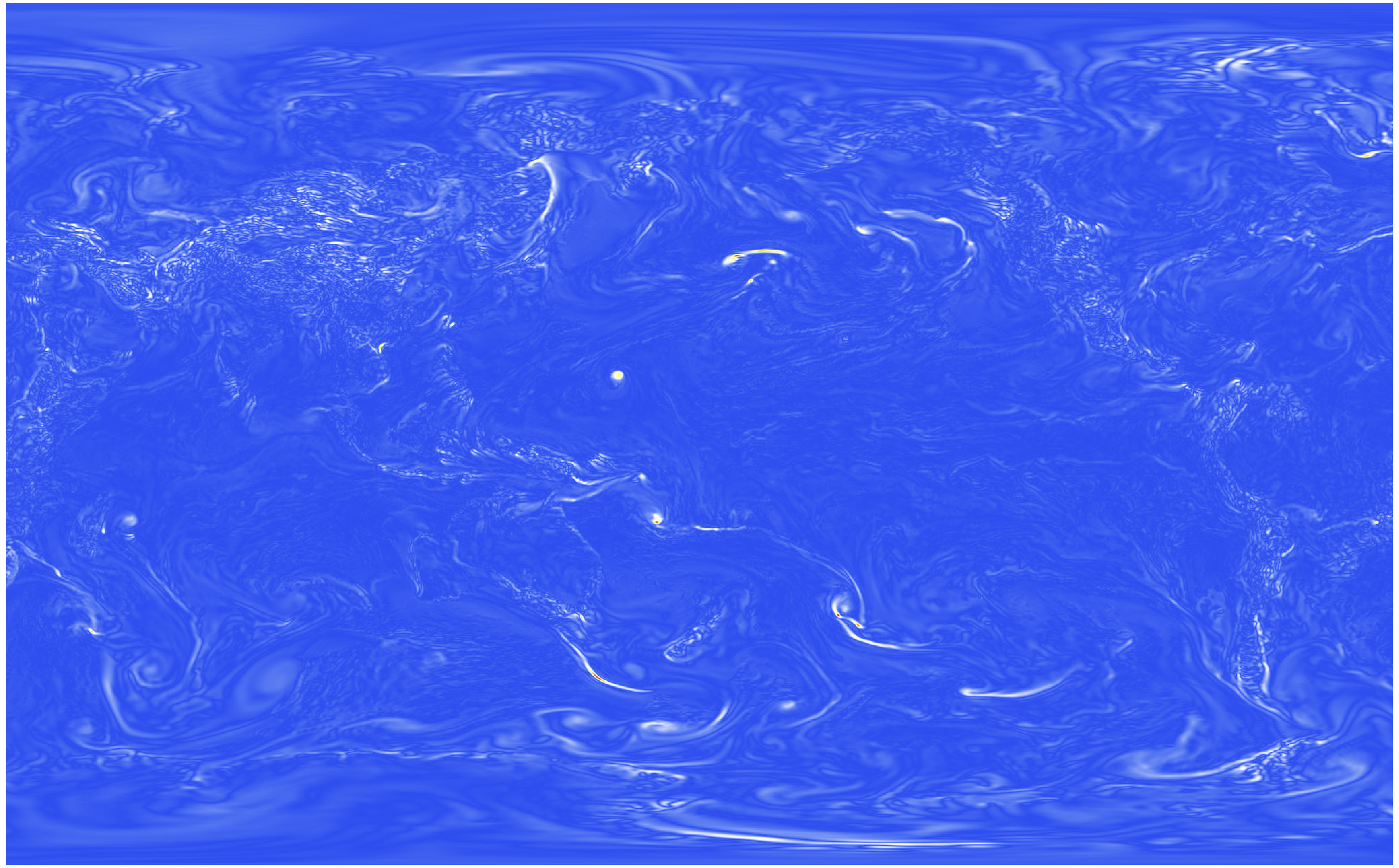
- Starting point:
  - Good distance function is critical for many machine learning applications
  - Standard ones from mathematics are often of limited utility

Motivation

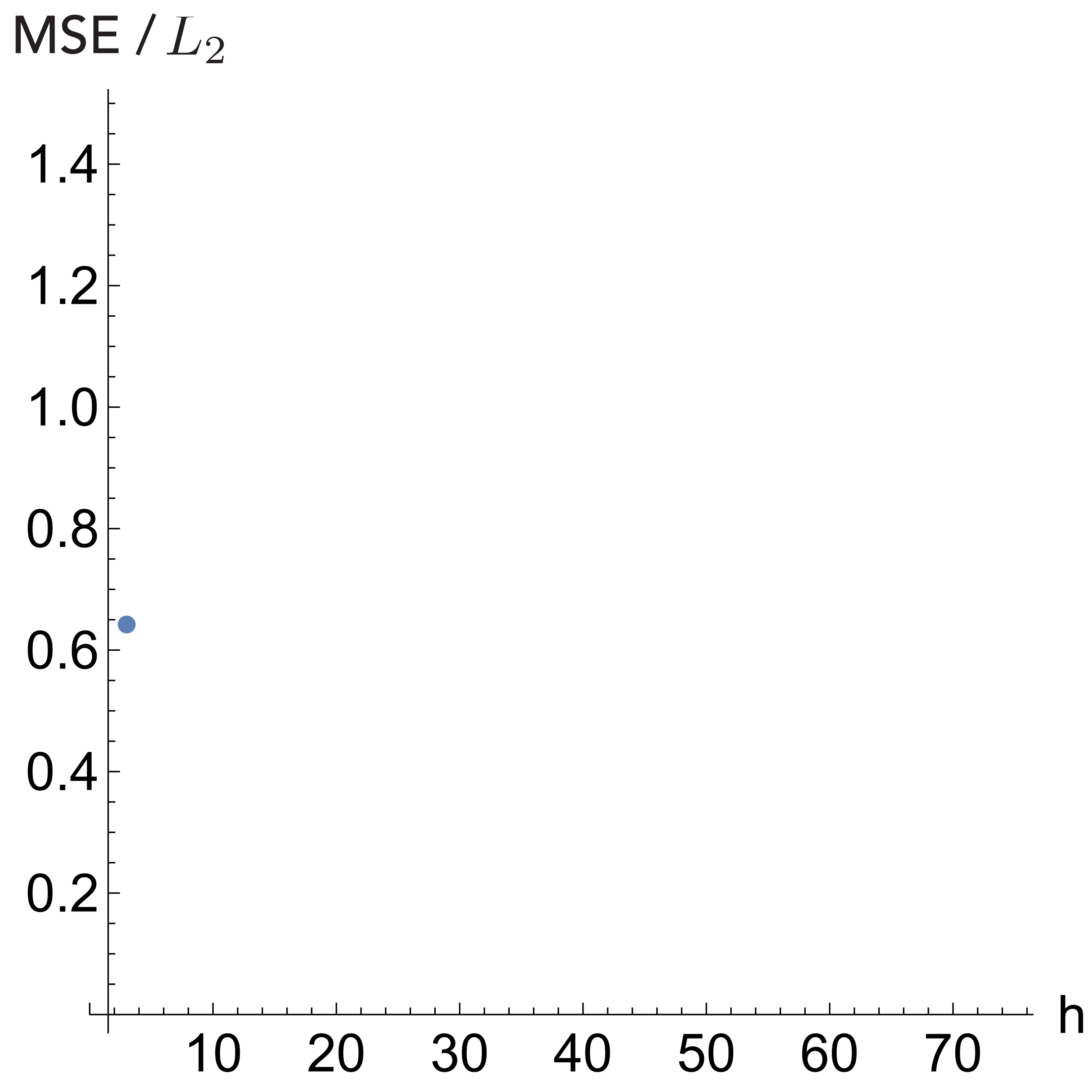


vorticity

Motivation



vorticity



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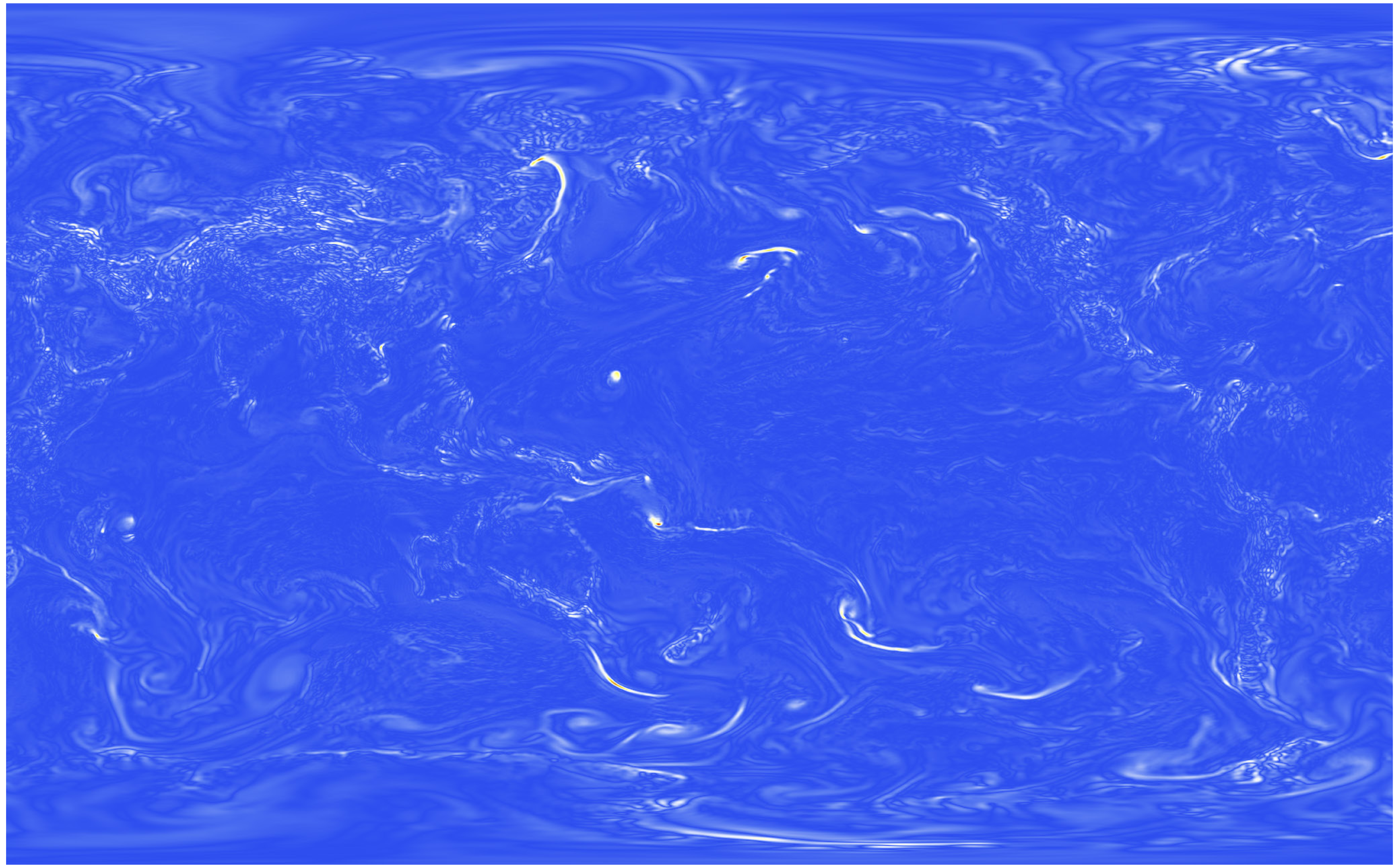

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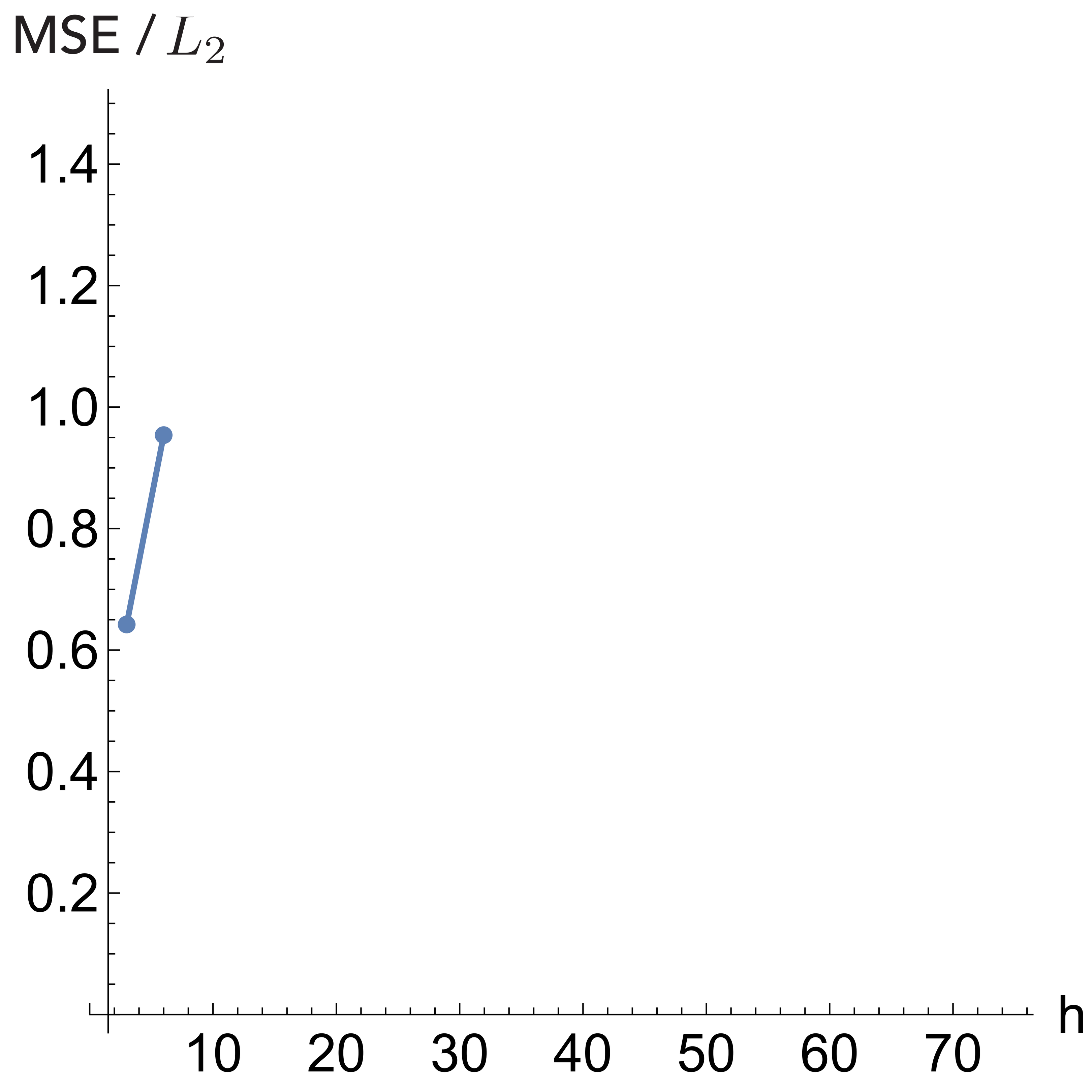

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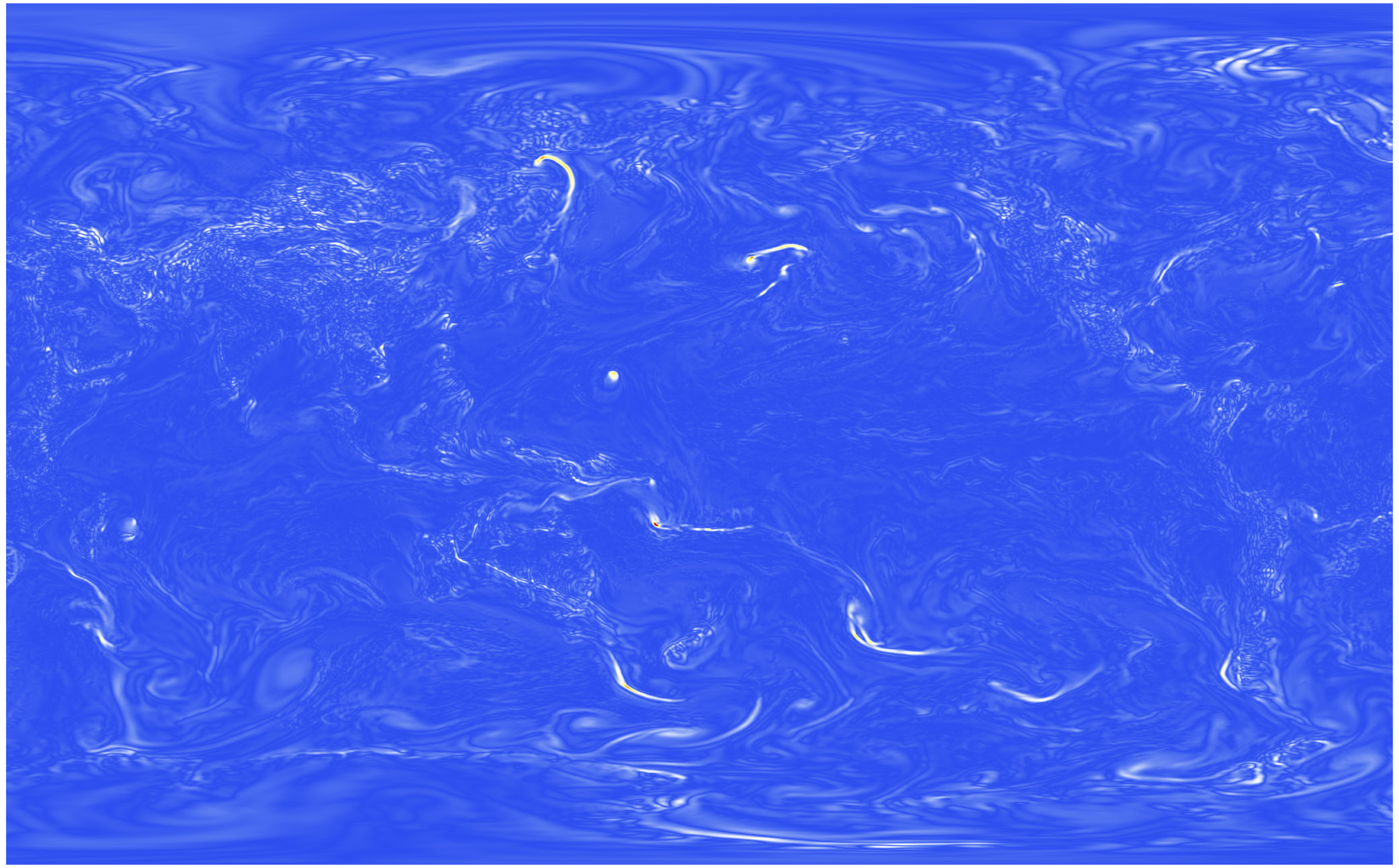

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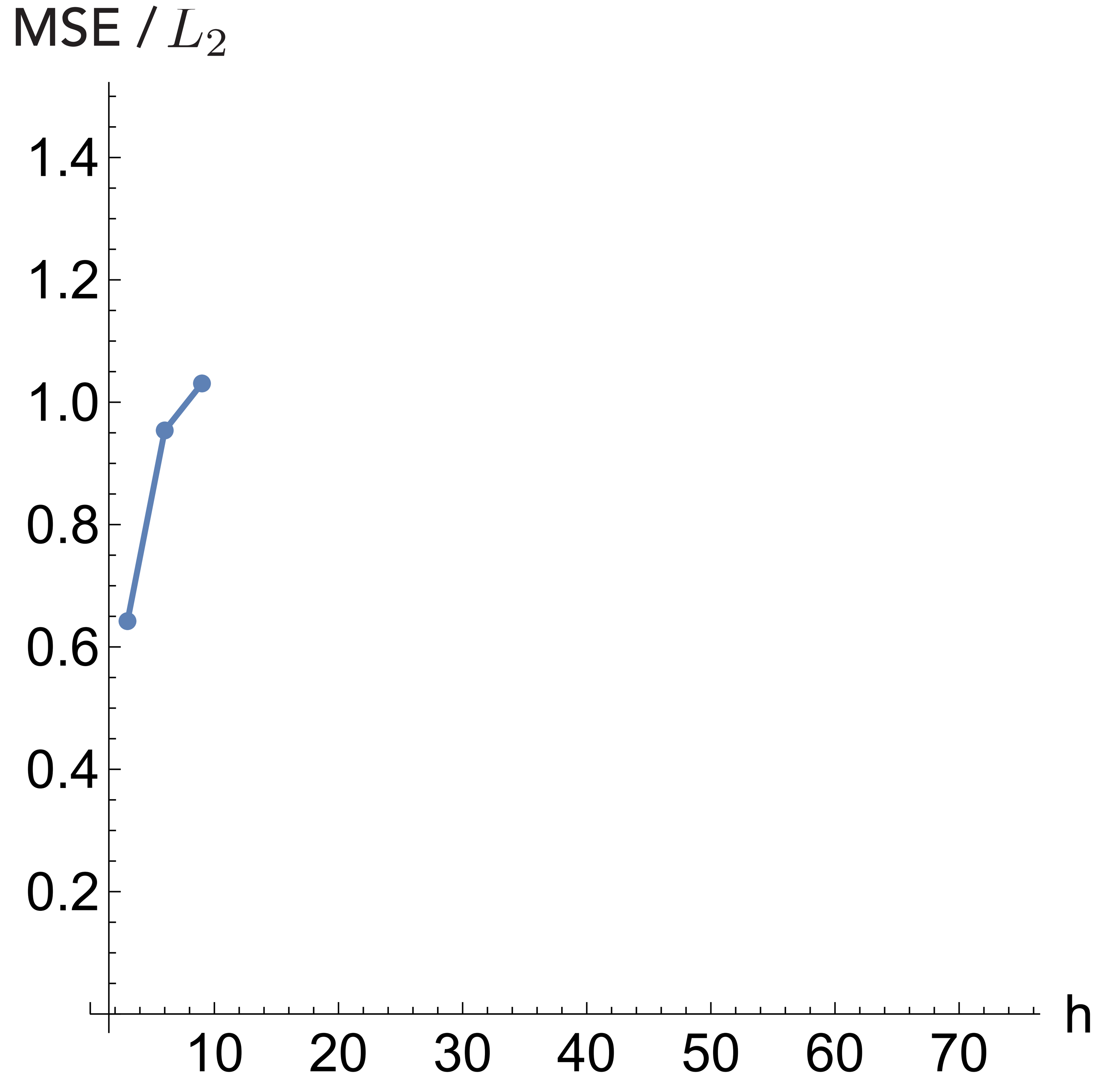

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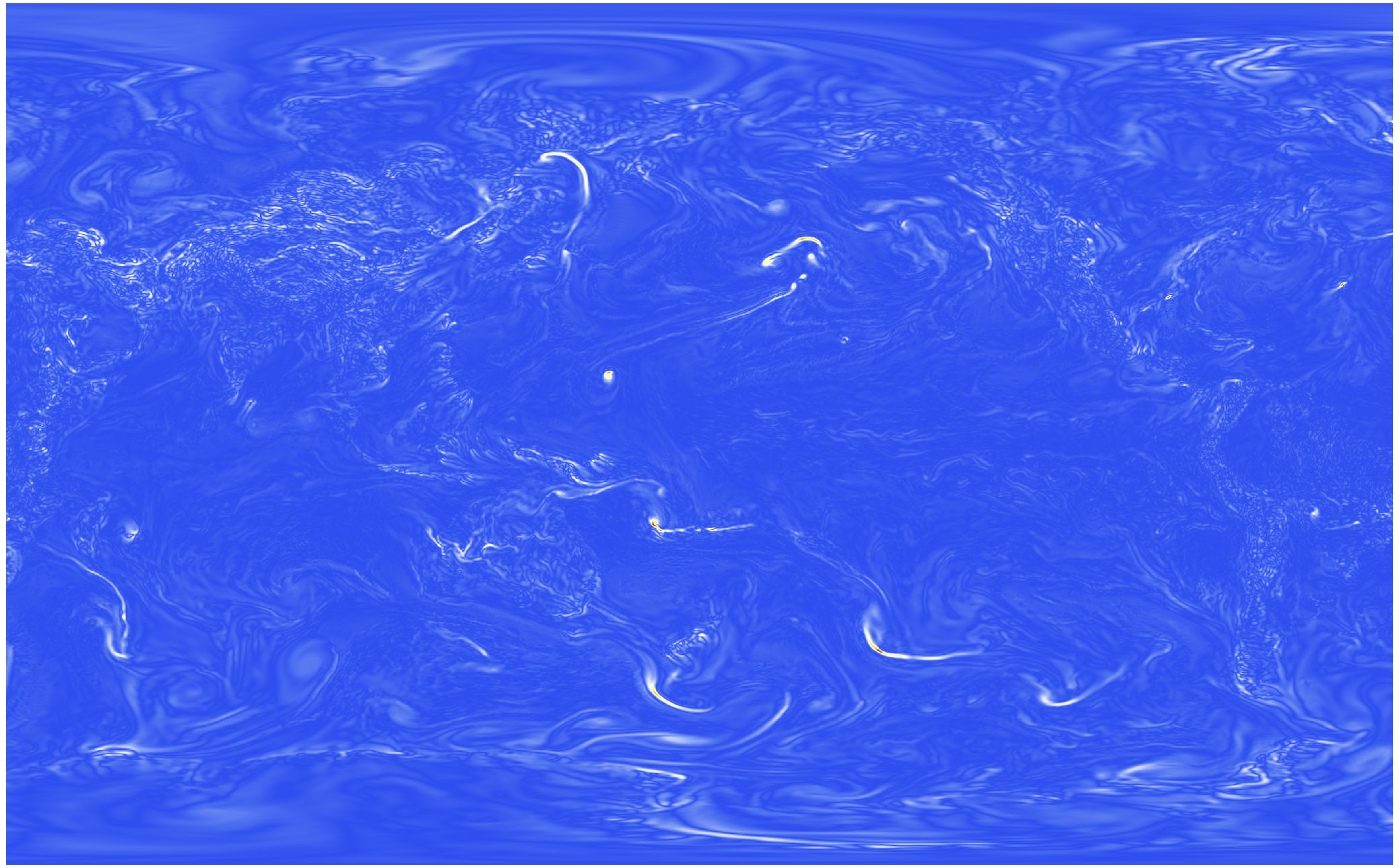

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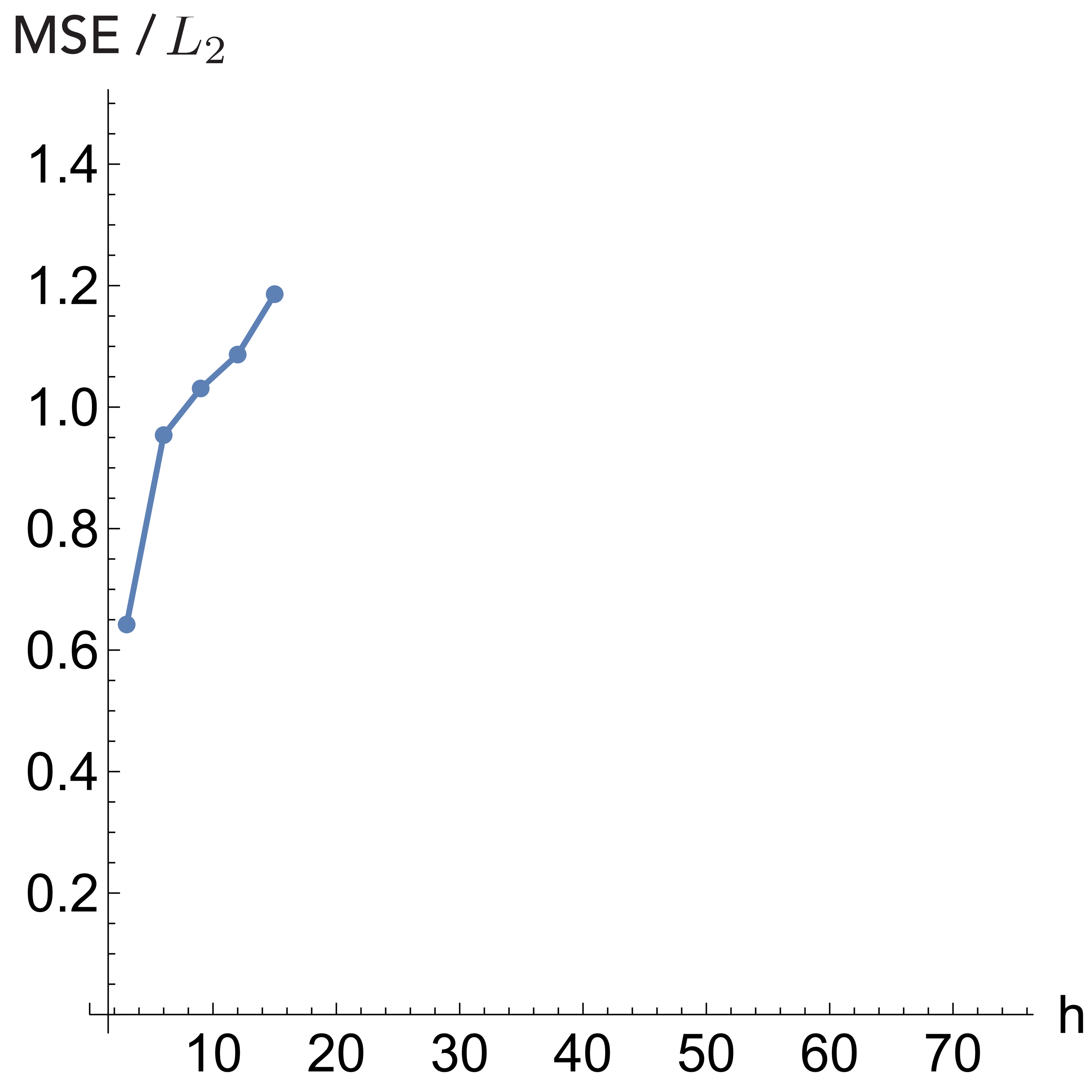

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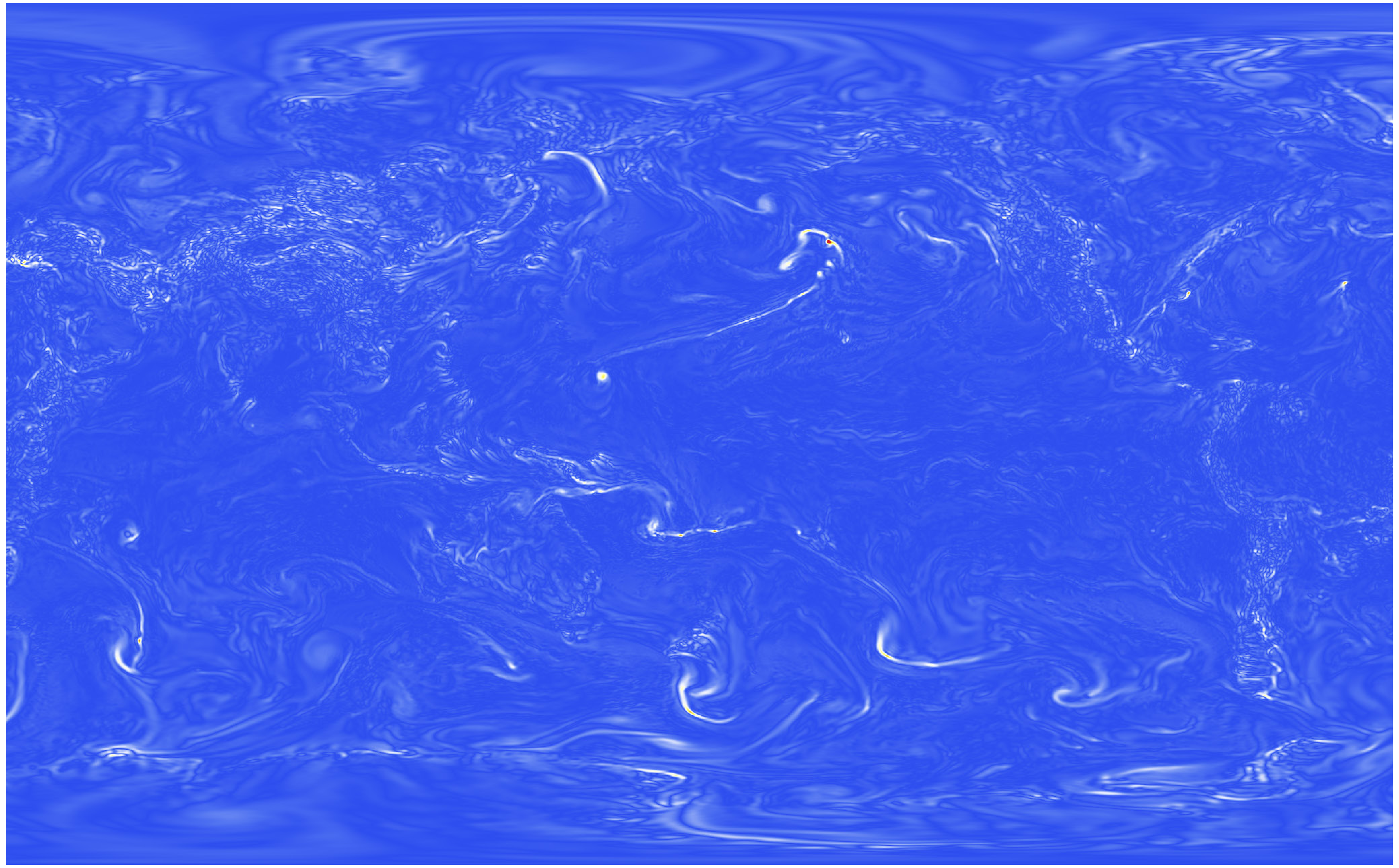

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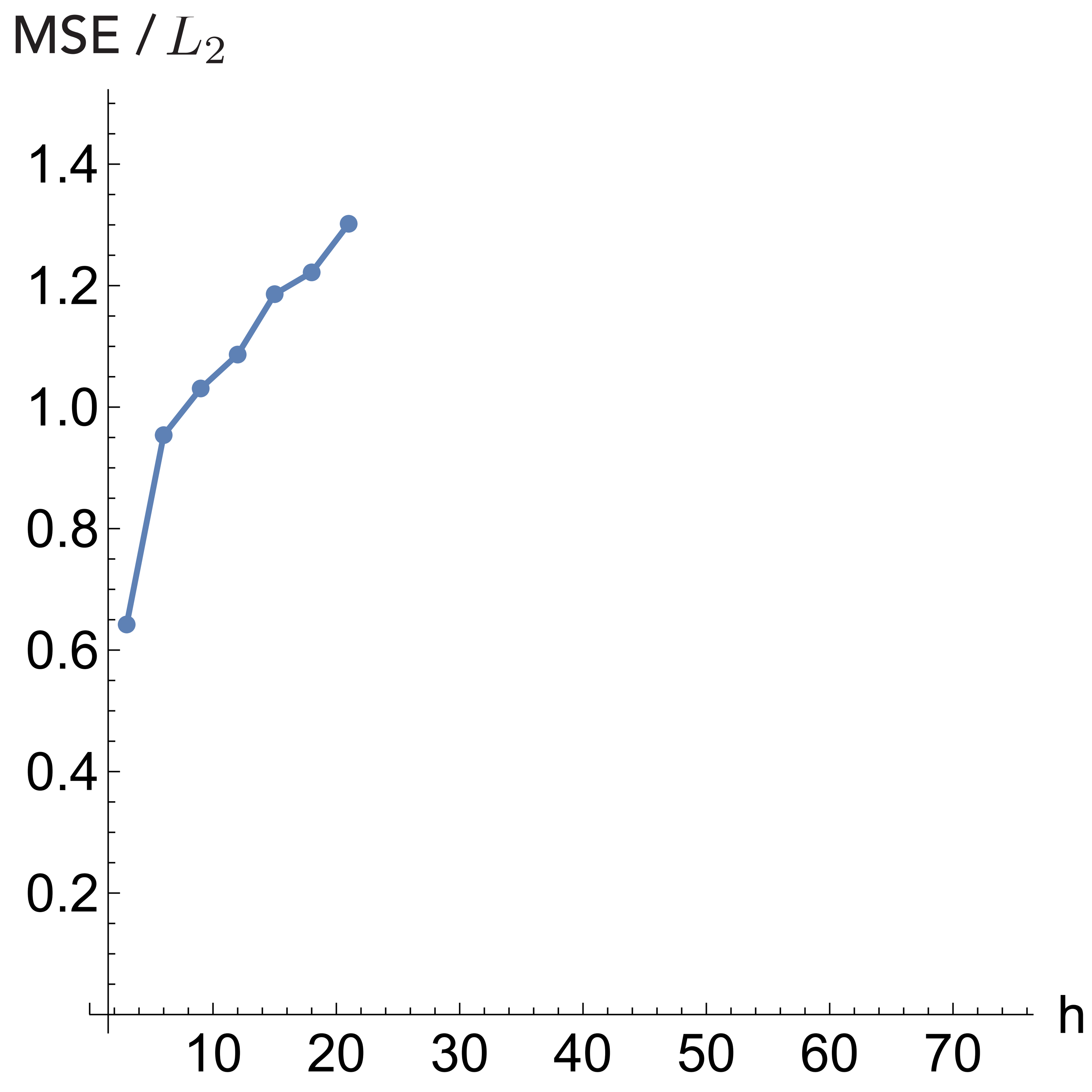

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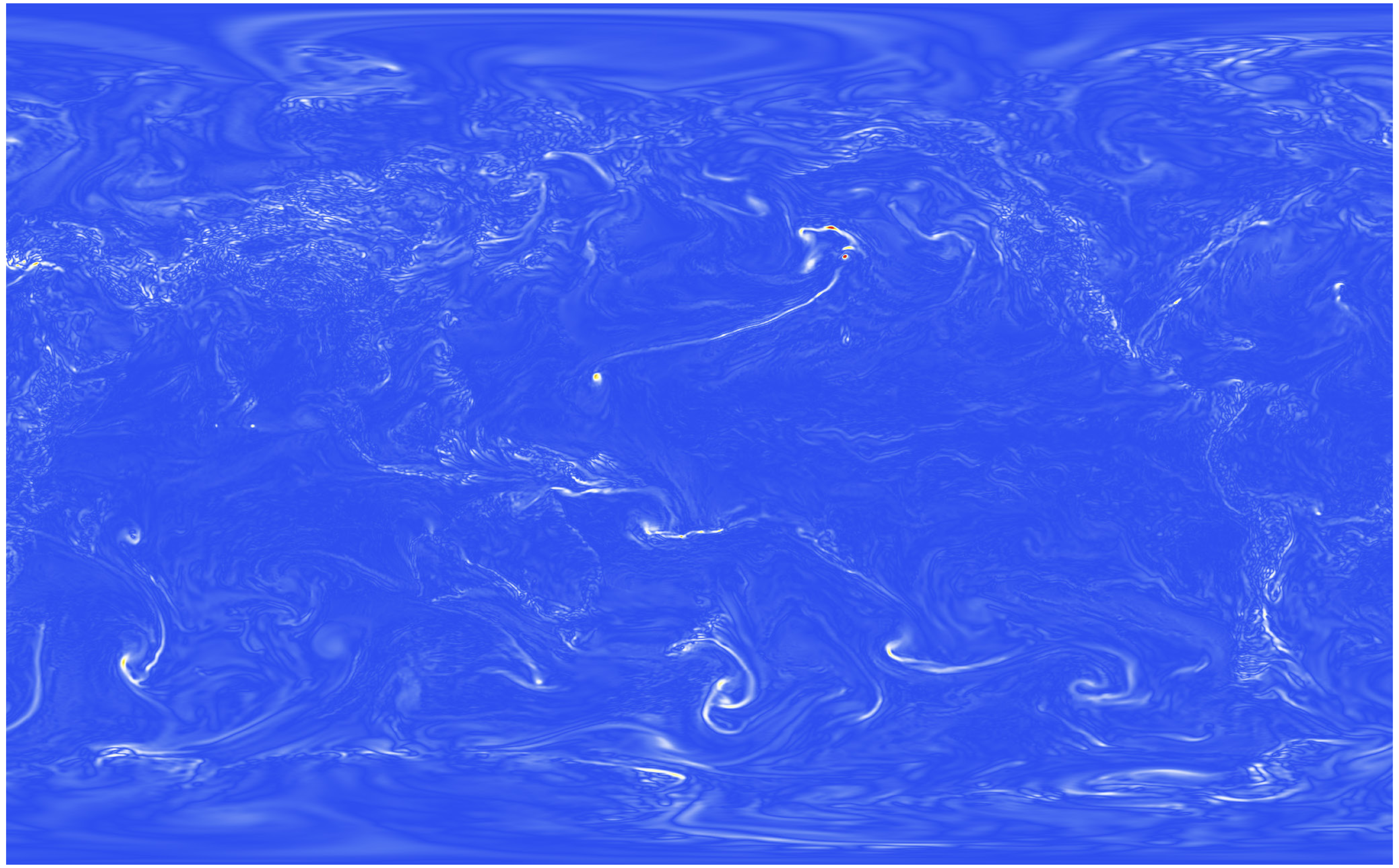

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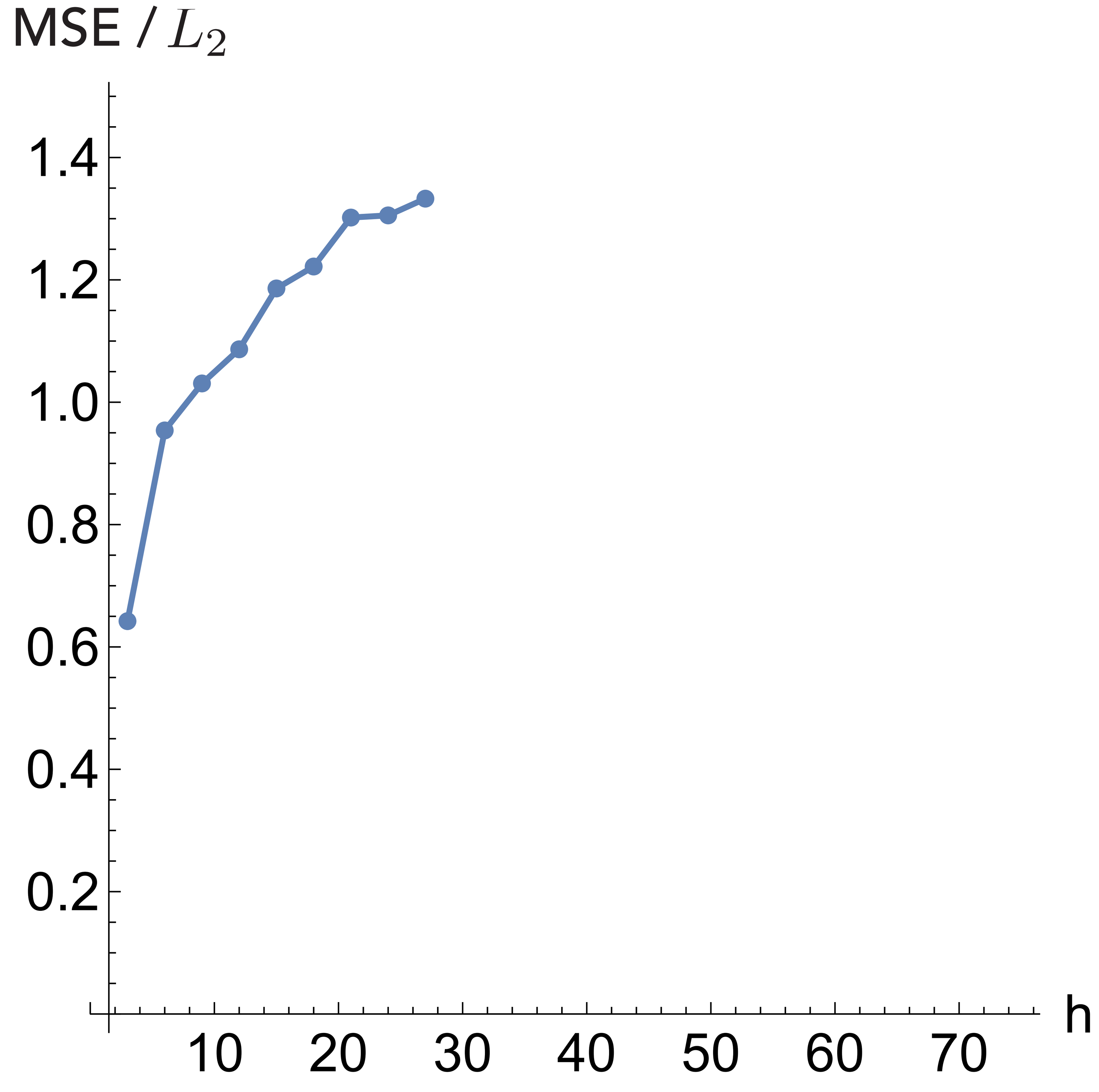

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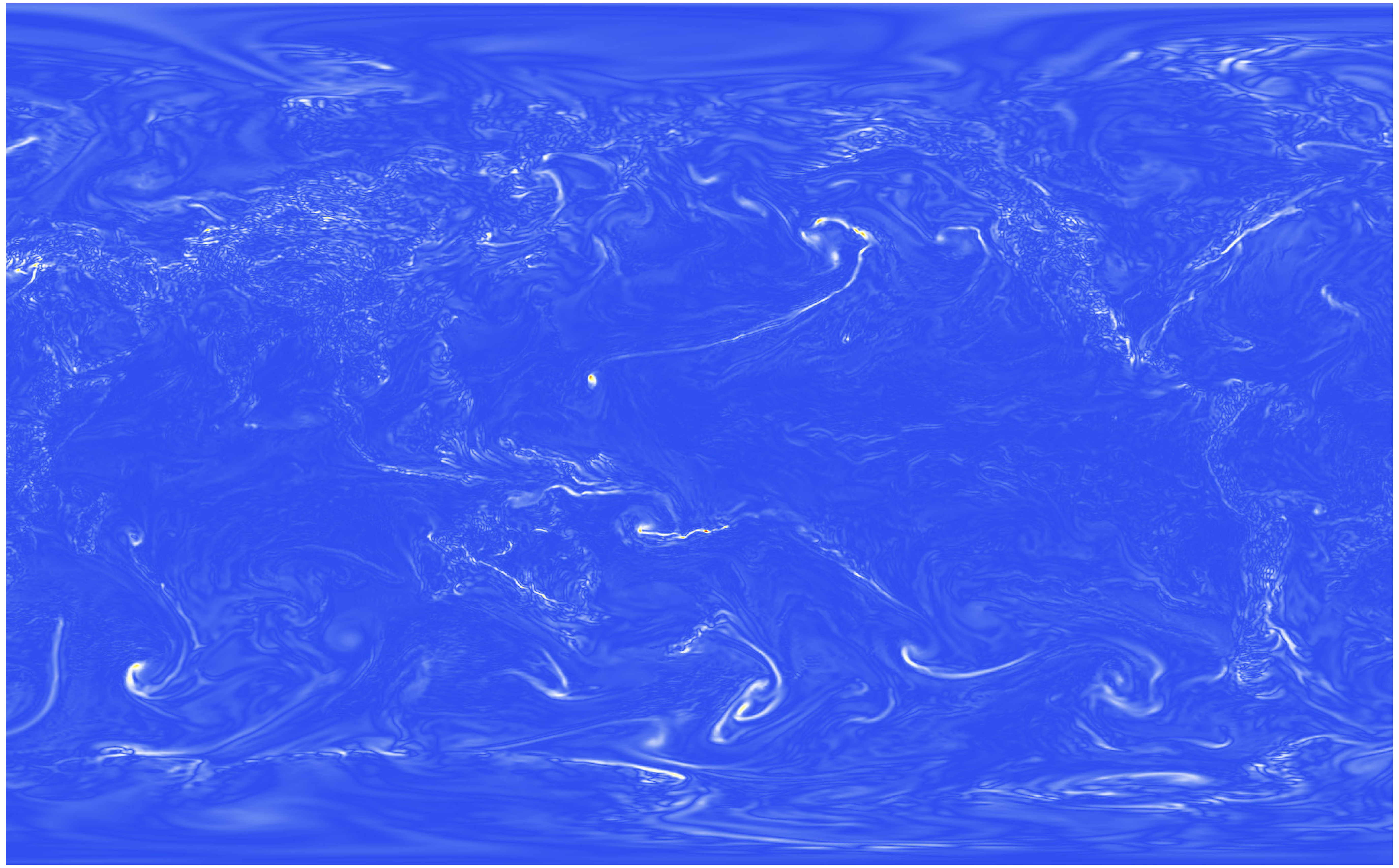

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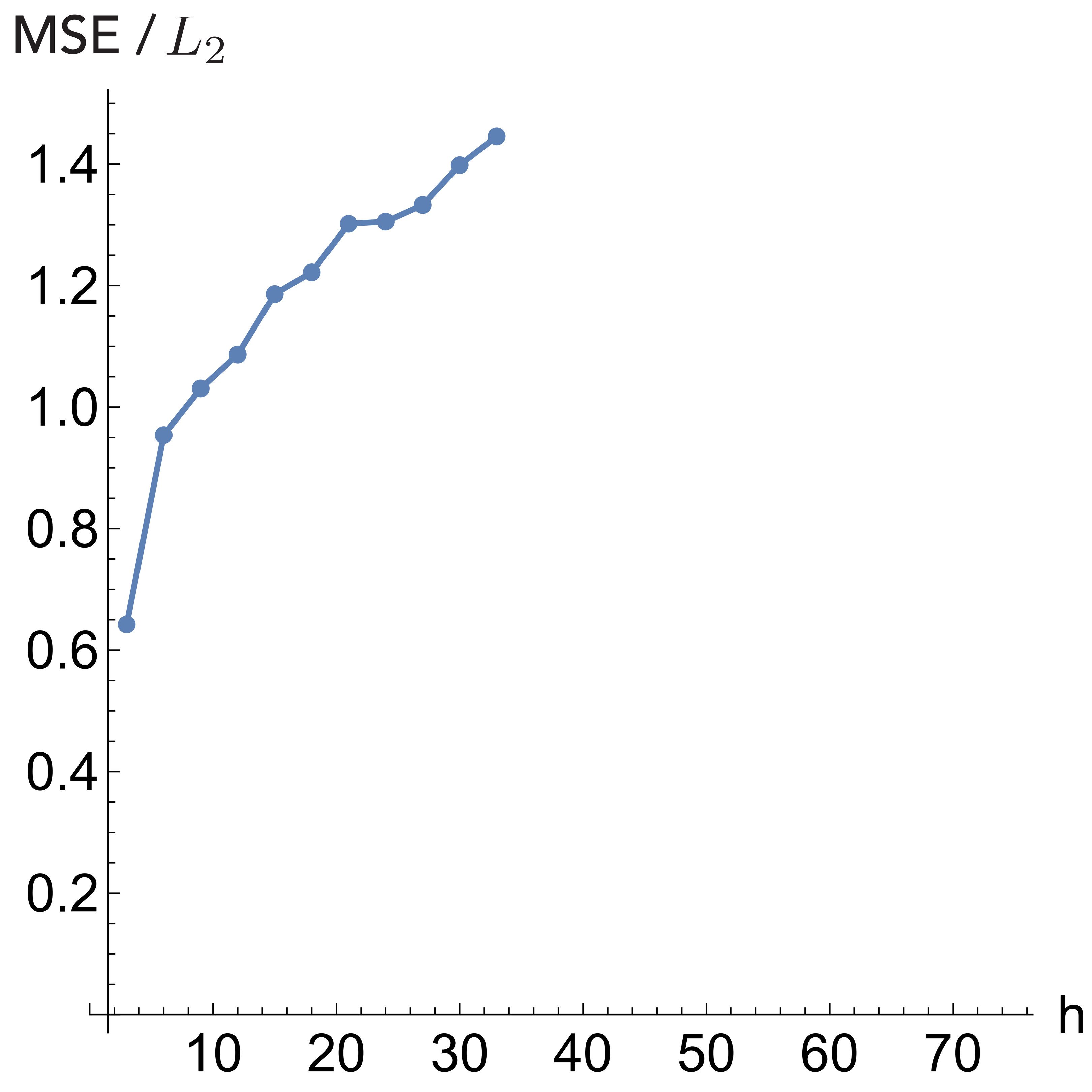

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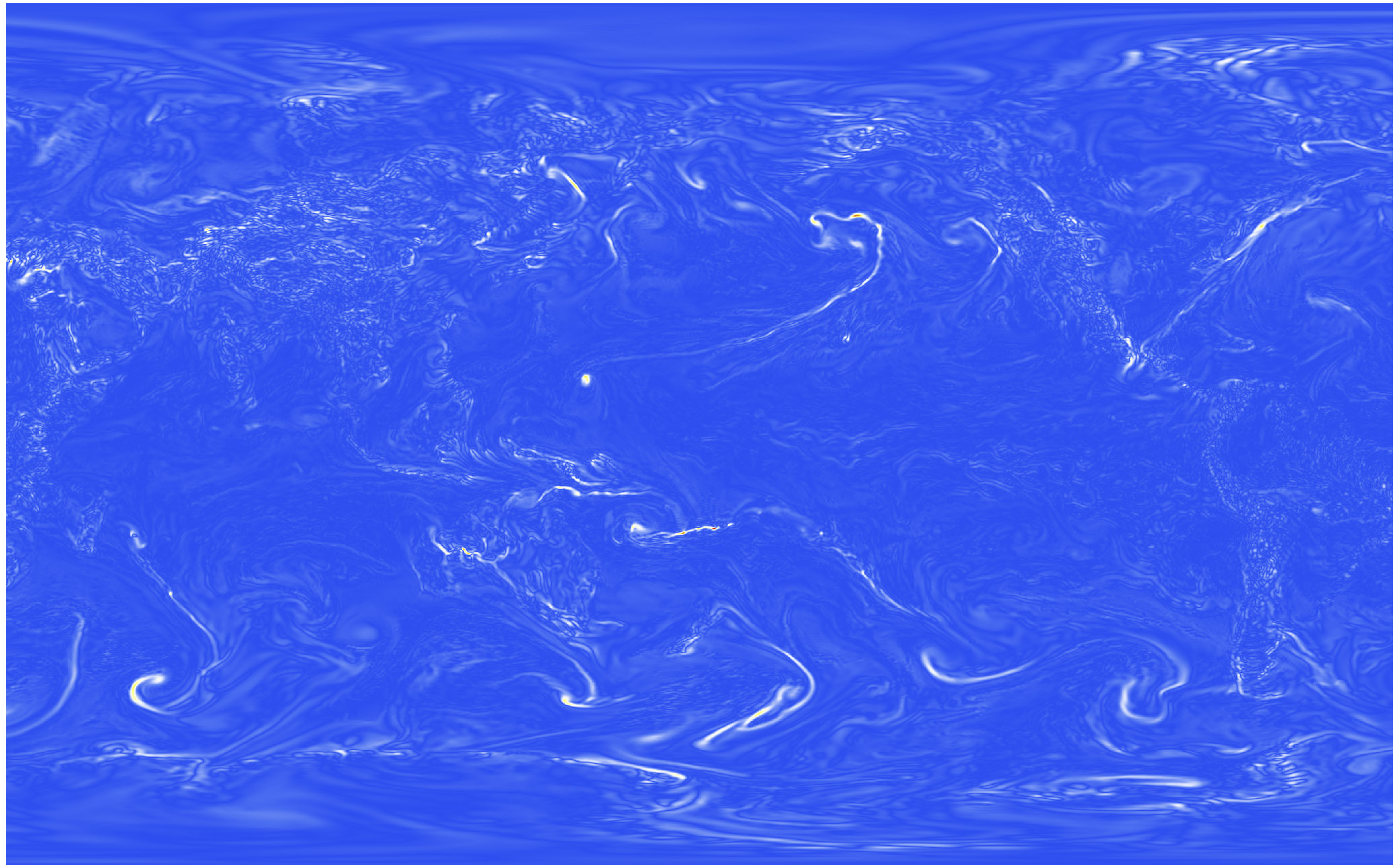

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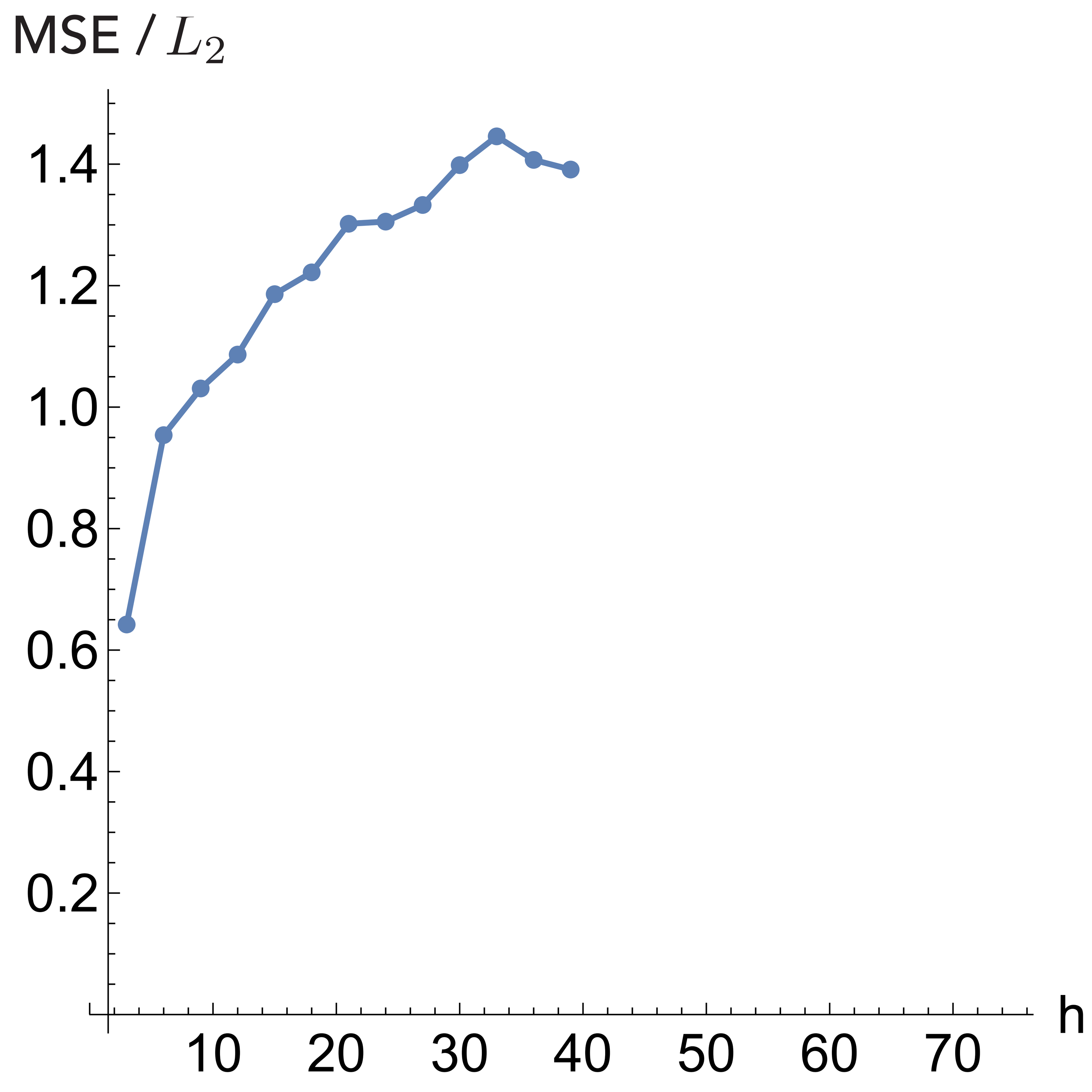

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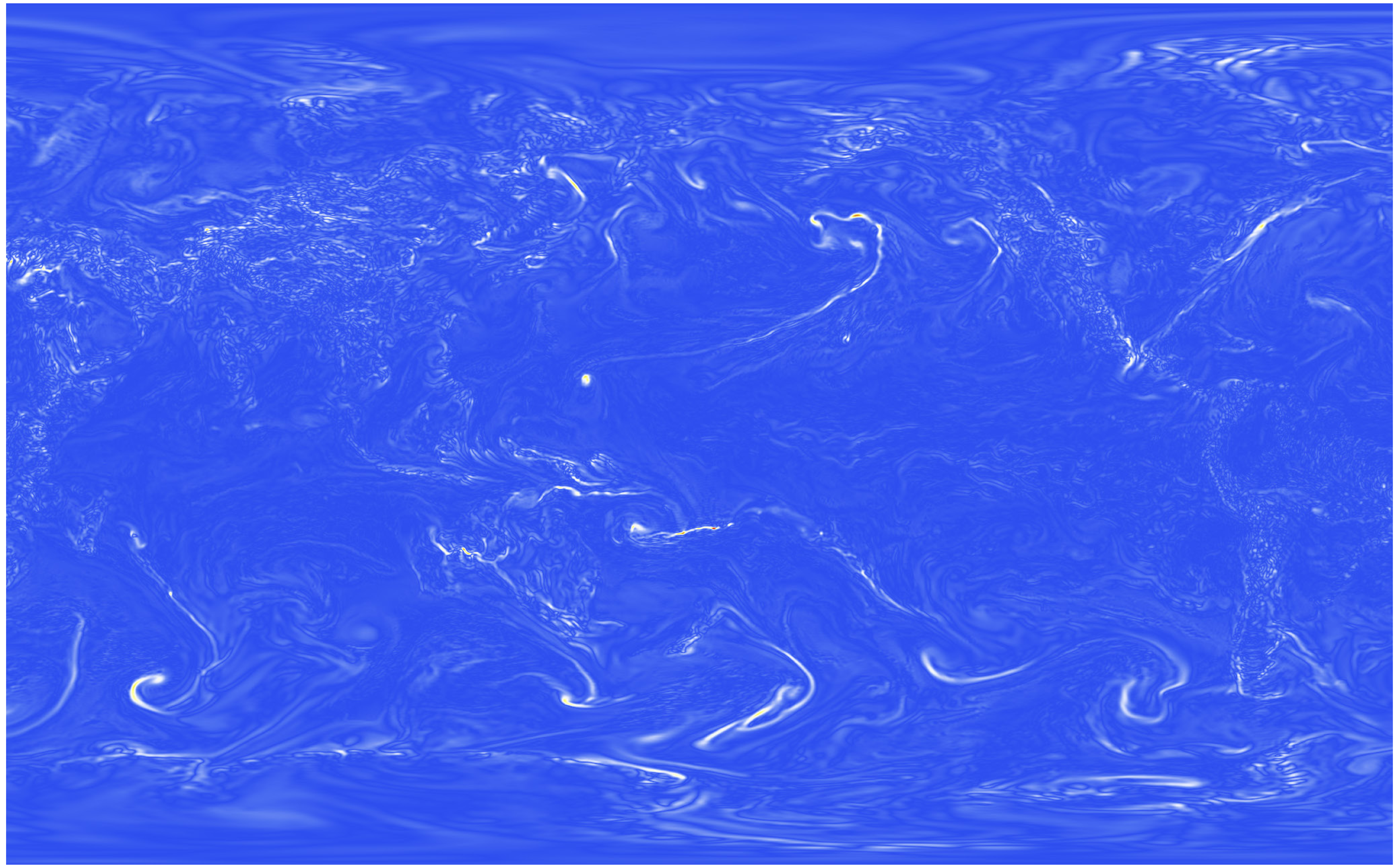

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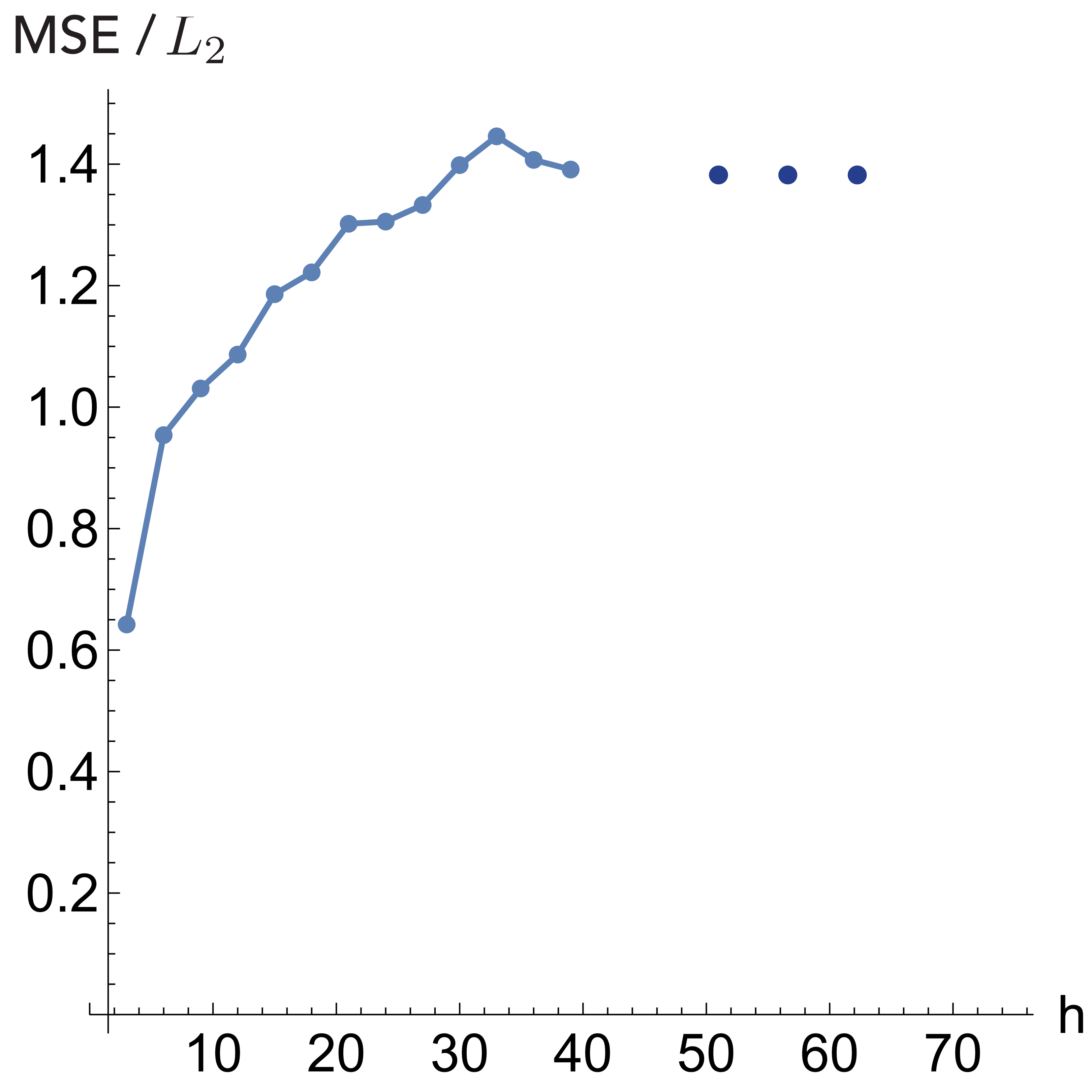

AtmoDist[1]

- Custom distance metric for vorticity + divergence (wind velocity vector field)
- Application: GAN-based super-resolution/downscaling
  - Recent work by Stengel et al.[2] as baseline

[1] S. Hoffmann and C. Lessig. Towards representation learning for atmospheric data. In NEURIPS 2021 Workshop on Climate Change (poster), 2021.
[2] 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.

Self-supervised representation learning

- Representation learning
  - Learn a task-independent representation of the data in the *feature space* of the neural network

$$\mathcal{N} : \mathbb{R}^n \to \mathbb{R}^{m_1} \to \cdots \to \mathbb{R}^{m_{j-1}} \to \mathbb{R}^m$$

- Self-supervised training
  - Train with "labels" or information intrinsic to the data

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feature spaces

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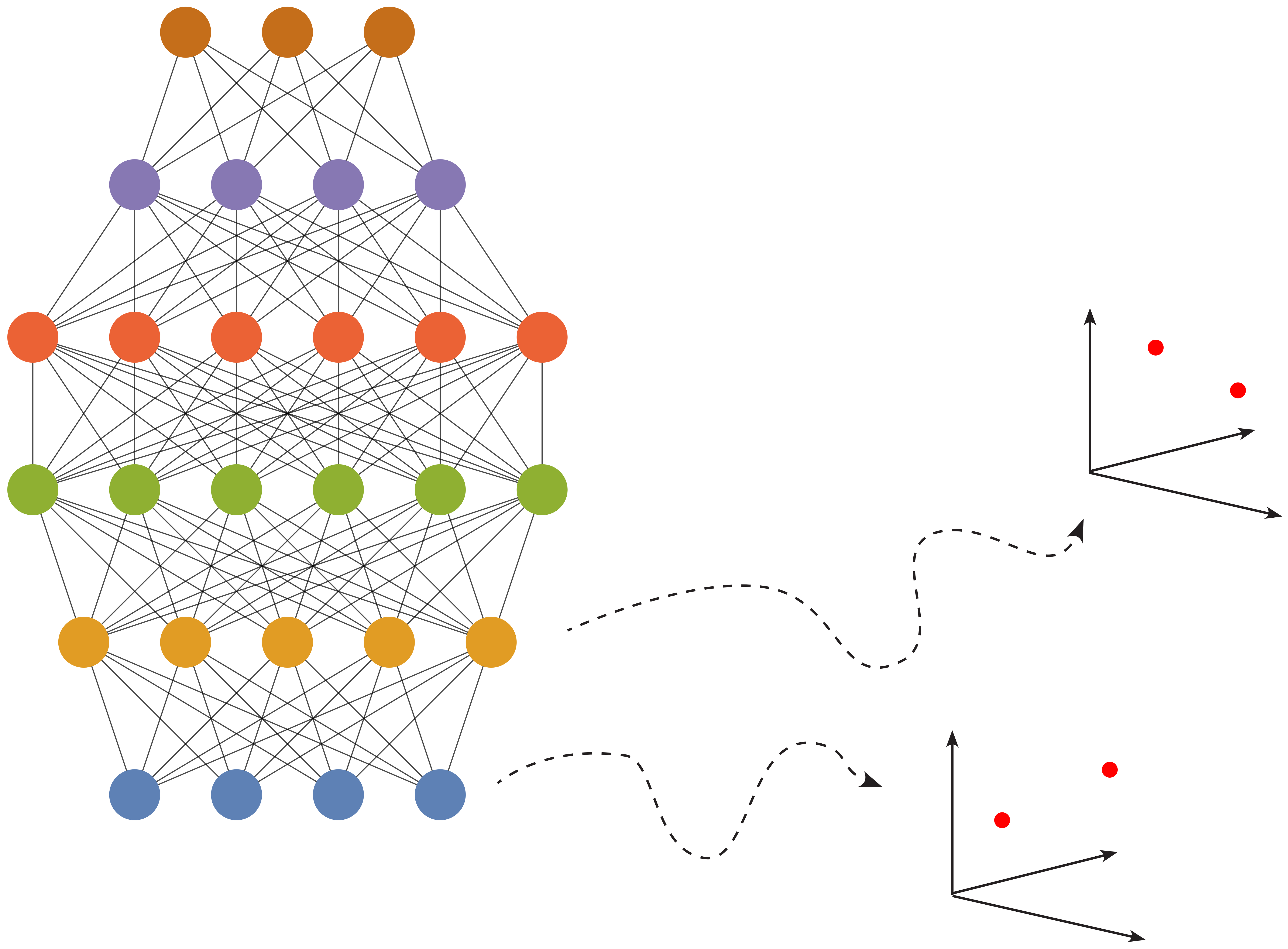
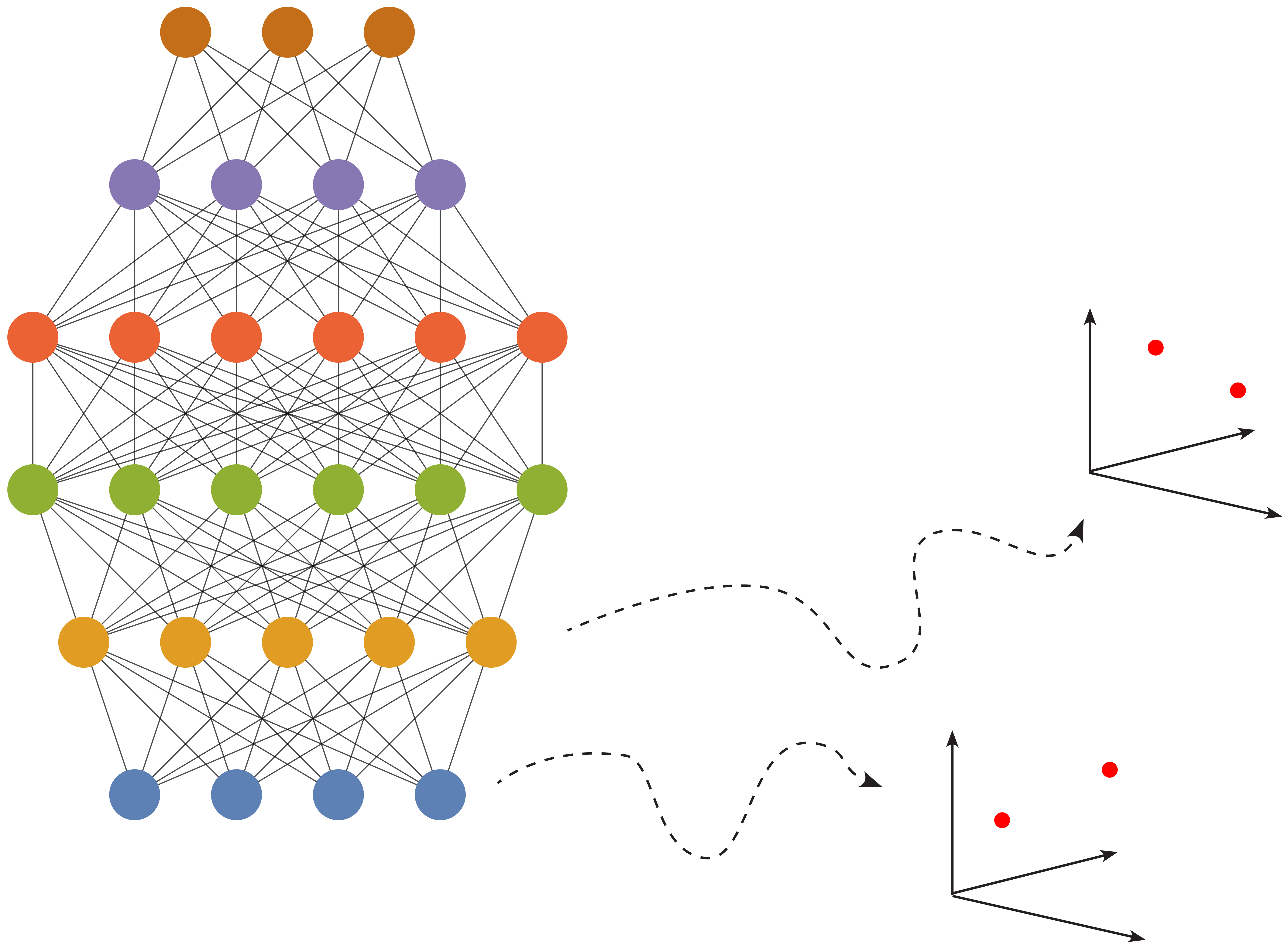
AtmoDist

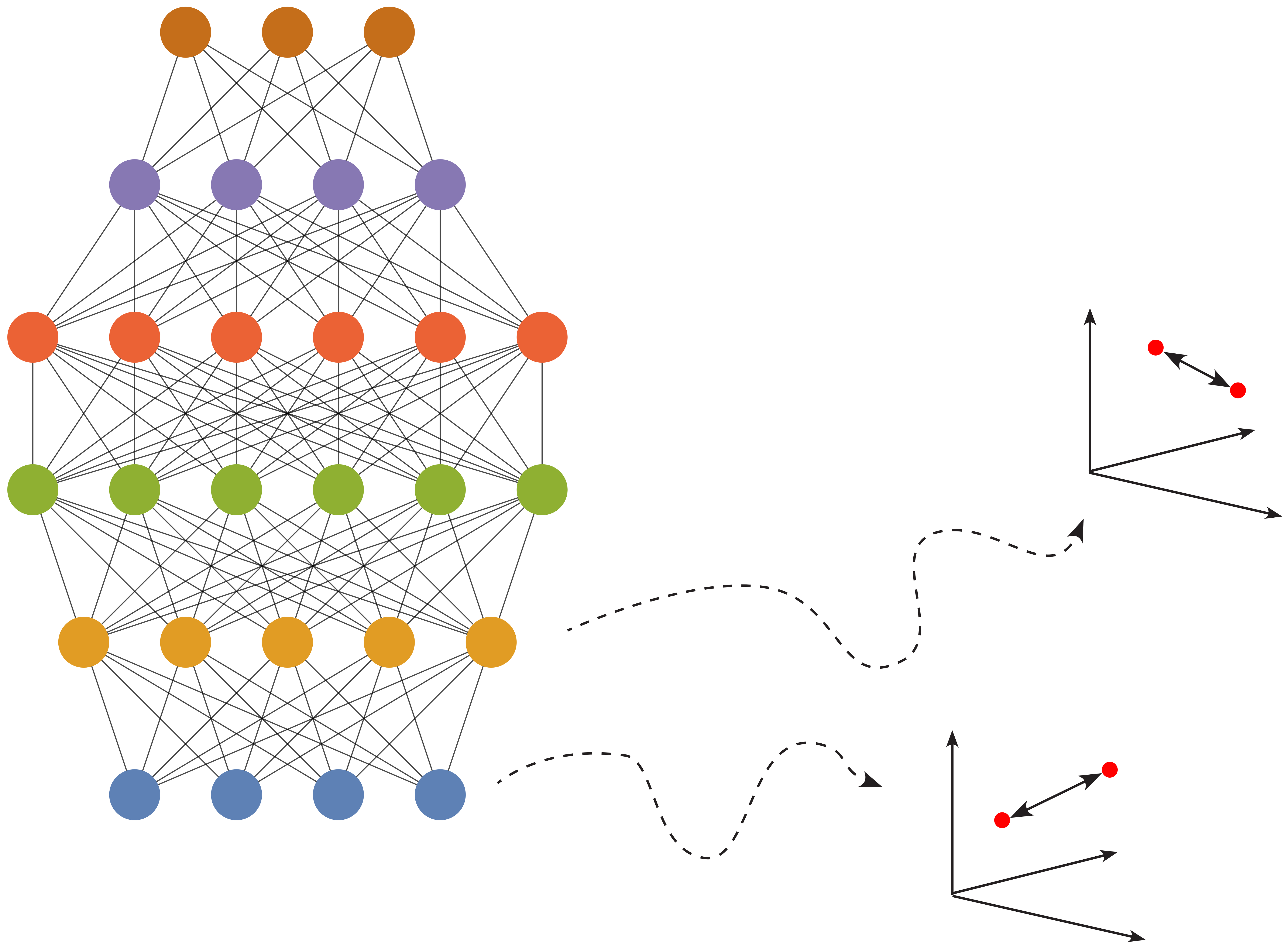


AtmoDist



Feature space is task / domain specific

AtmoDist



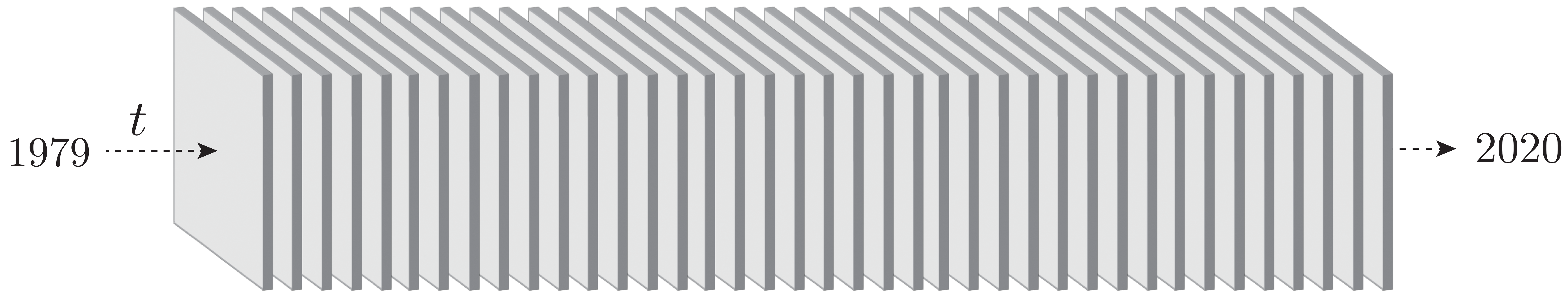
Feature space
is task / domain
specific

Compute distance
there!

AtmoDist

- ERA5 provides well curated data set for training
  - Close to observations
  - Several 100 TB
  - But unlabelled

AtmoDist



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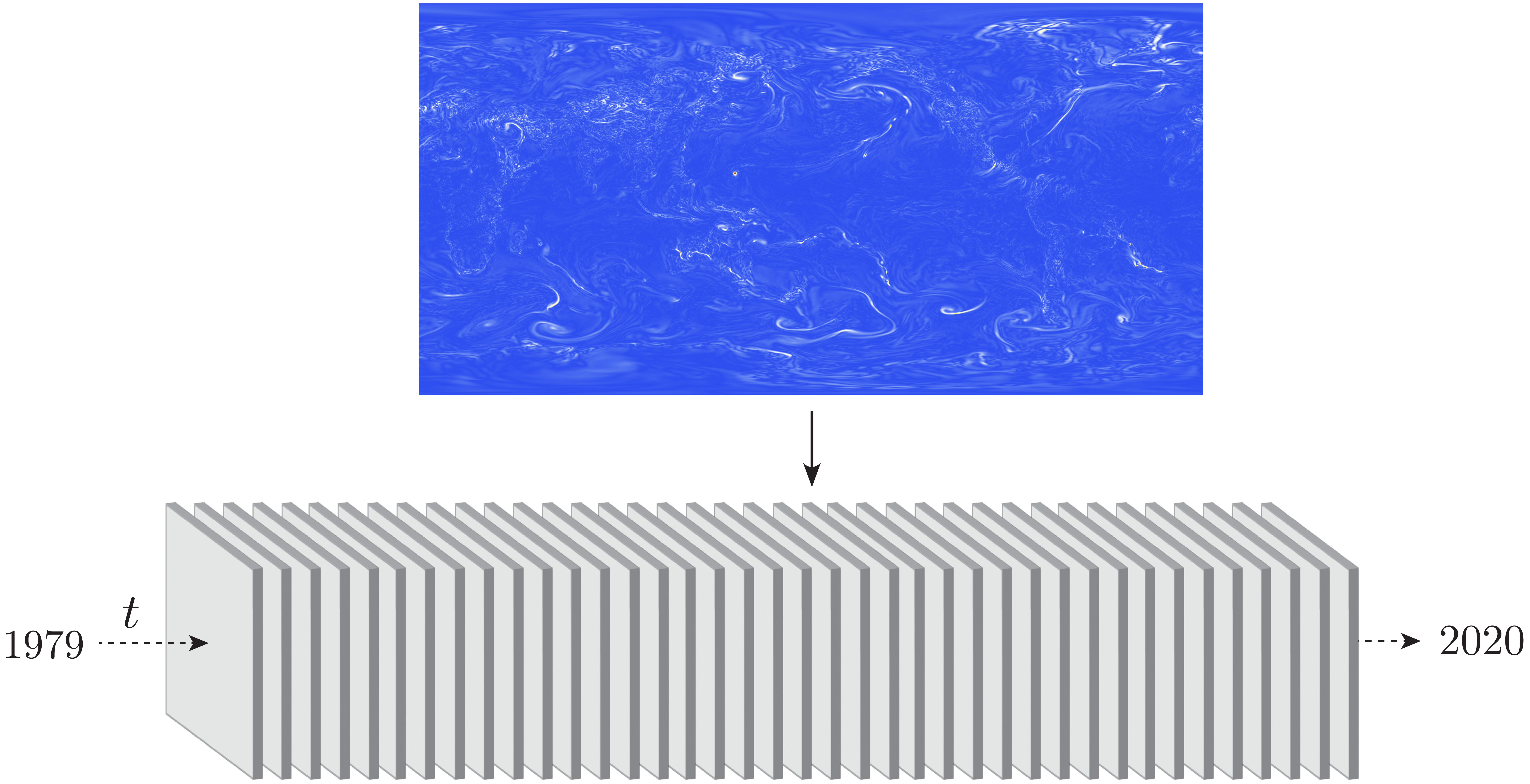

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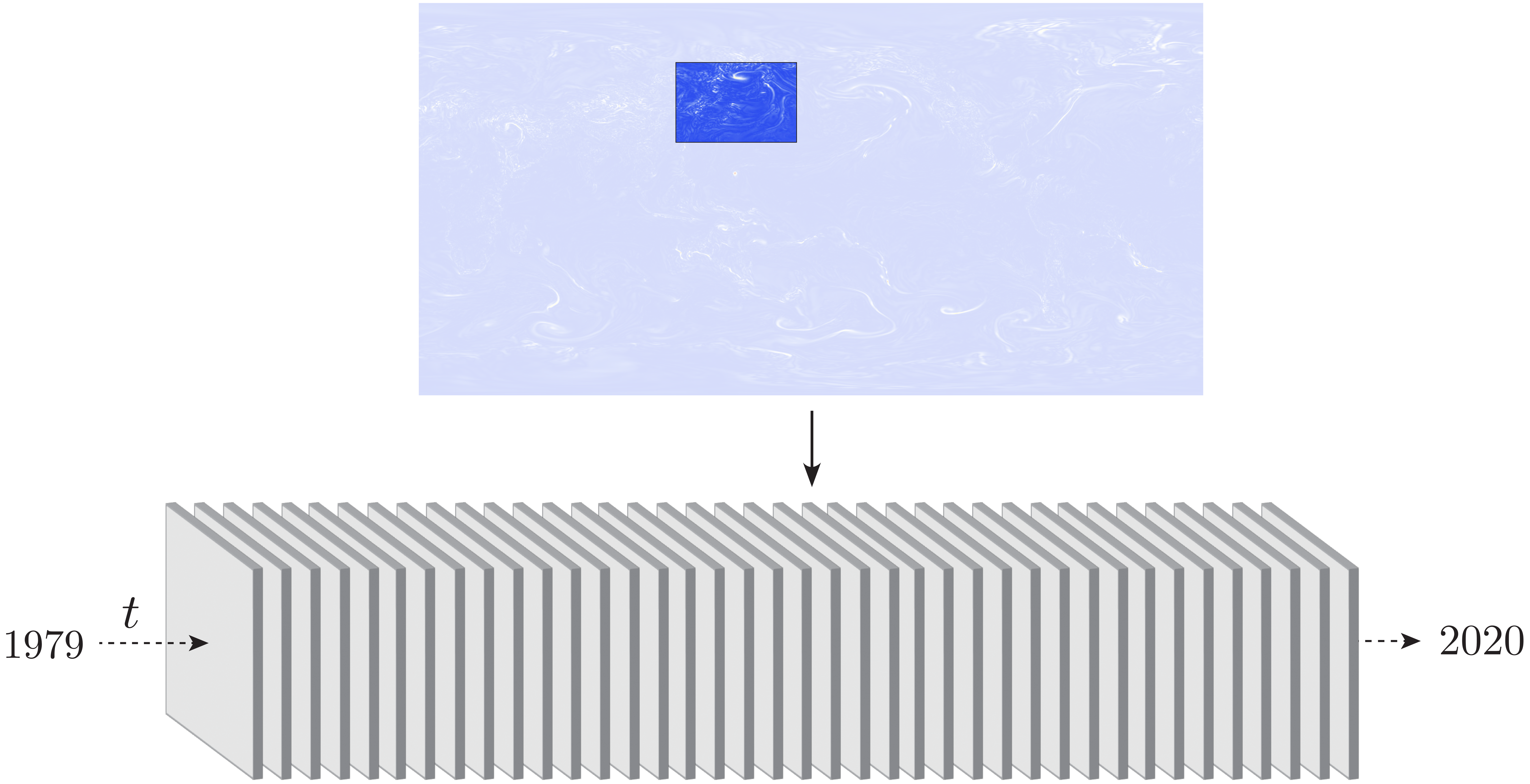

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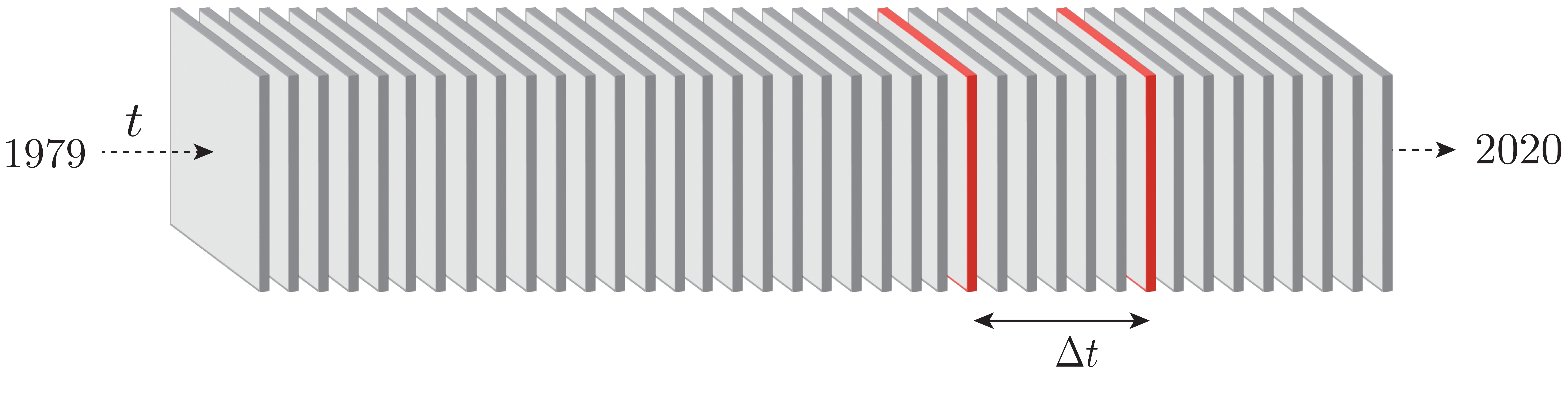

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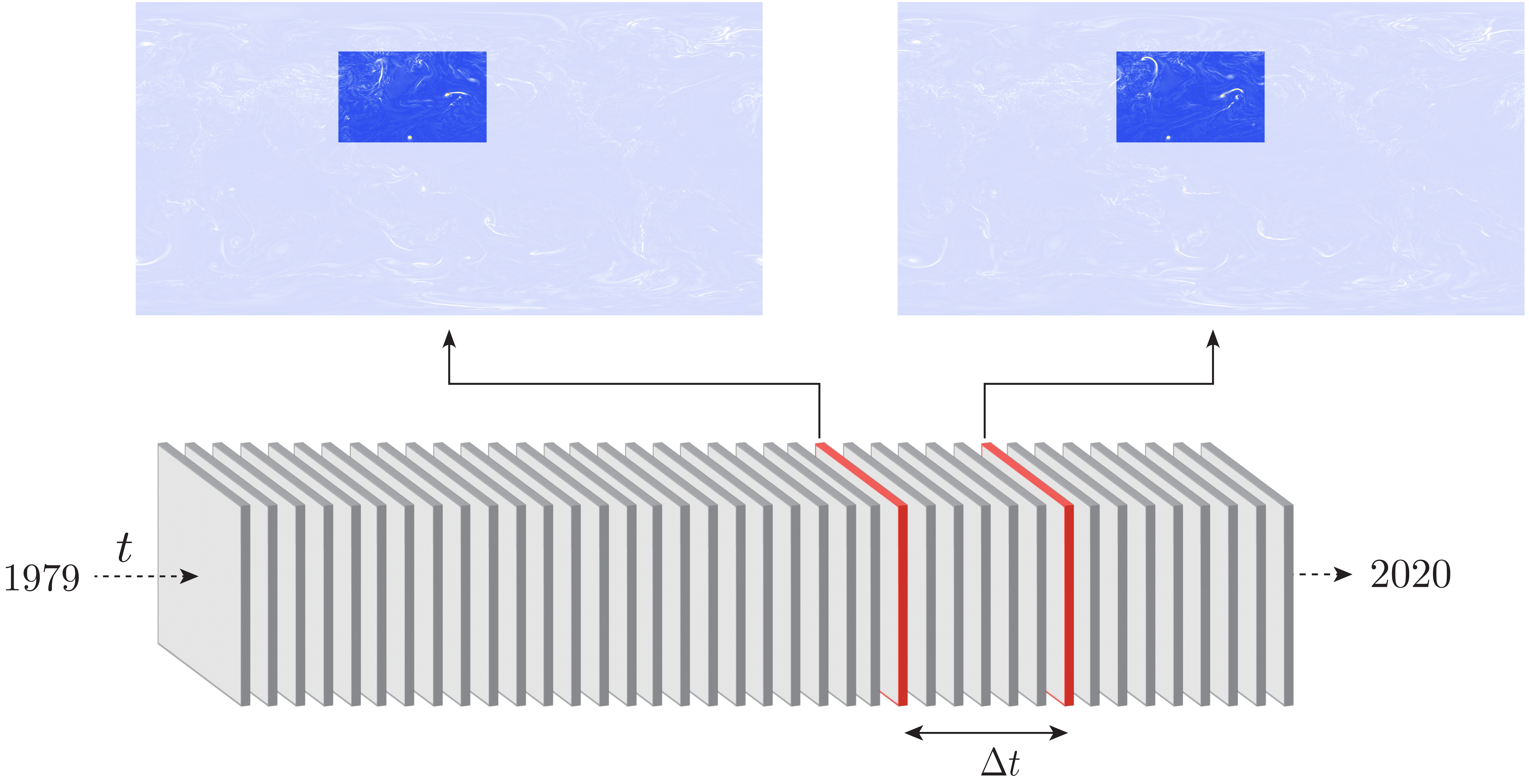

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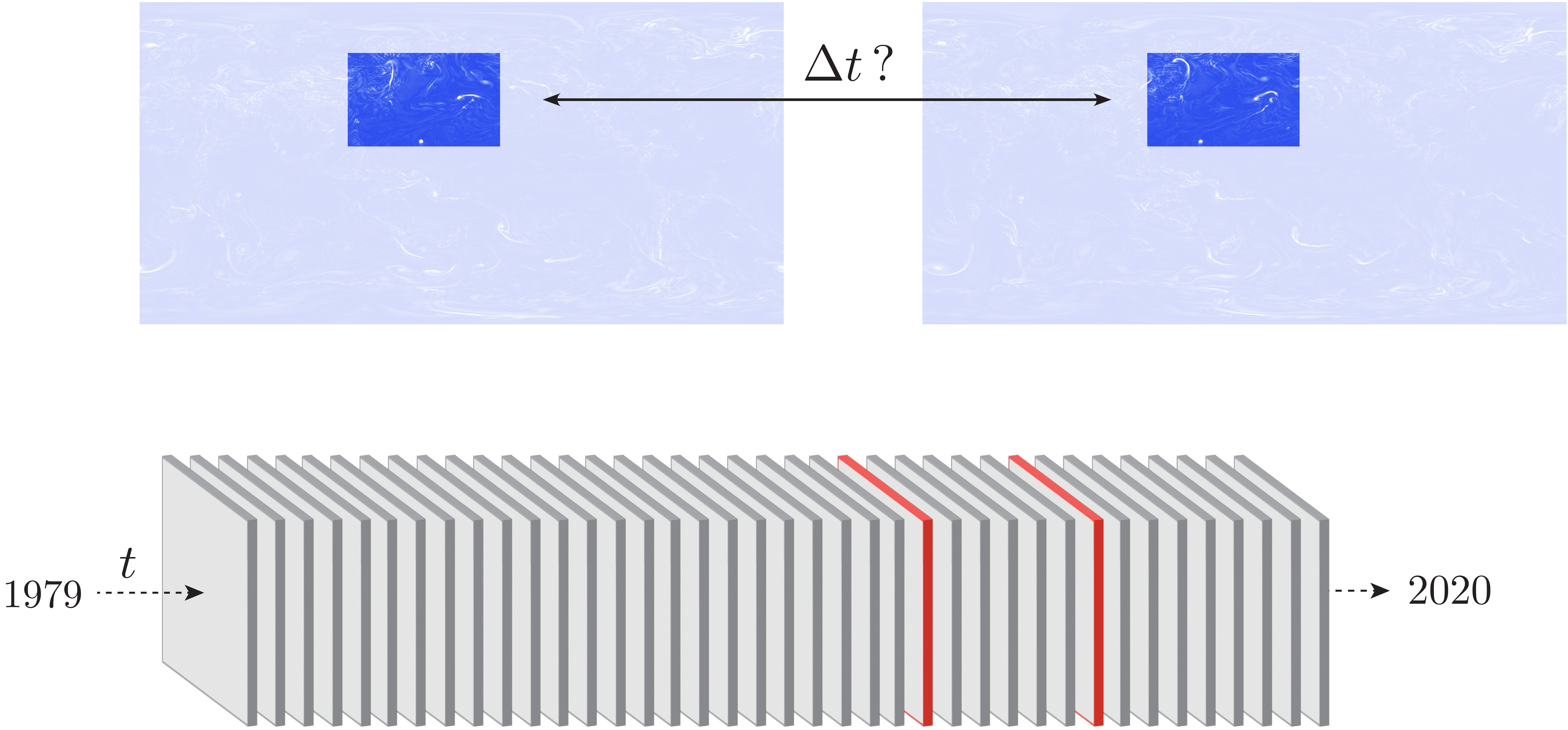

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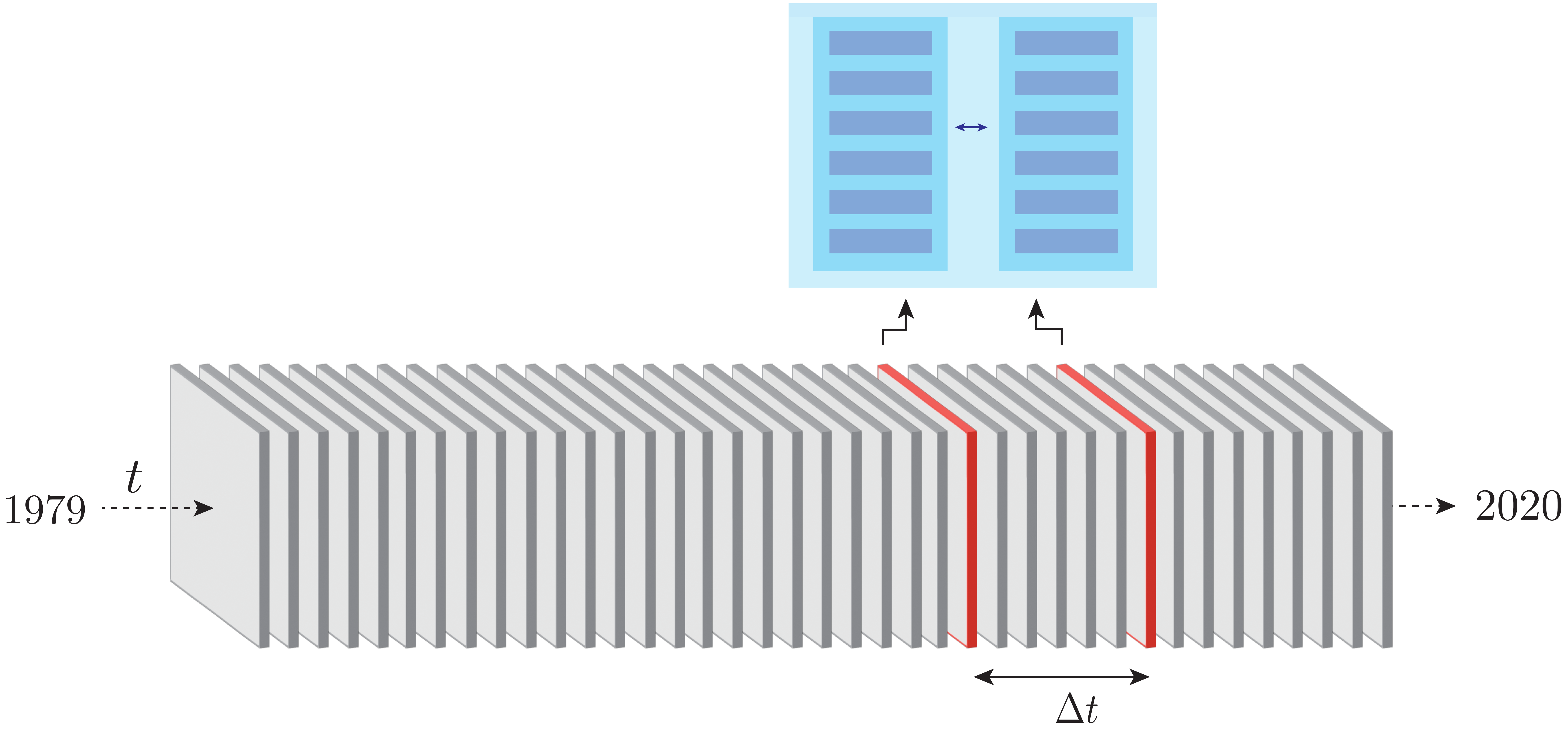

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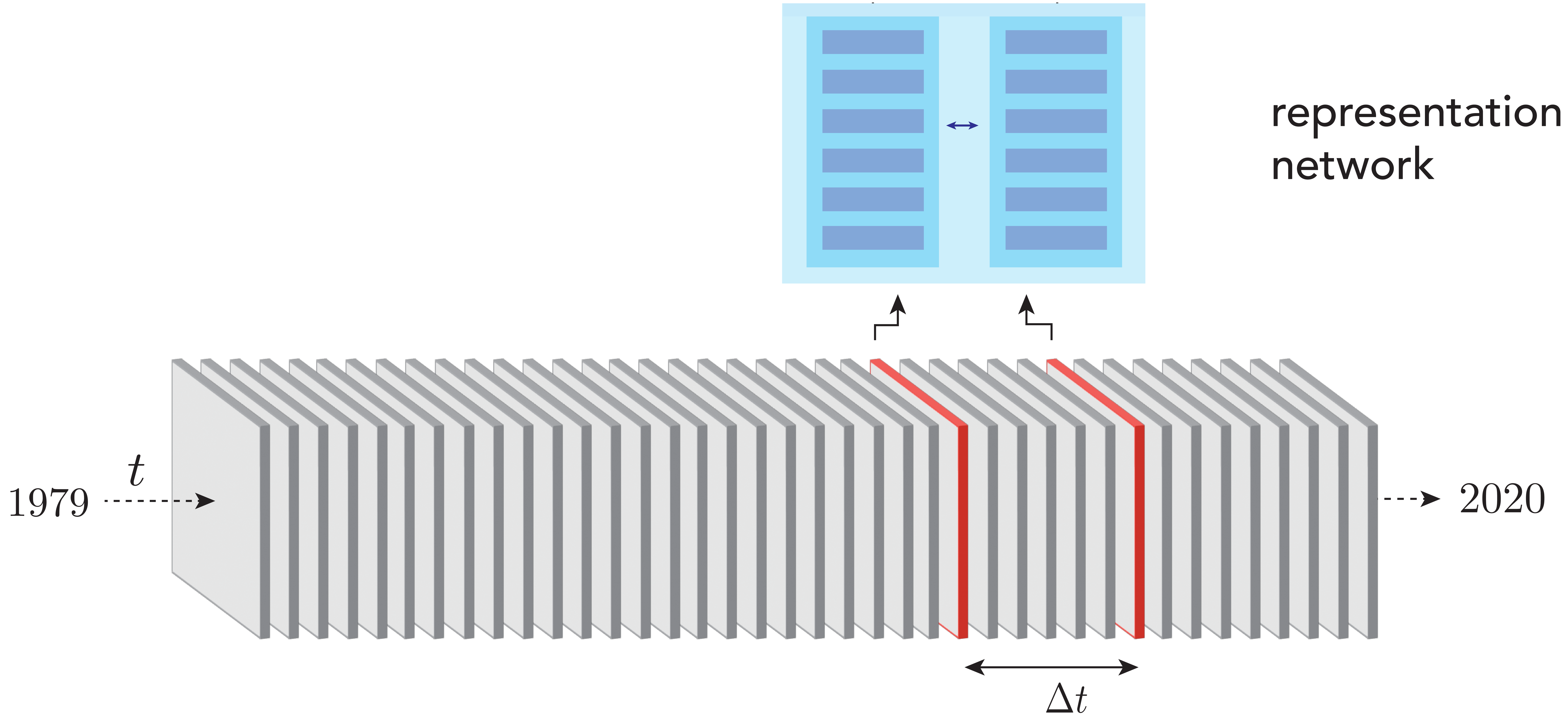

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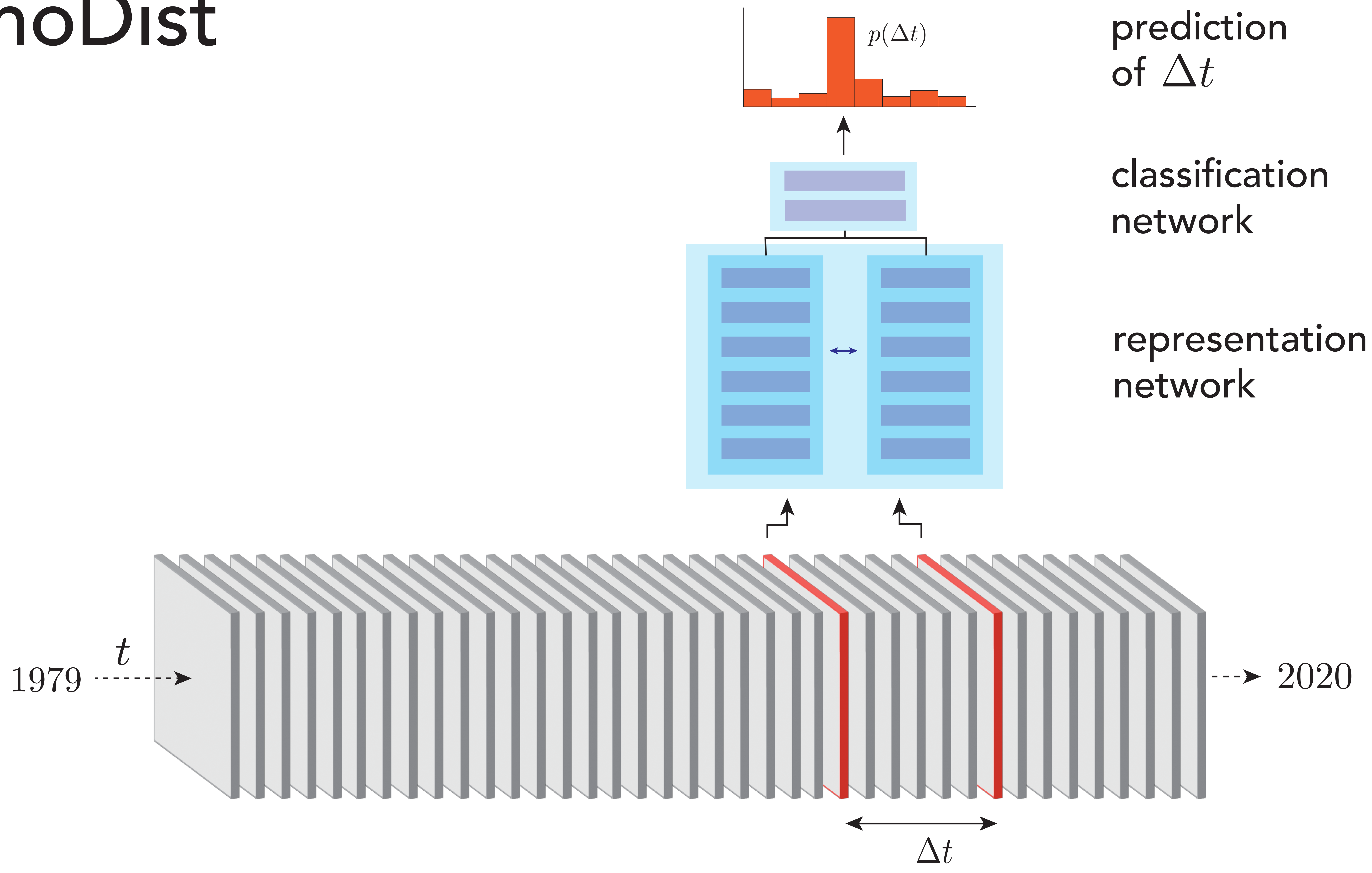
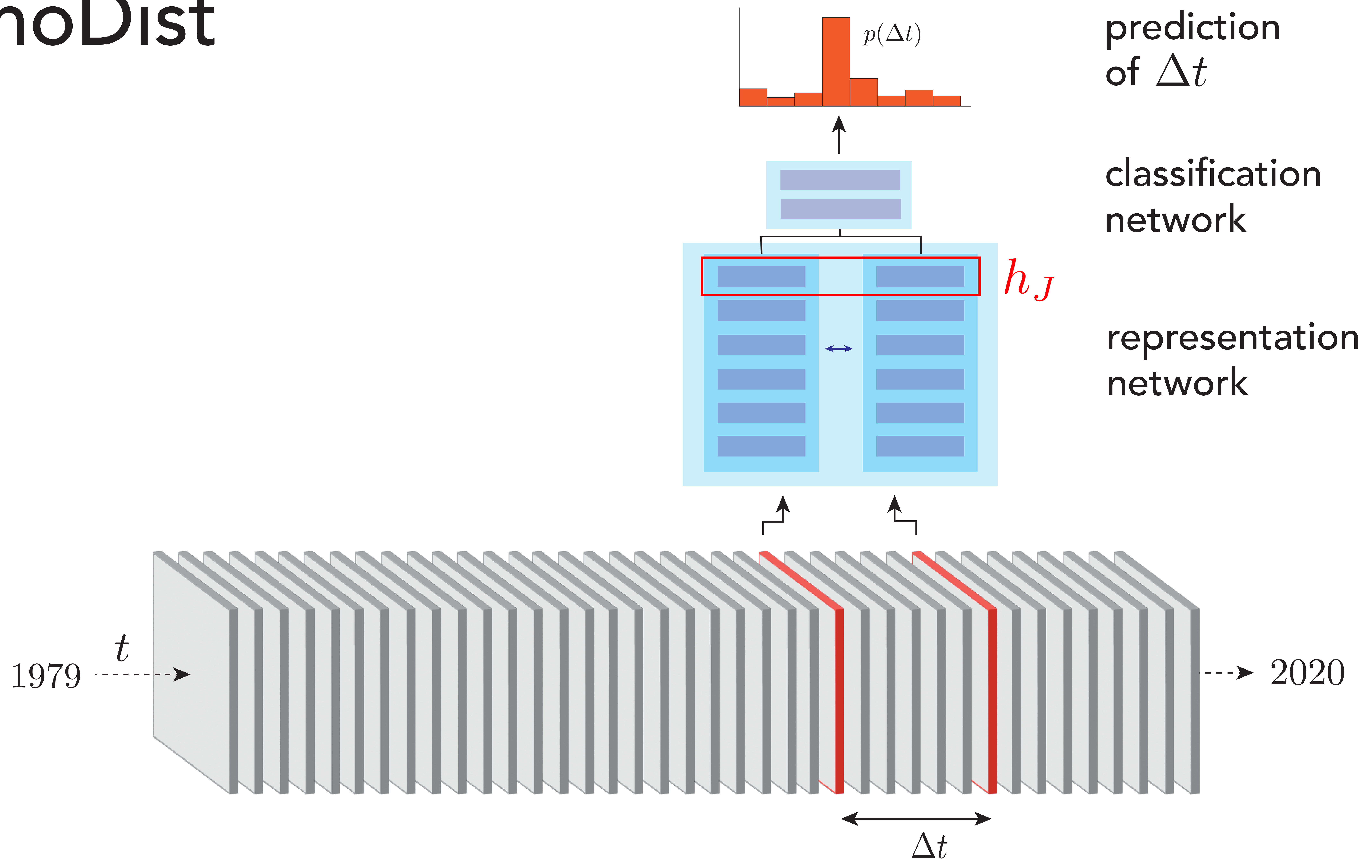


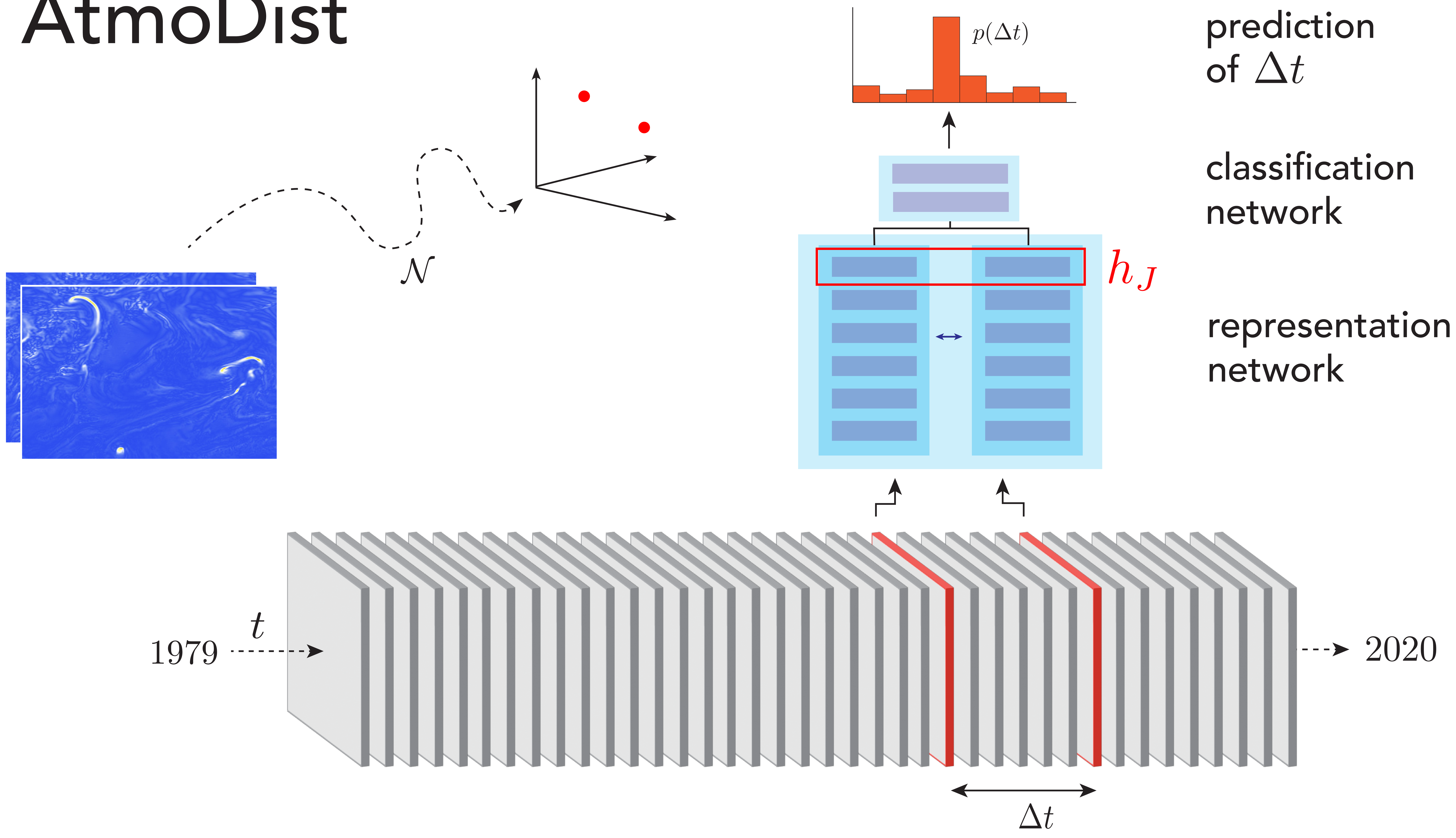
$p(\Delta t)$
prediction of Δt
classification network
representation network
t
1979
2020
Δt

AtmoDist



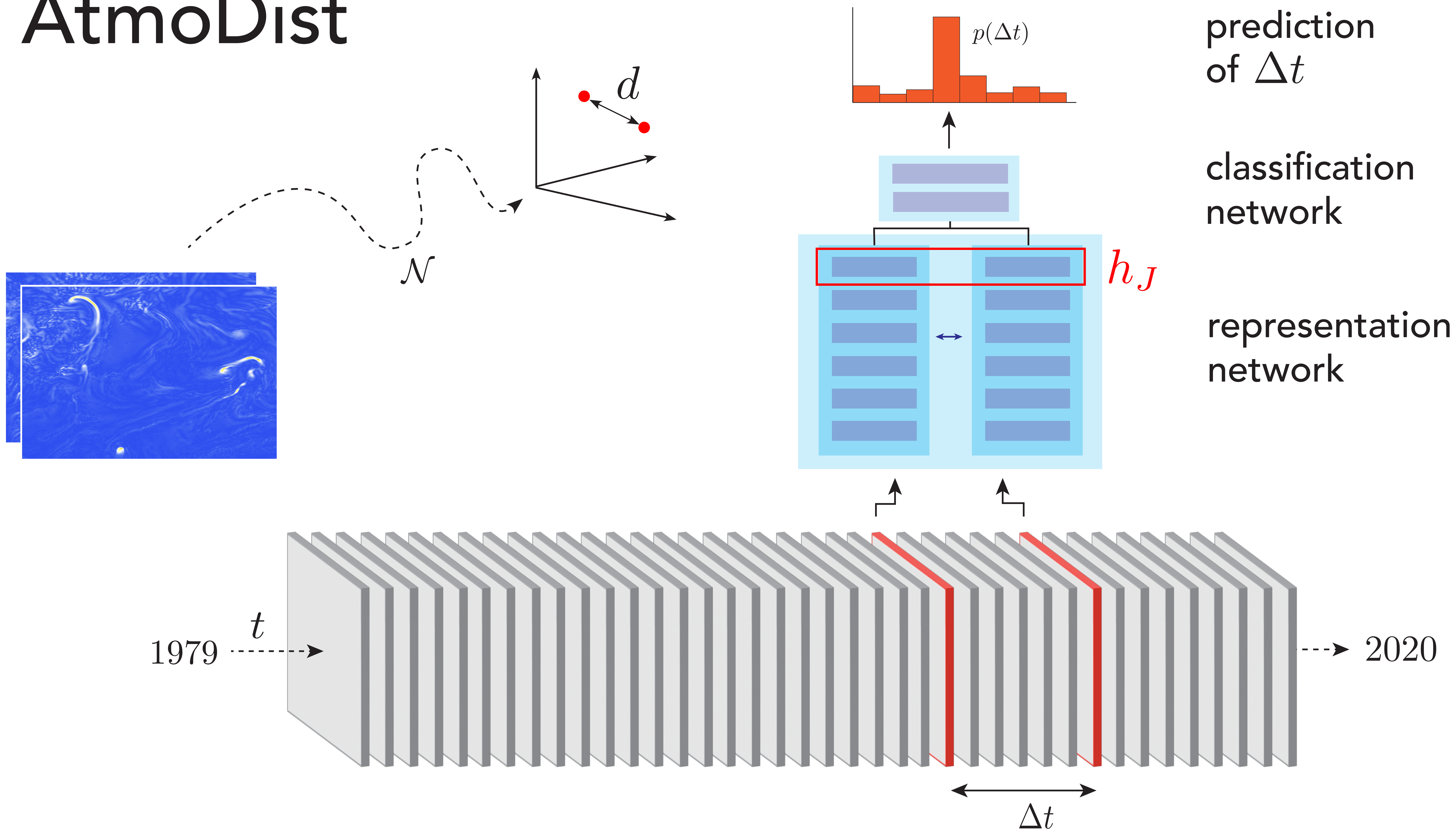
$p(\Delta t)$
prediction of Δt
classification network
h_J
representation network
1979
t
2020
Δt

AtmoDist



$p(\Delta t)$
prediction of Δt
classification network
h_J
representation network
$\mathcal{N}$
t
1979
2020
Δt

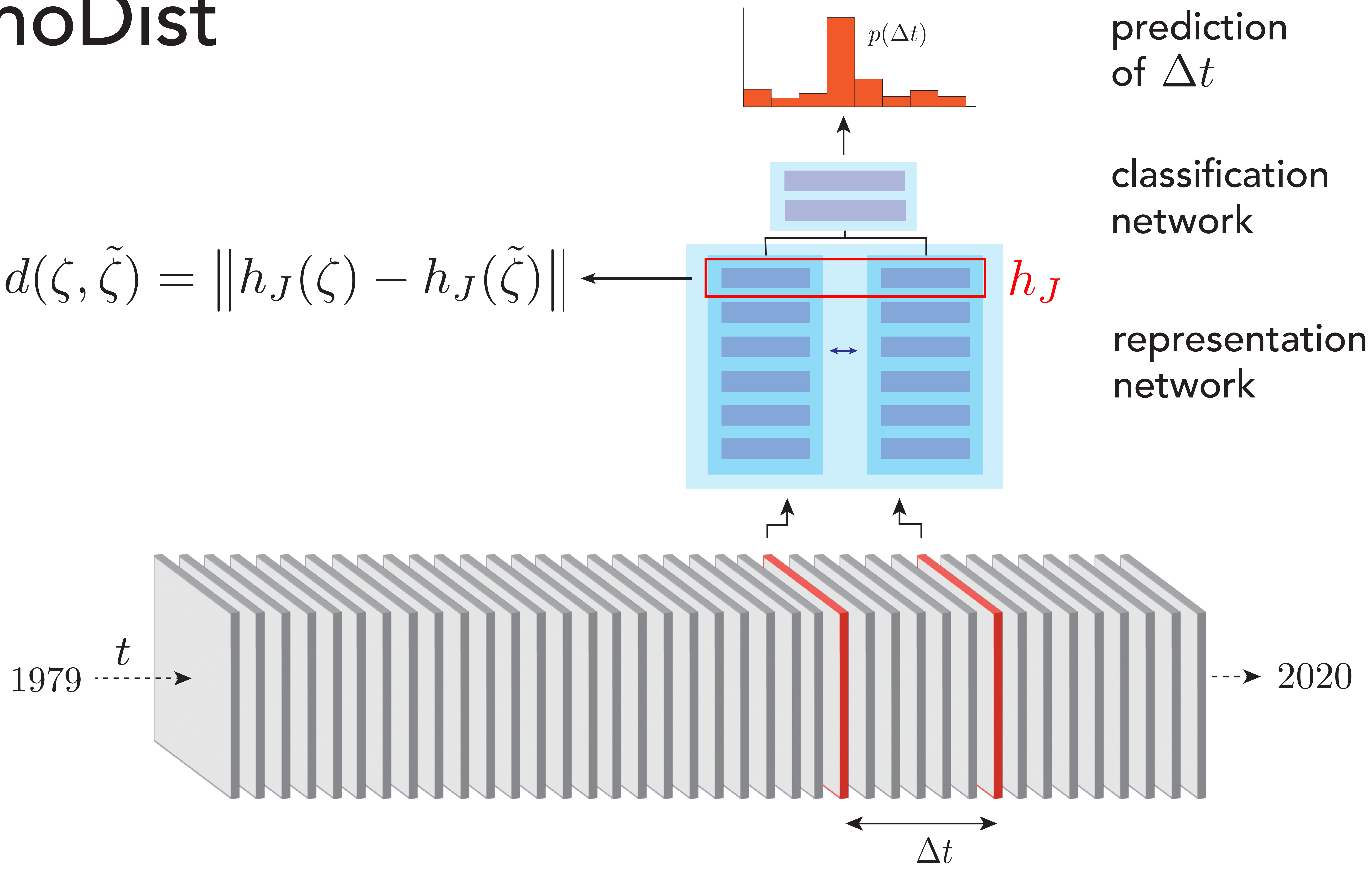
AtmoDist



d
$\mathcal{N}$
$p(\Delta t)$
prediction of Δt
classification network
h_J
representation network
1979
t
2020
Δt

AtmoDist

$$d(\zeta, \tilde{\zeta}) = \left\| h_J(\zeta) - h_J(\tilde{\zeta}) \right\|$$



AtmoDist: data

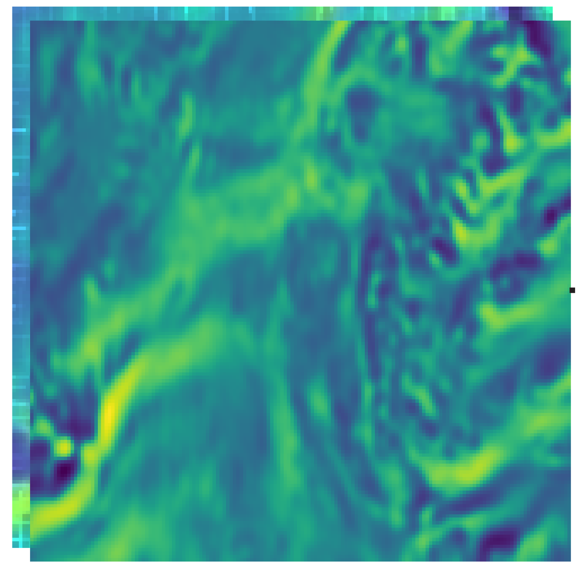
- ERA5[1] reanalysis 1979-2006
  - Training: 1979-1998; Evaluation: 1999-2006 (58,440 training slices and 17,536 evaluation ones)
  - Vorticity and divergence
  - 1280 × 2560 grids sampled into 160 x 160 patches
  - One vertical layer (≈ 883 hPa)

[1] Hersbach et al., The ERA5 global reanalysis, Quarterly Journal of the Royal Meteorological Society, 146 (730), 2020.

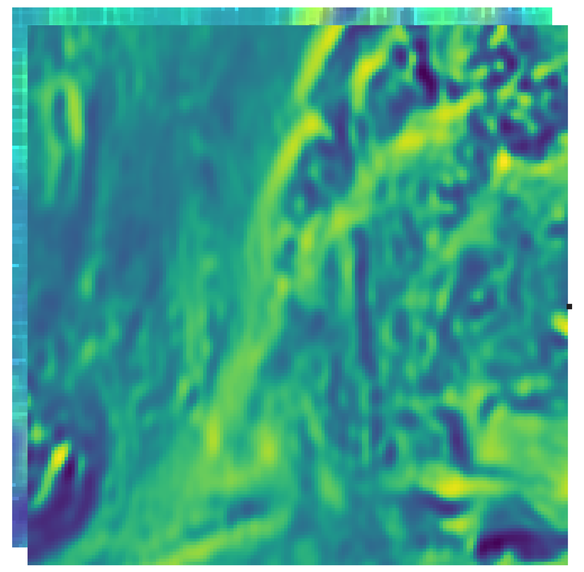
AtmoDist: network

vorticity,
divergence

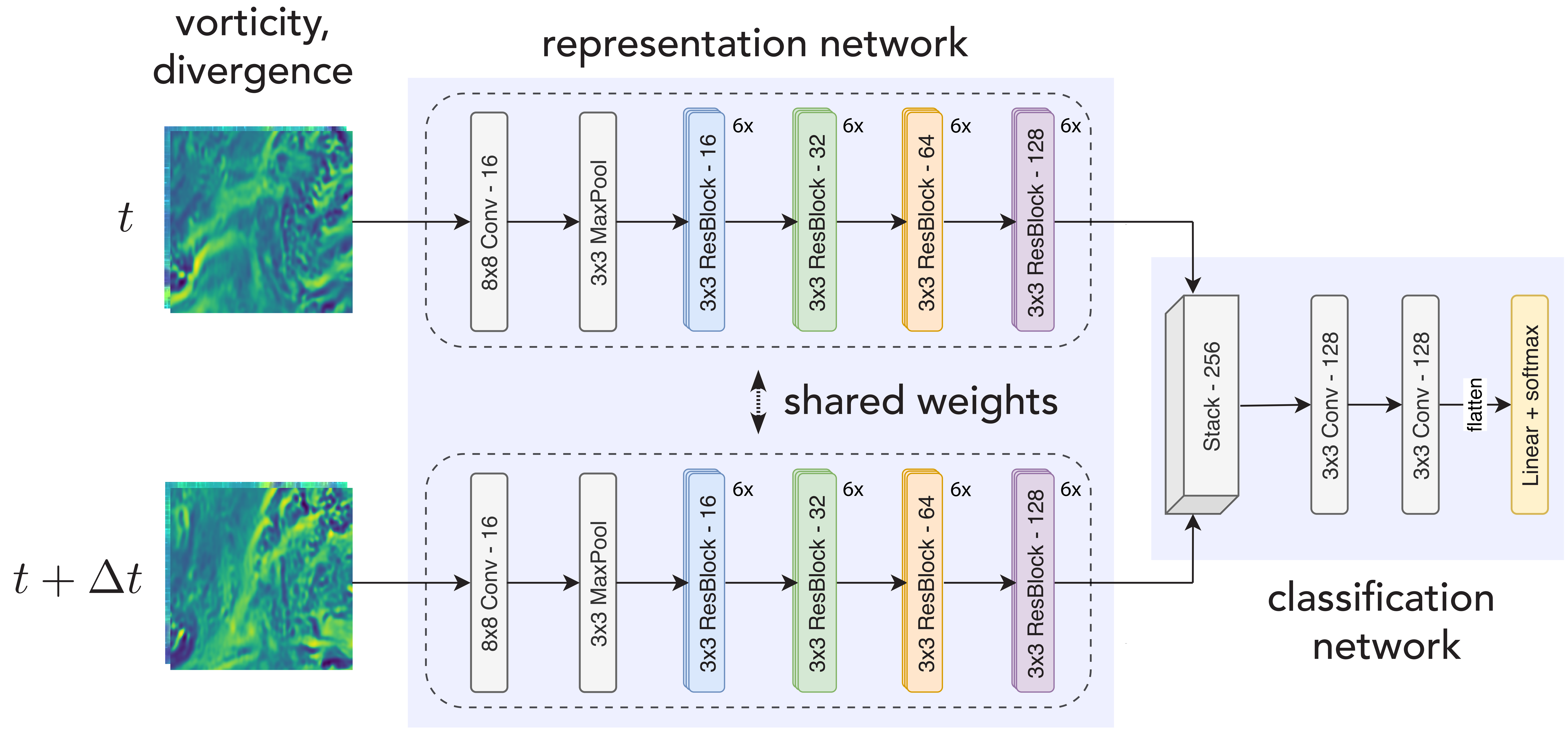
t



$t + \Delta t$



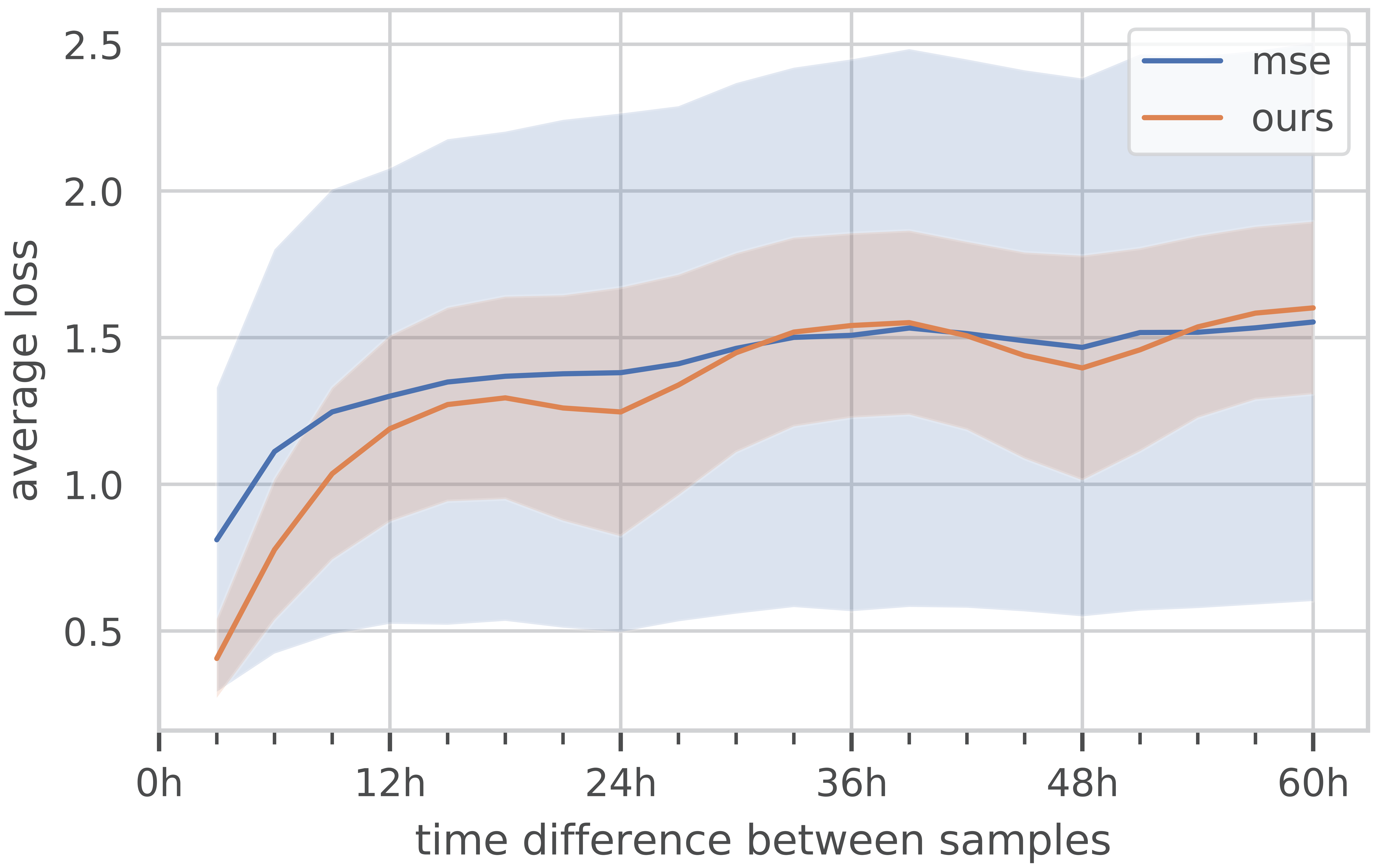
AtmoDist: network



2.27 million parameters

AtmoDist: network

AtmoDist: evaluation



Super-resolution using AtmoDist

- Objective: down-scaling / upsampling of coarse fields

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  - Only 4X super-resolution in our work

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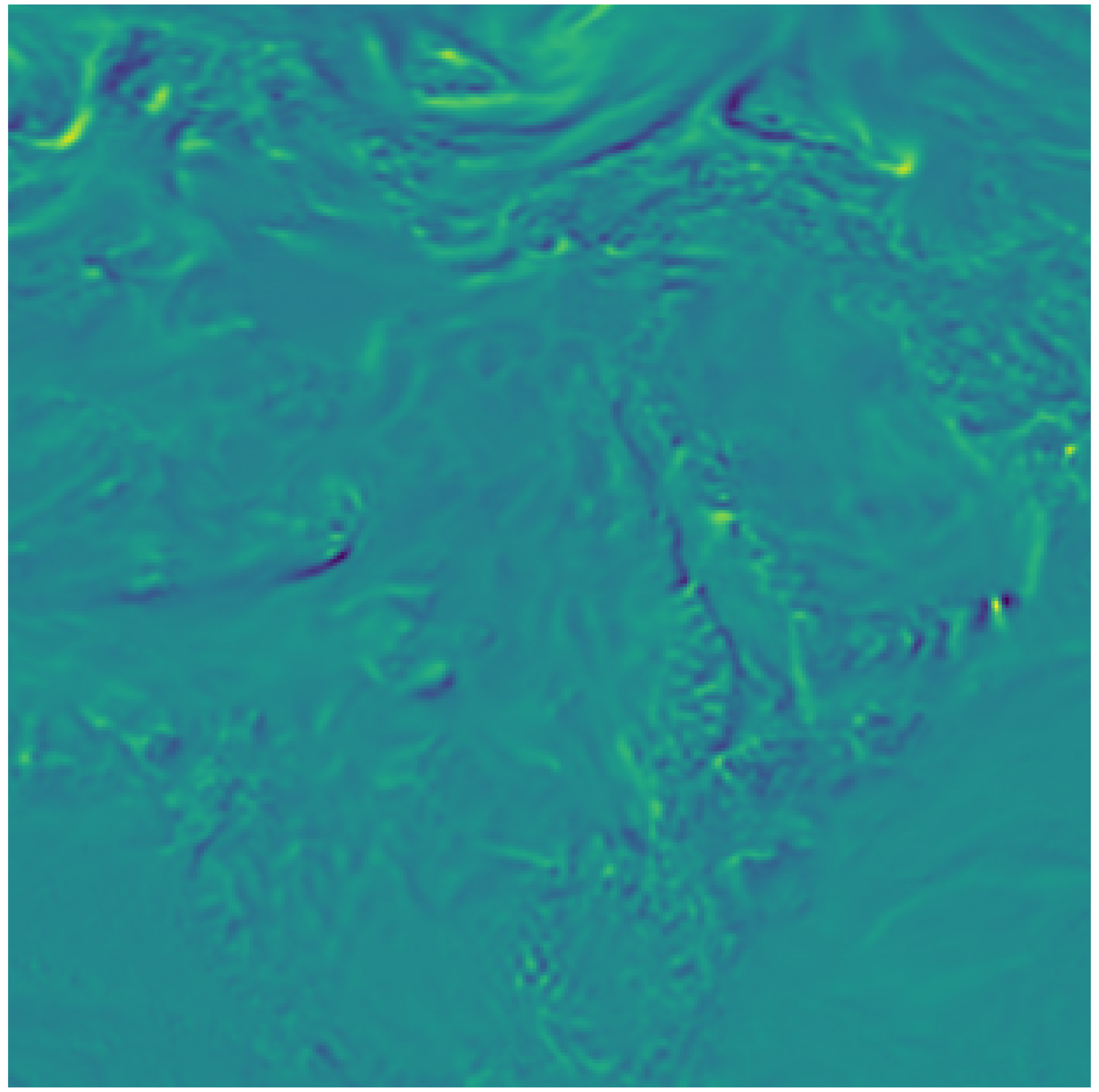
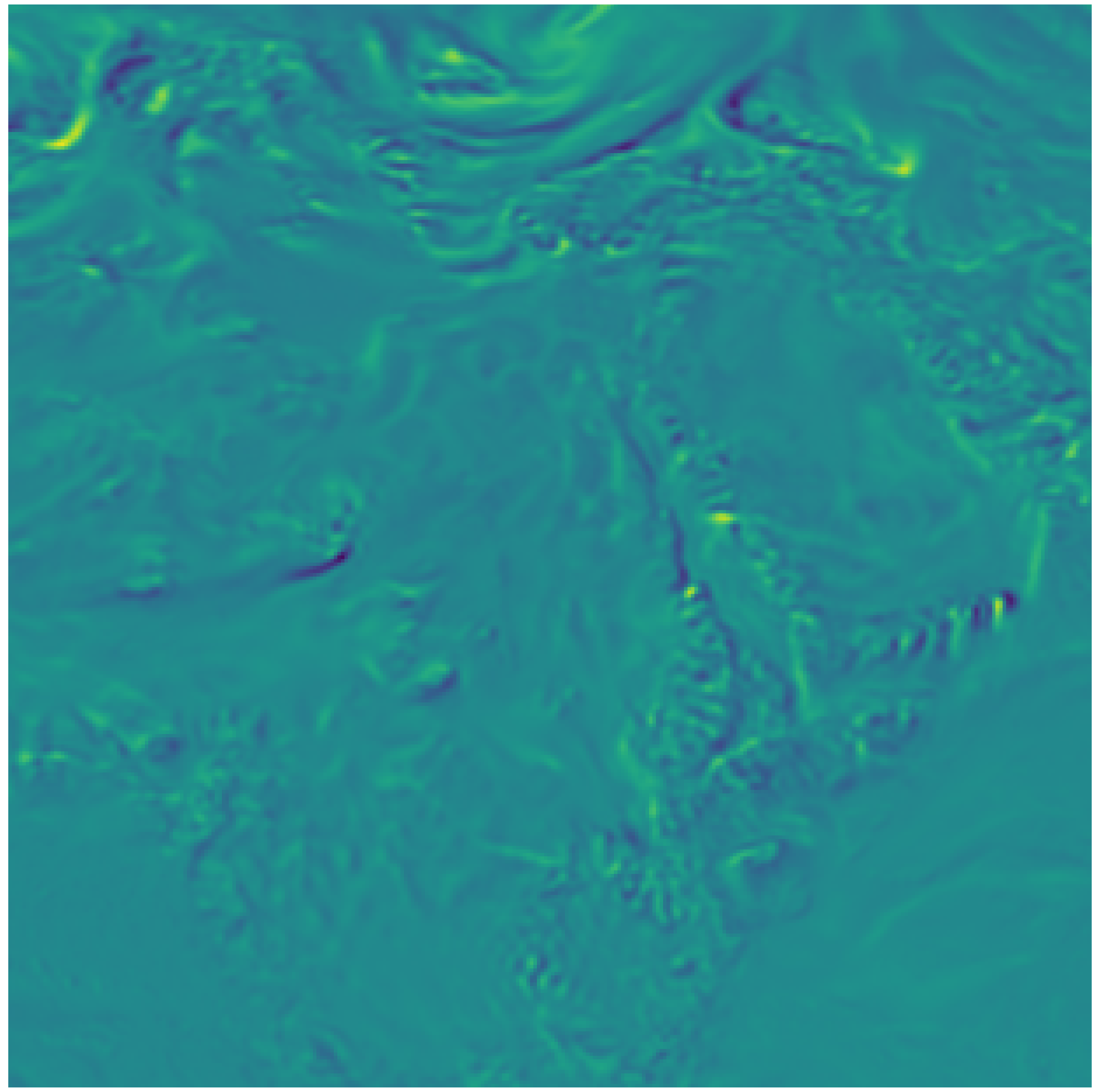
Super-resolution using AtmoDist

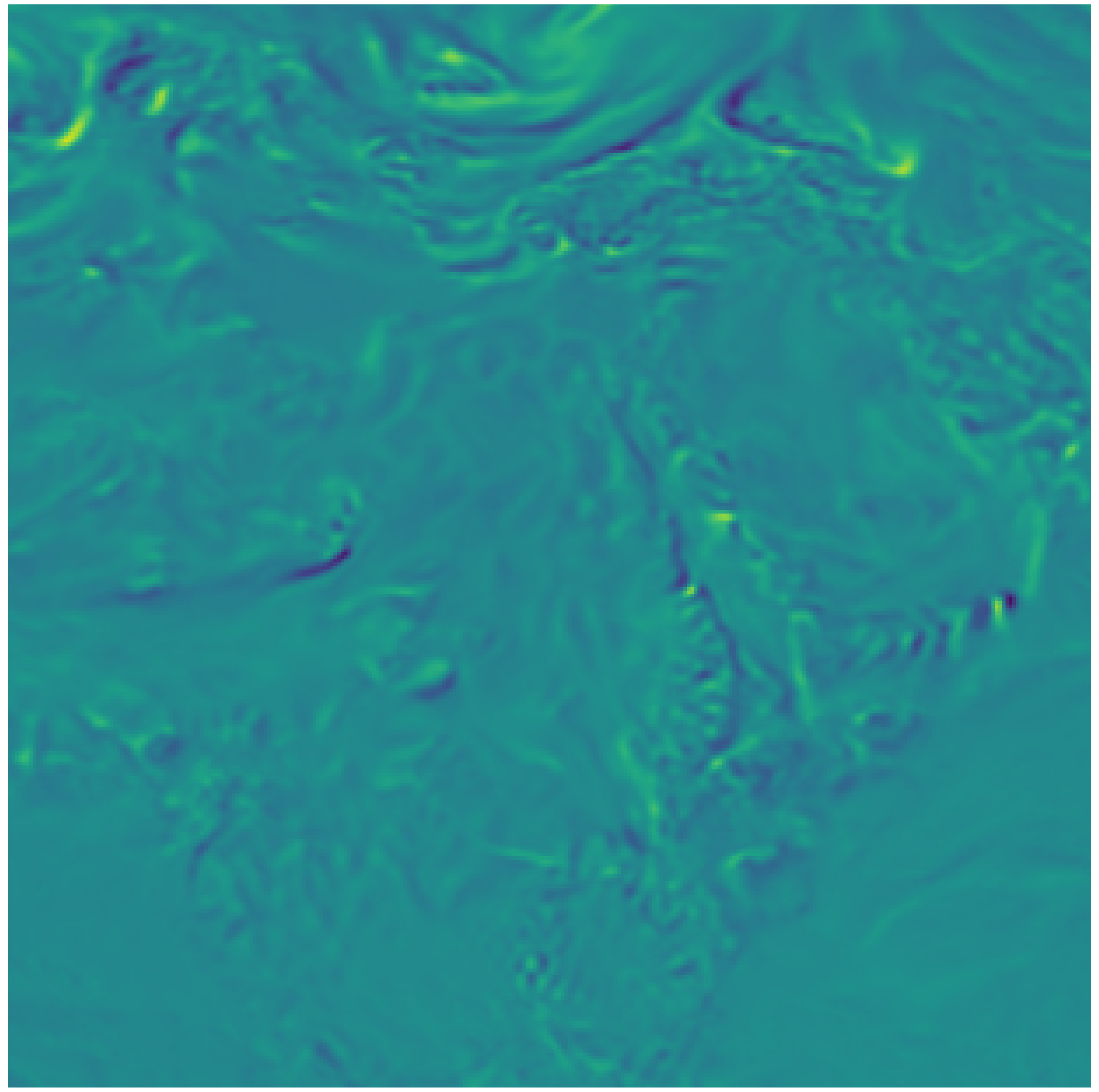
ours



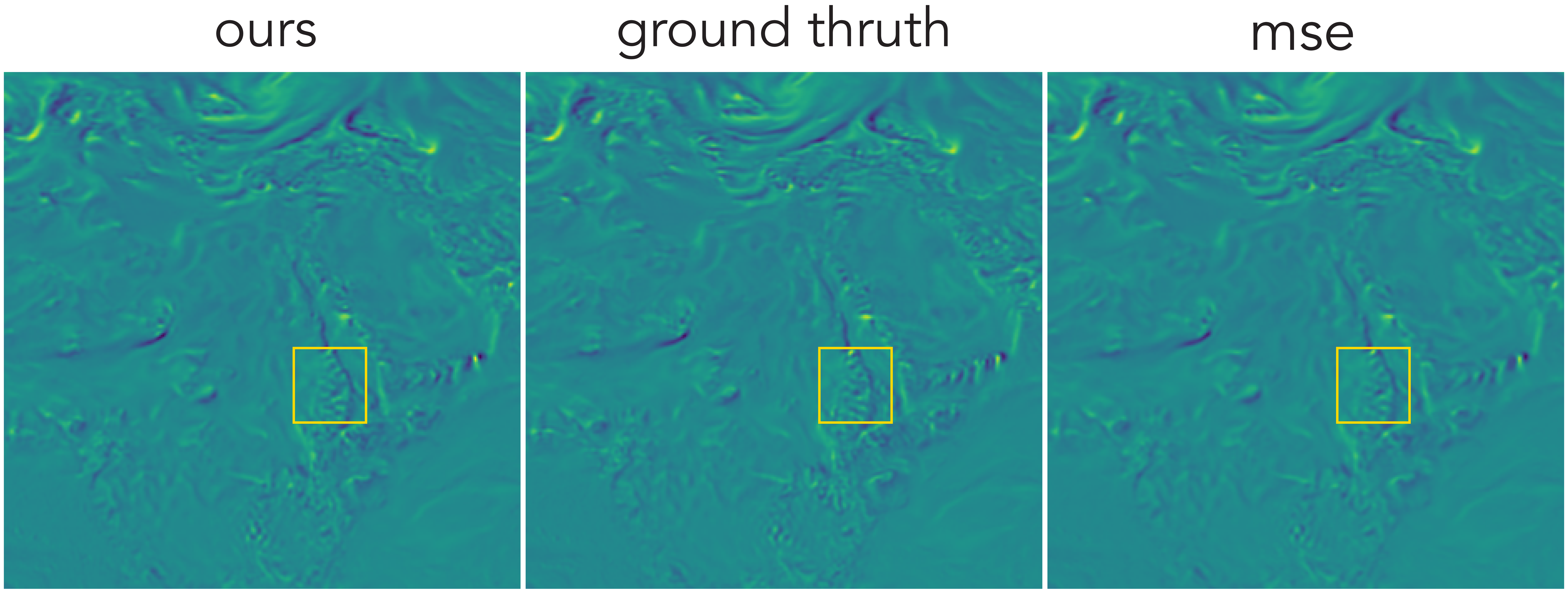
ground thruth



mse

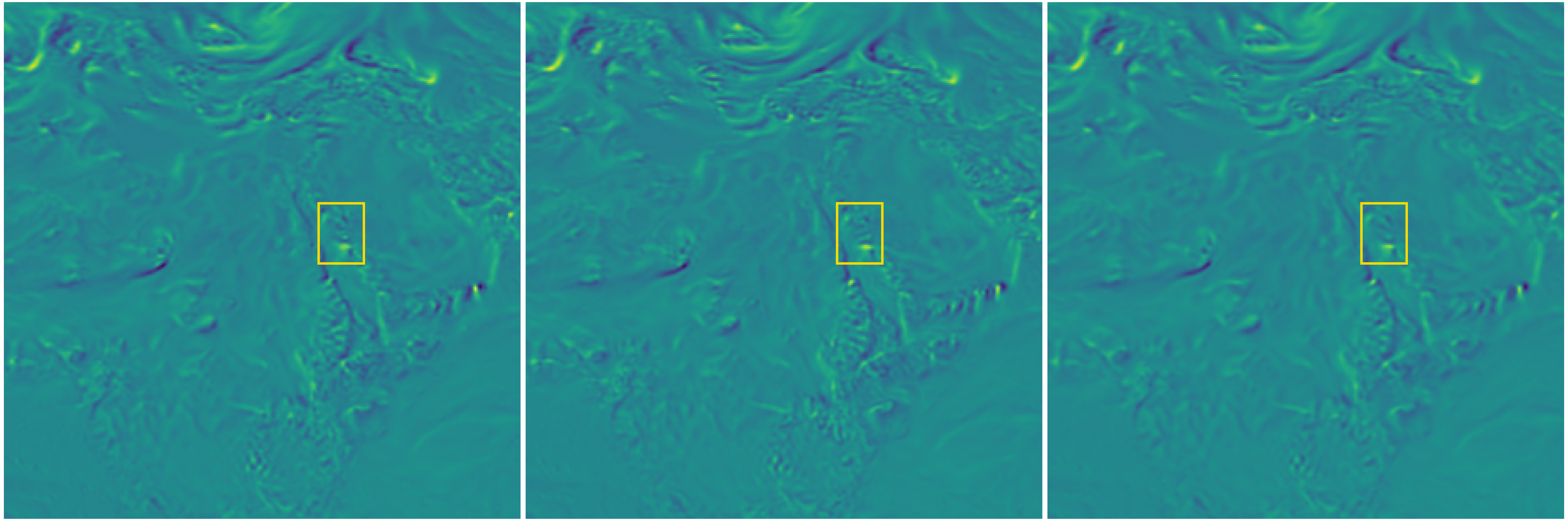


Super-resolution using AtmoDist



Super-resolution using AtmoDist

ours ground thruth mse



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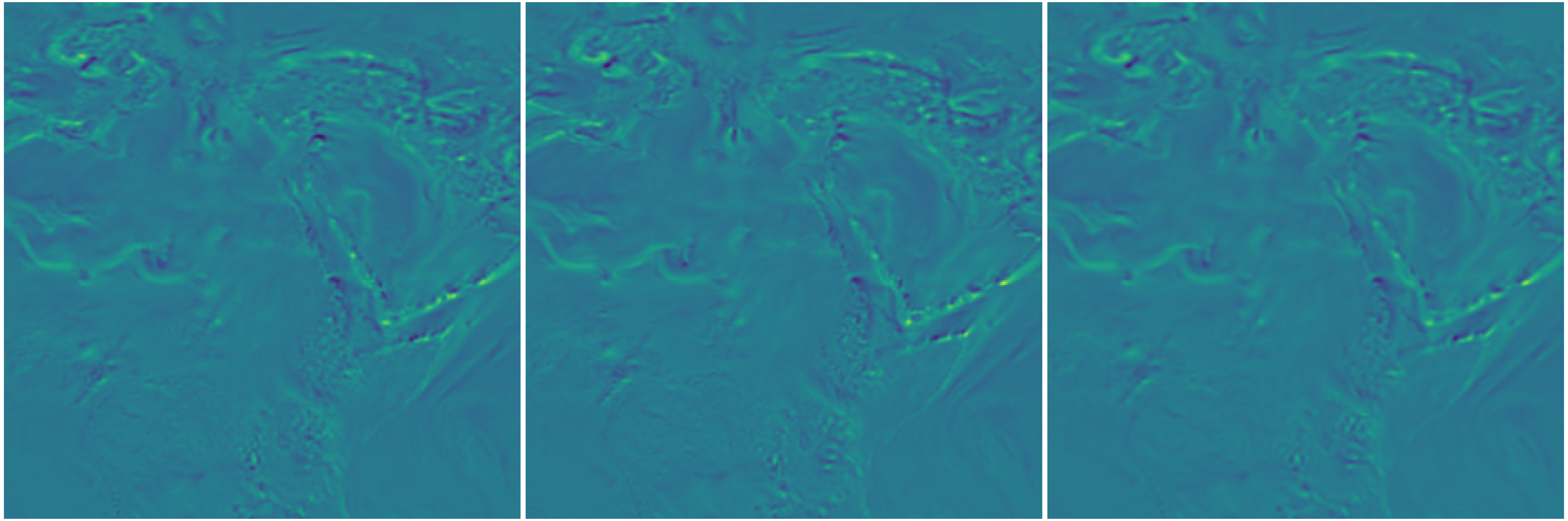

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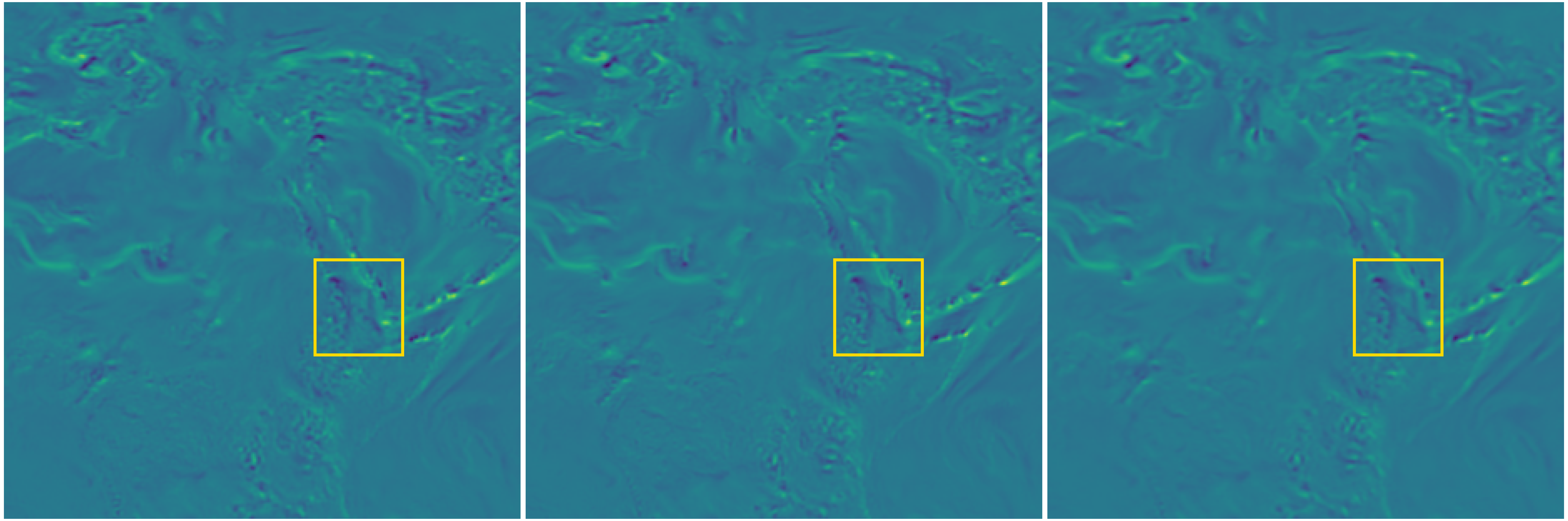

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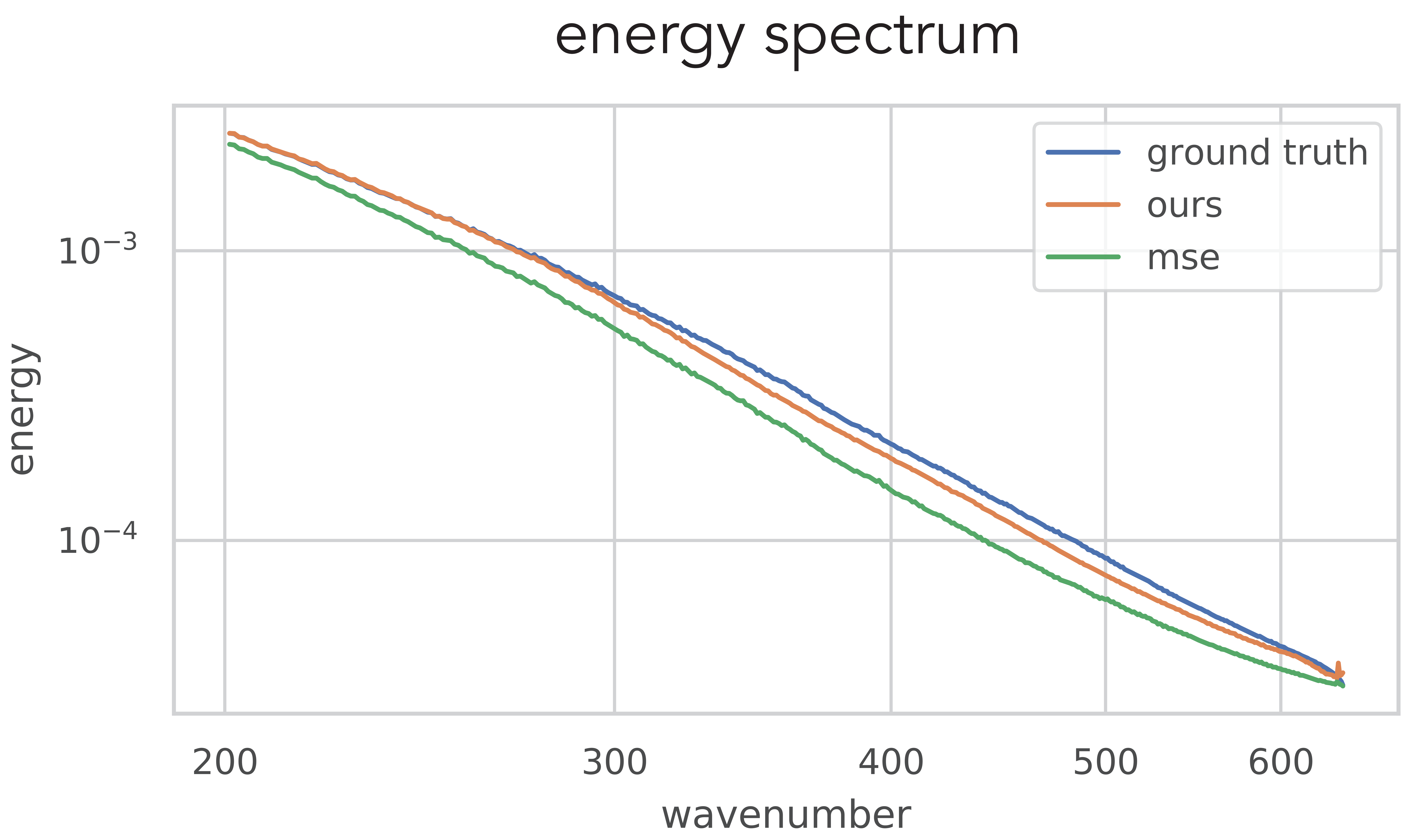

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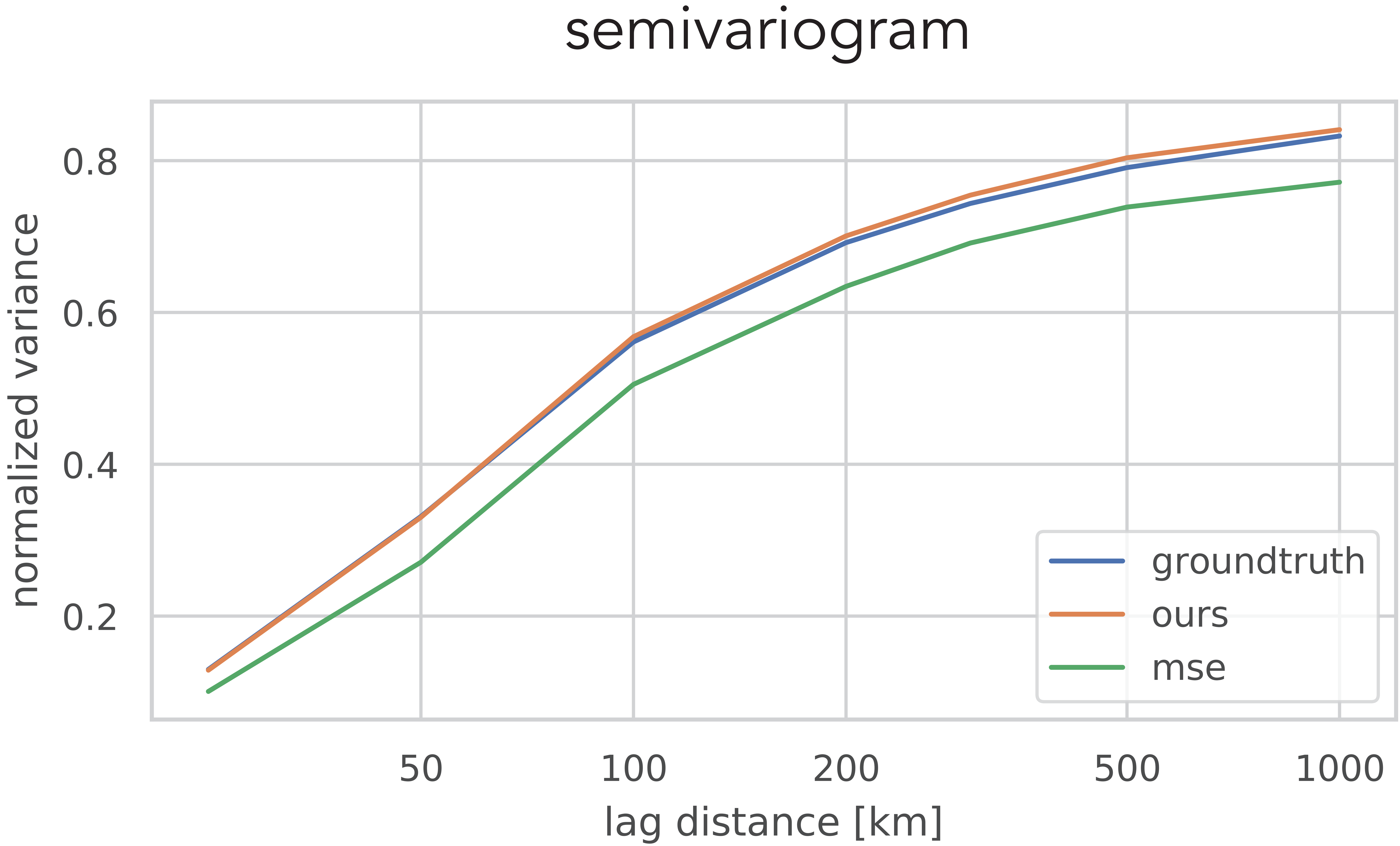

Super-resolution using AtmoDist

- Local statistics by averaging over super-resolution predictions for entire reanalysis data set
- 150 big cities as locations

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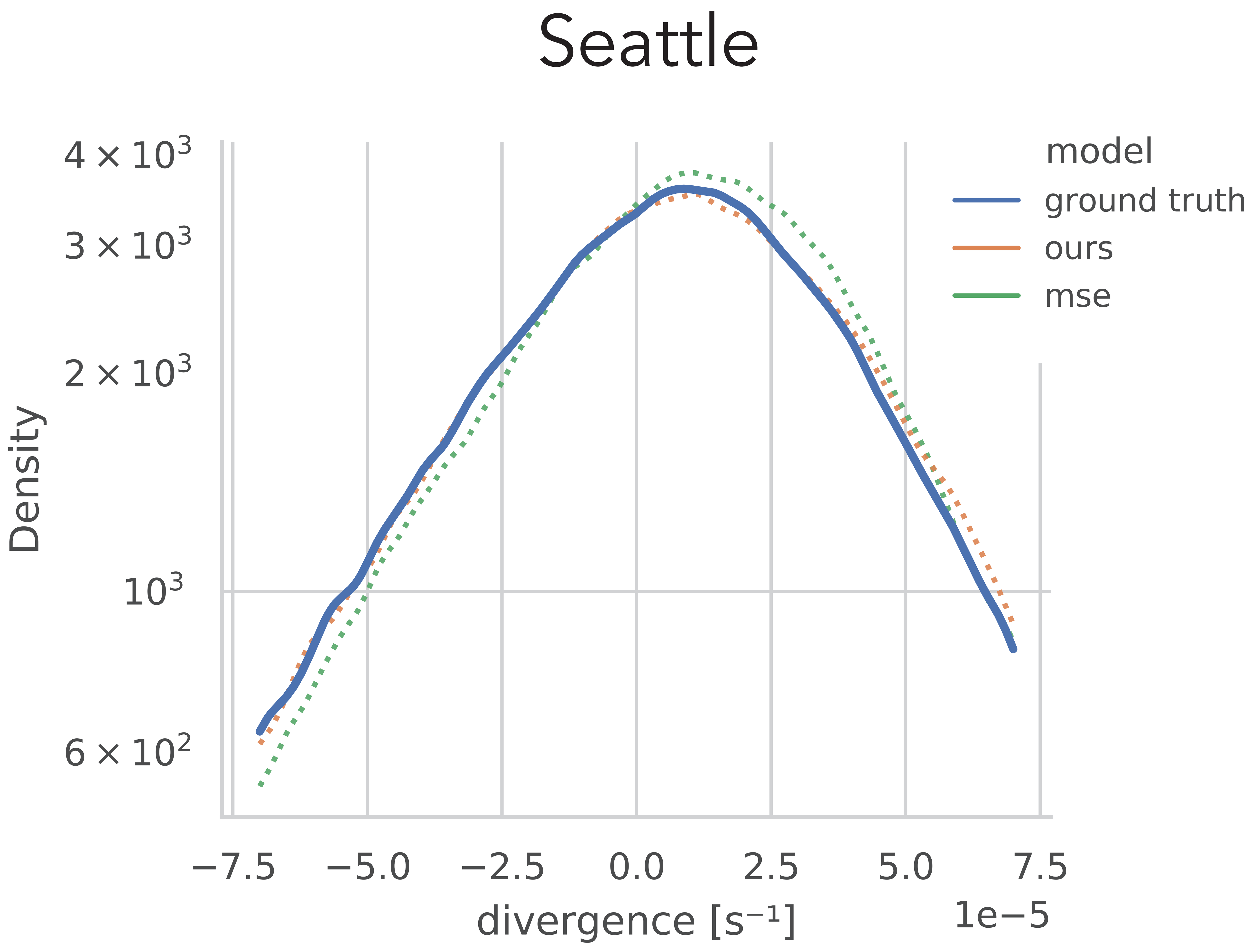
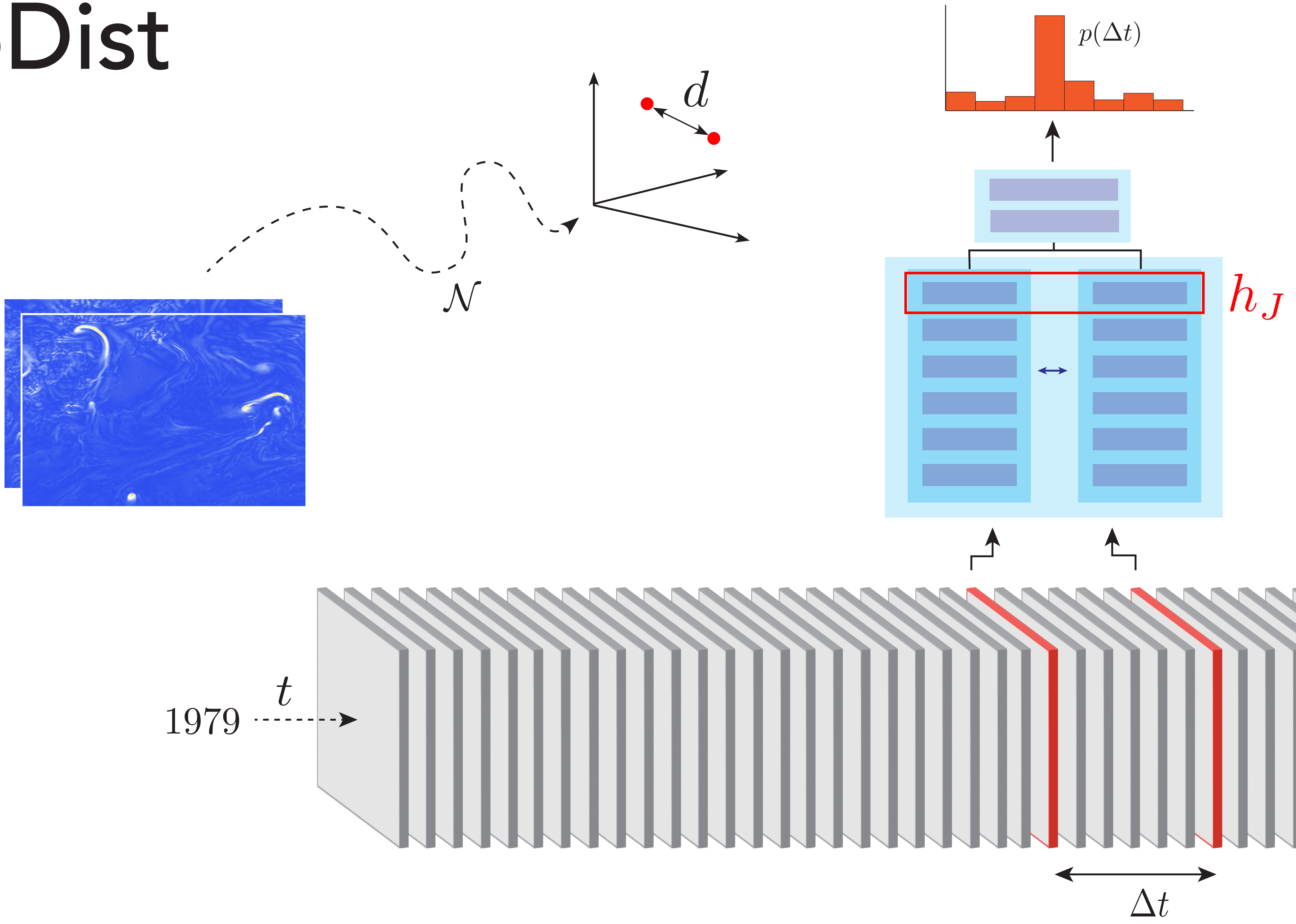


AtmoDist

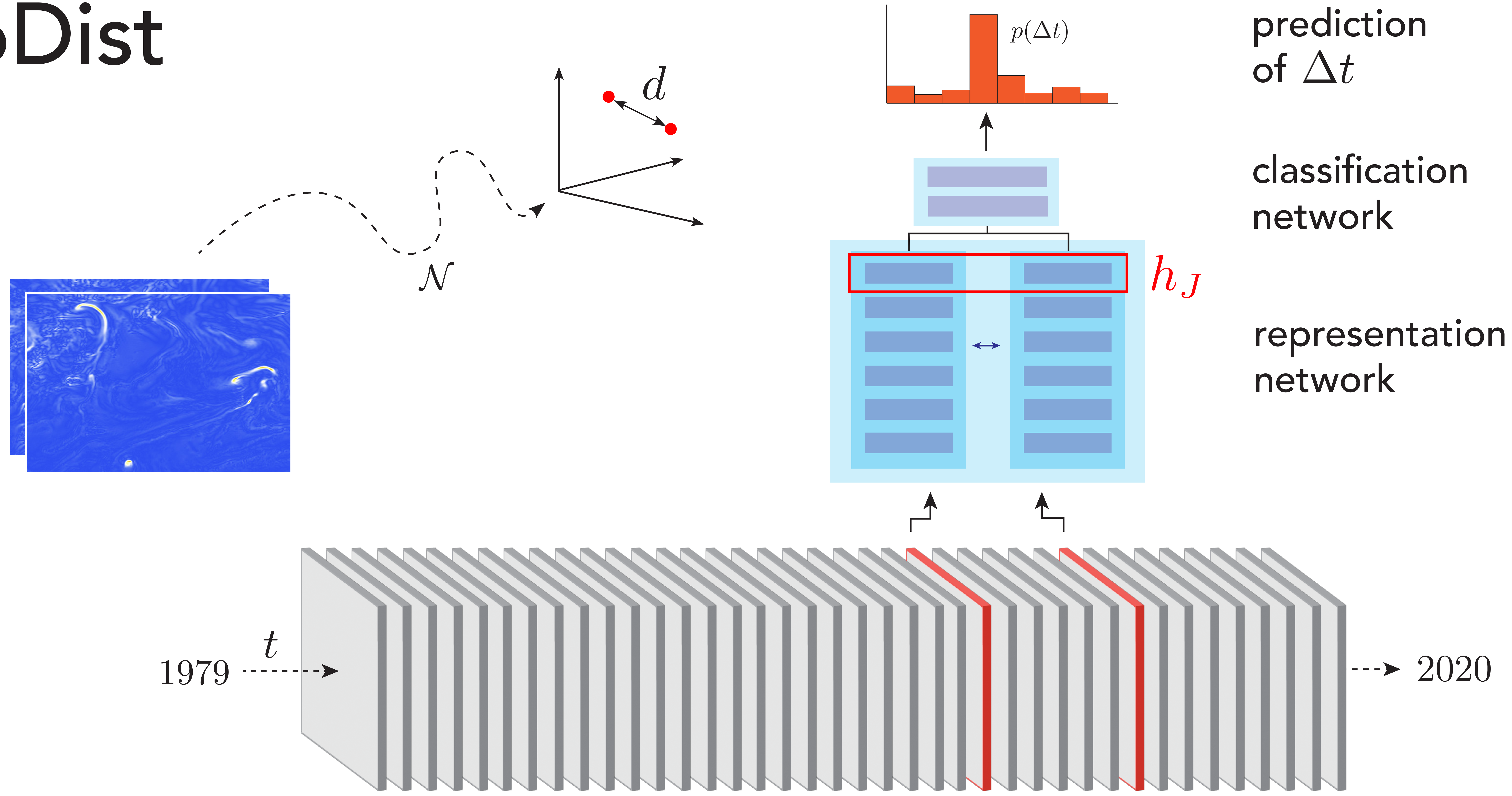


prediction of Δt

classification network

representation network

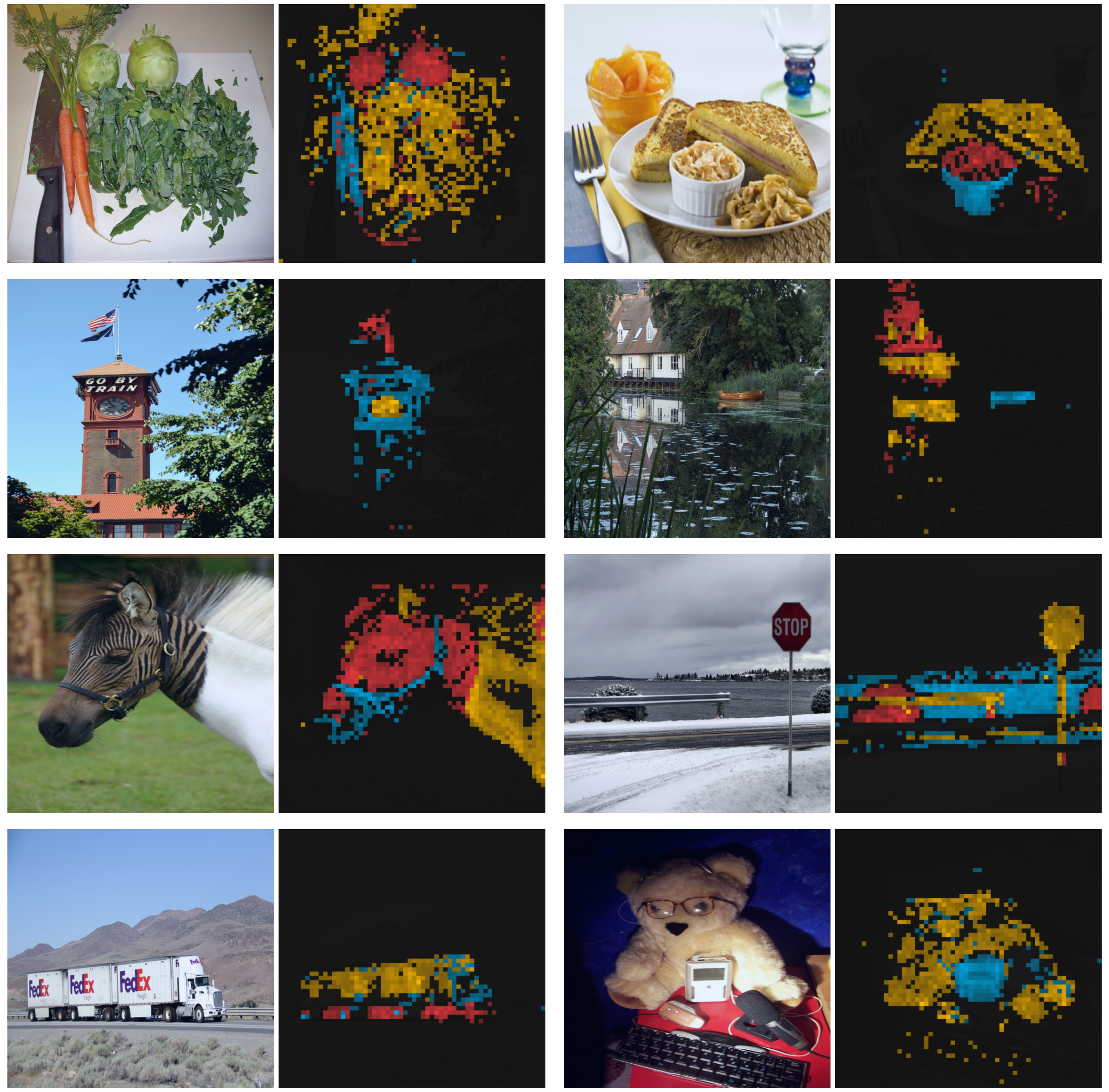
AtmoDist



New results next week at EGU 2022 (Session: Machine learning for Earth System modelling, room N1 on Tuesday, 24 May 2022, 10:26 CEST)

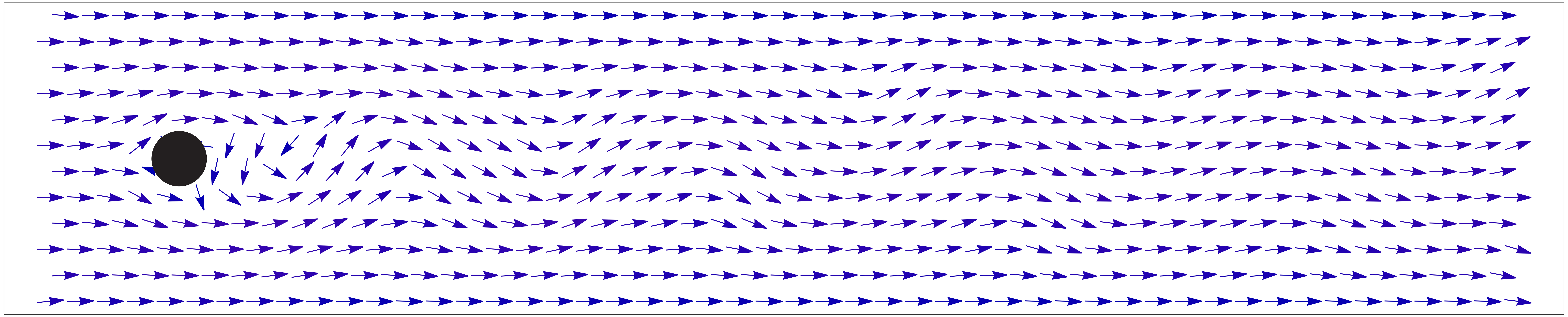
Transformers and attention

A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. N. Gomez, L. Kaiser, and I. Polosukhin. Attention is all you need. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 30. Curran Associates, Inc., 2017.

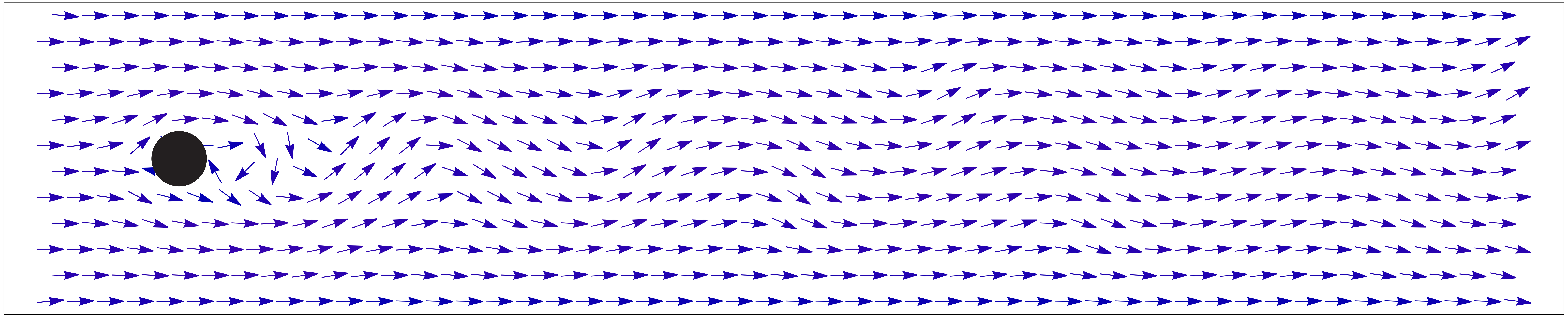


M. Caron, H. Touvron, I. Misra, H. Jegou, J. Mairal, P. Bojanowski, and A. Joulin. Emerging properties in self-supervised vision transformers. CoRR, abs/2104.14294, 2021.

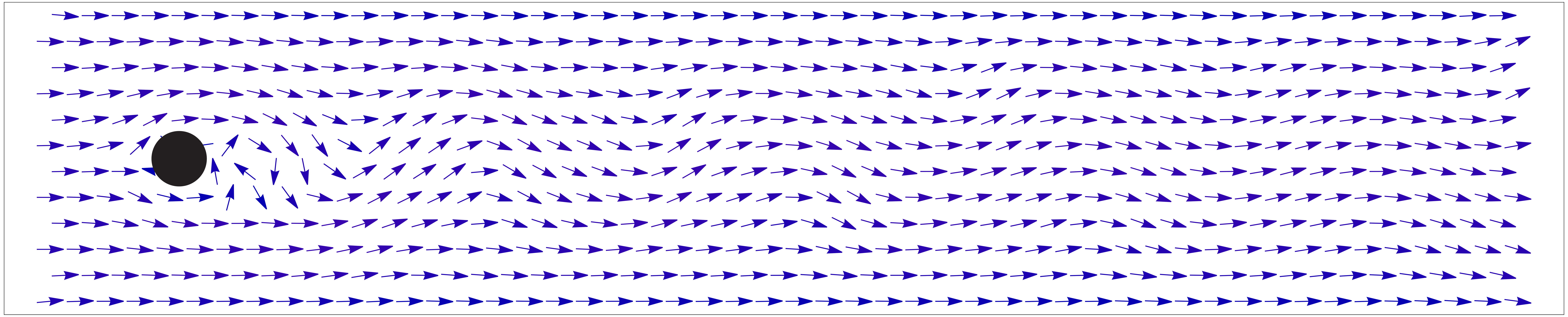
Transformers and attention



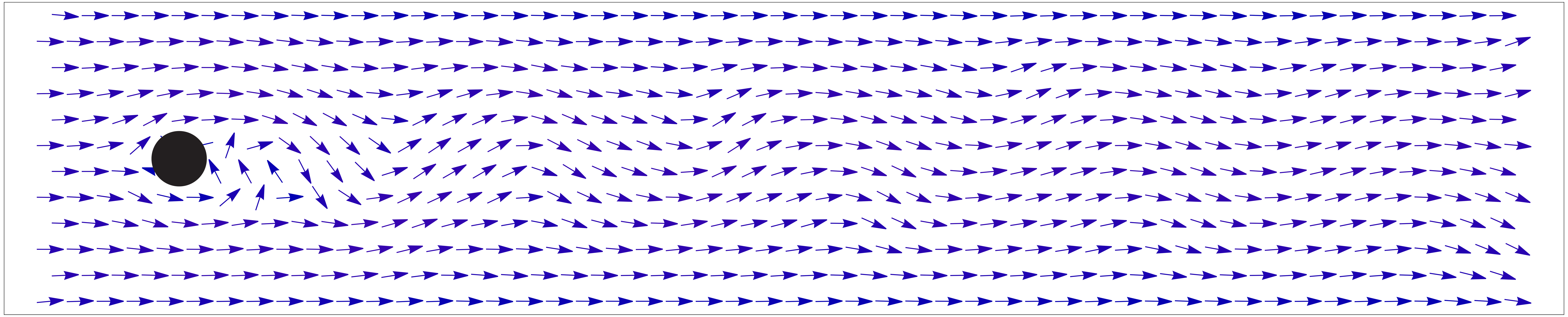
Transformers and attention



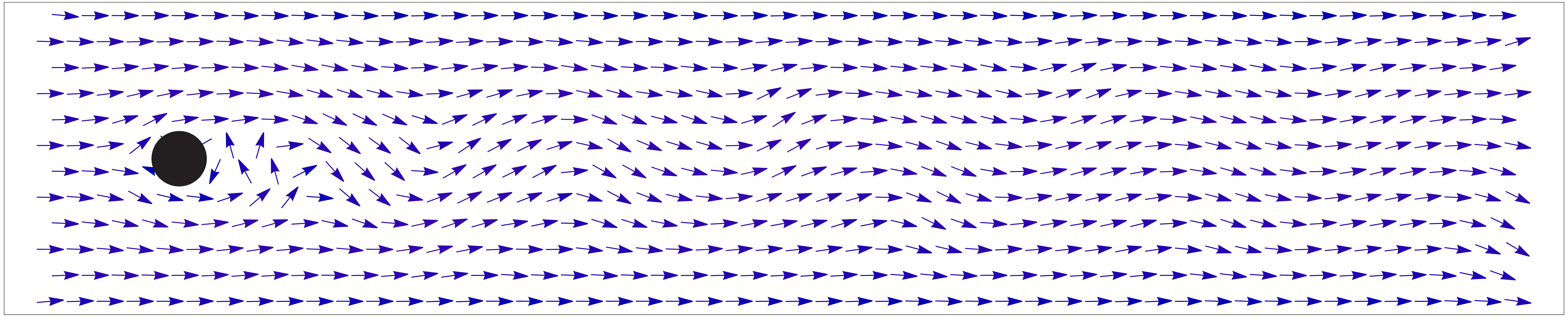
Transformers and attention



Transformers and attention



Transformers and attention



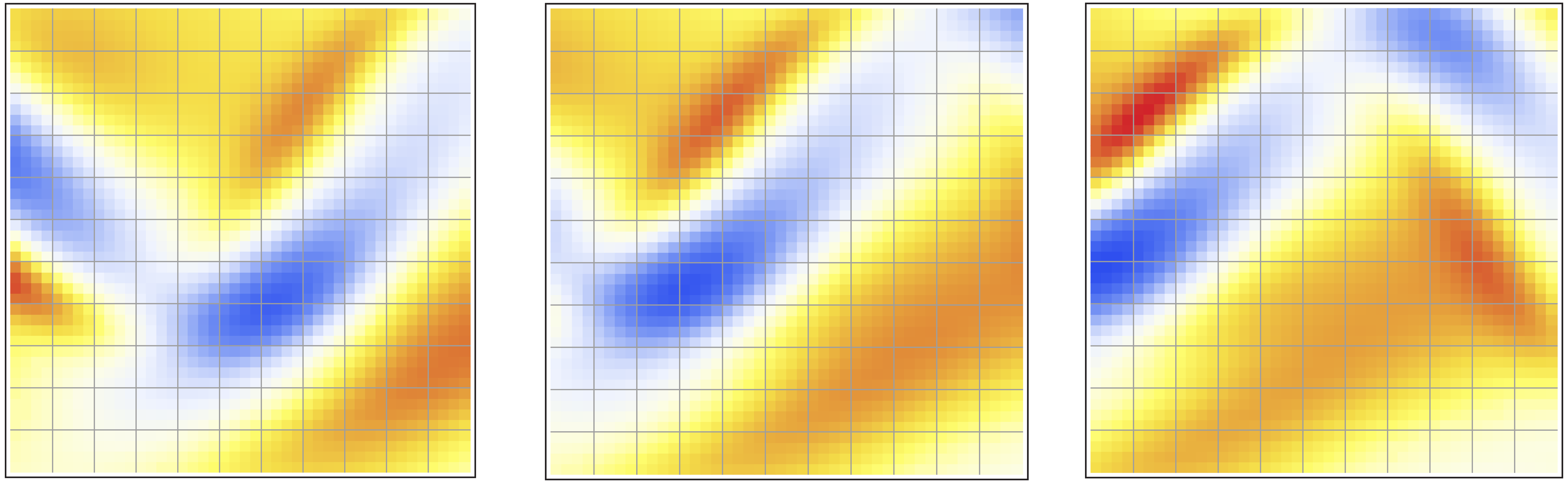
Fluid flow (vorticity)

Fluid flow (vorticity)

training with varying position
and spherical eccentrity

Fluid flow (vorticity)

t-2 t-1 t



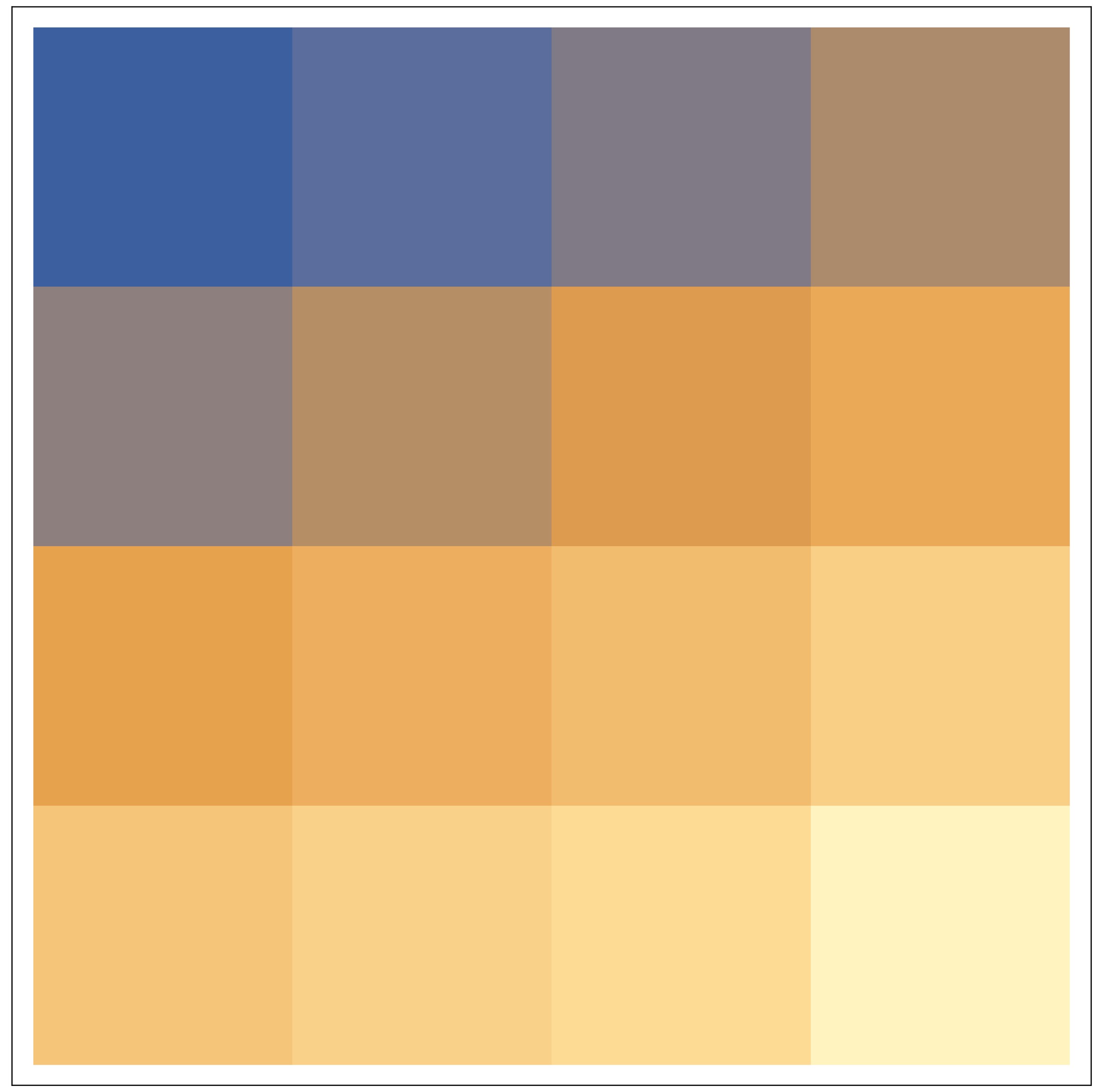
Fluid flow (vorticity)

Fluid flow

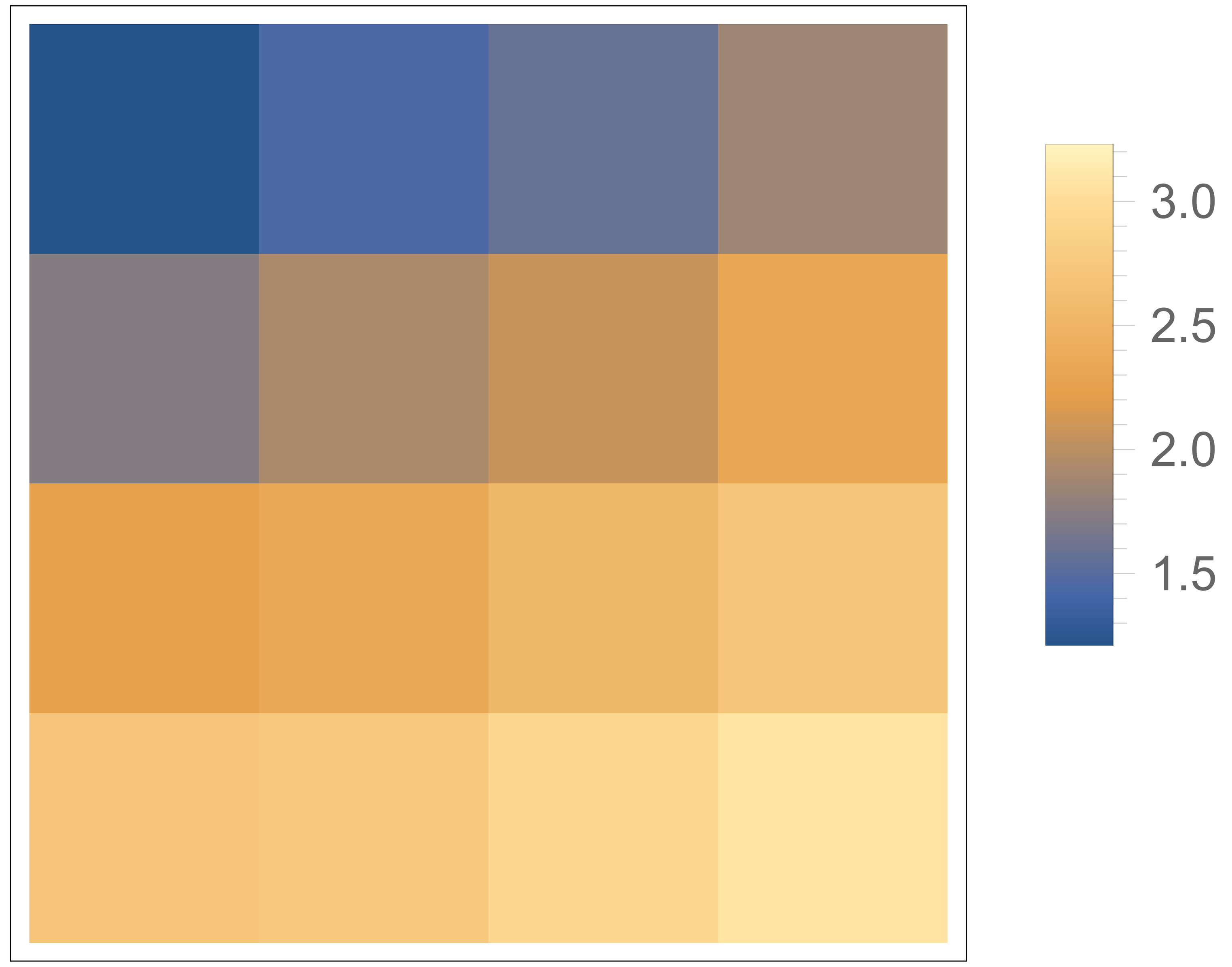

Prediction
Reference
10.0
7.5
5.0
2.5
0
10
5
−5
2
4
6
8
10
12
14
16
Reference
Prediction 1
Prediction 2

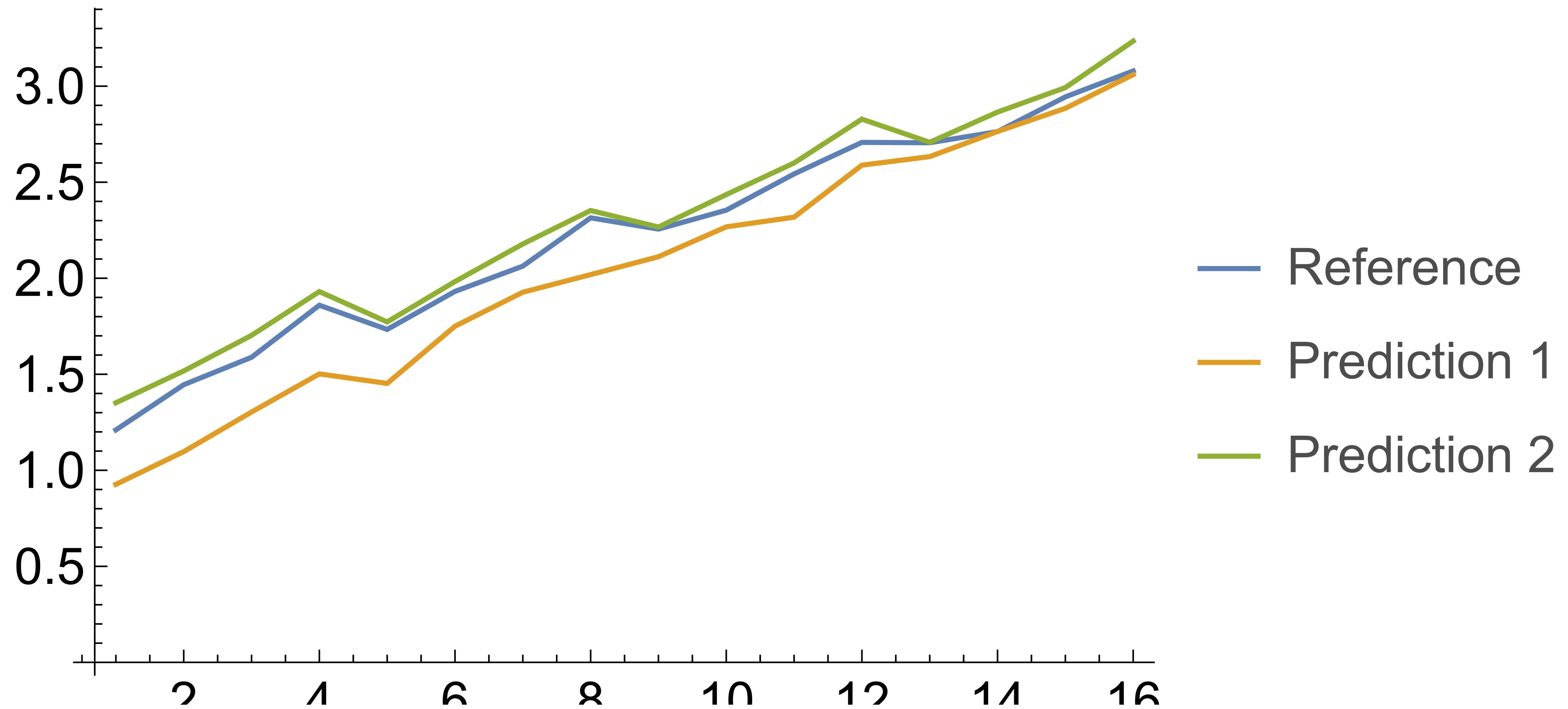
Fluid flow

Prediction

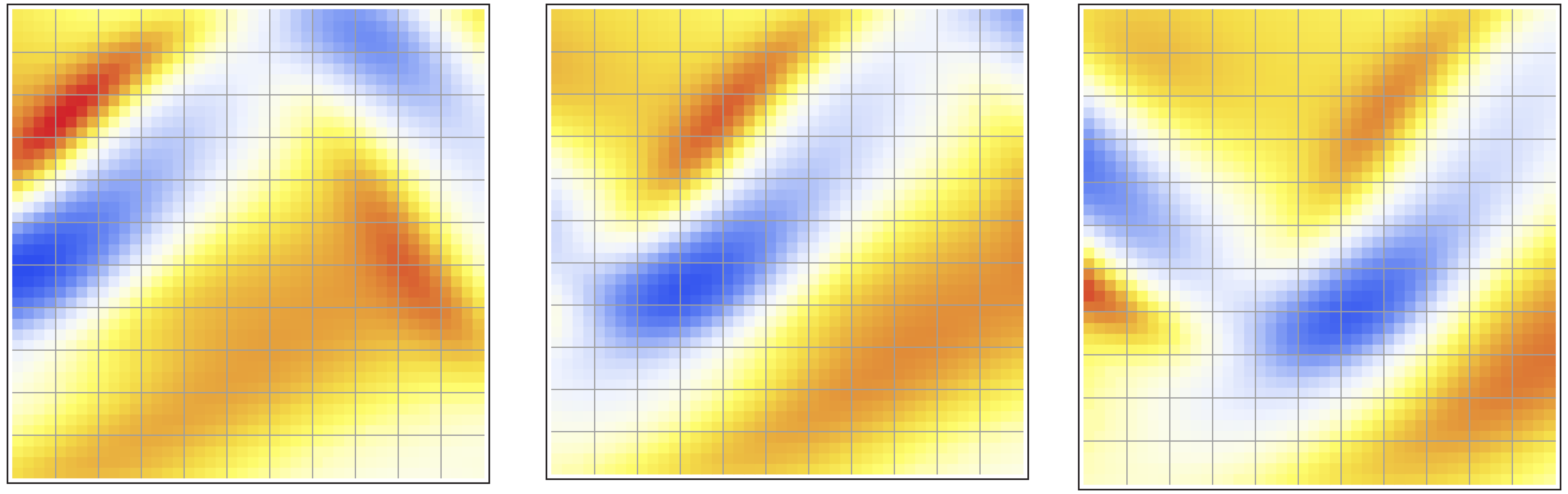


Reference



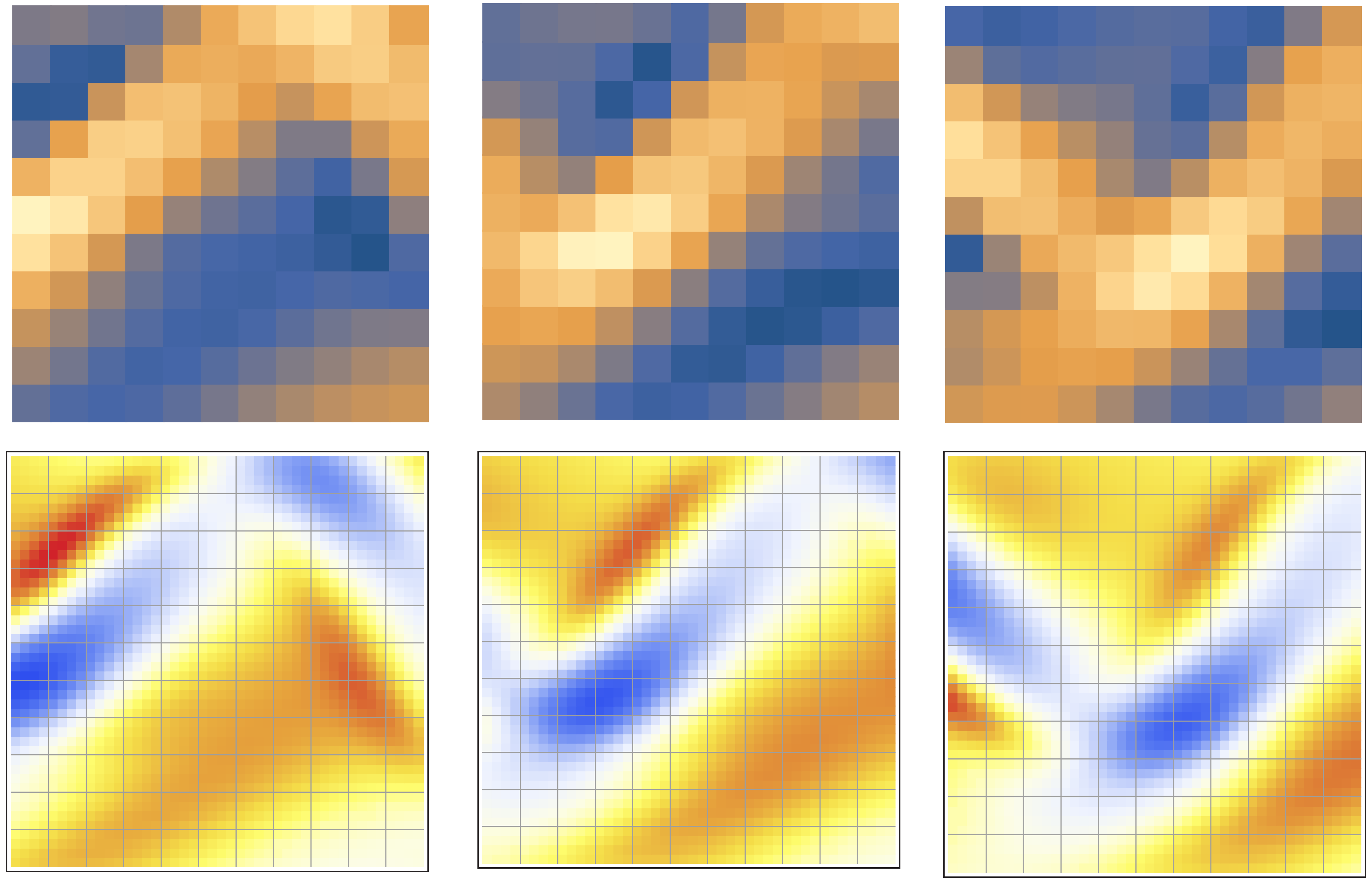


Fluid flow



t-2 t-1 t

Fluid flow



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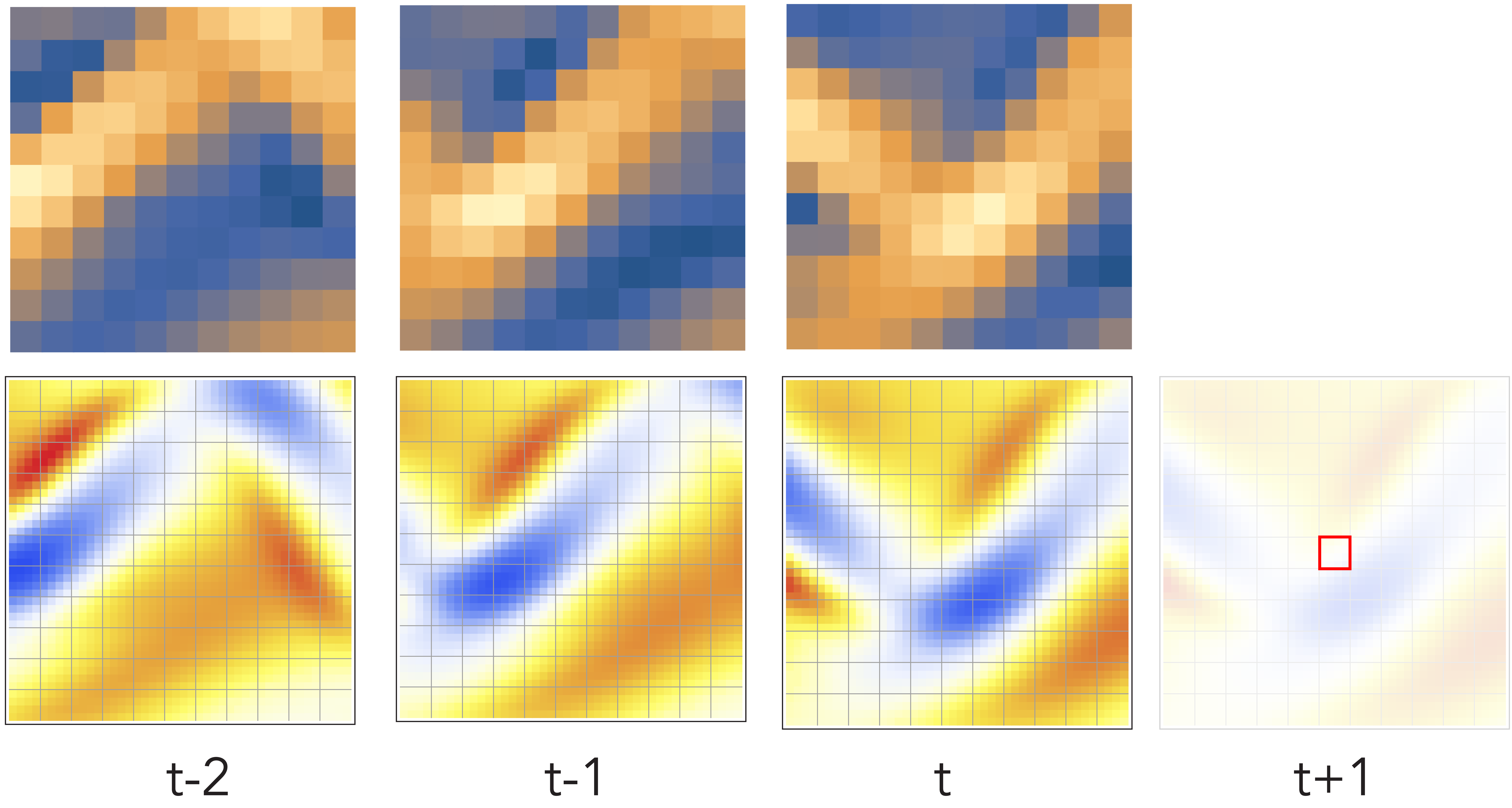

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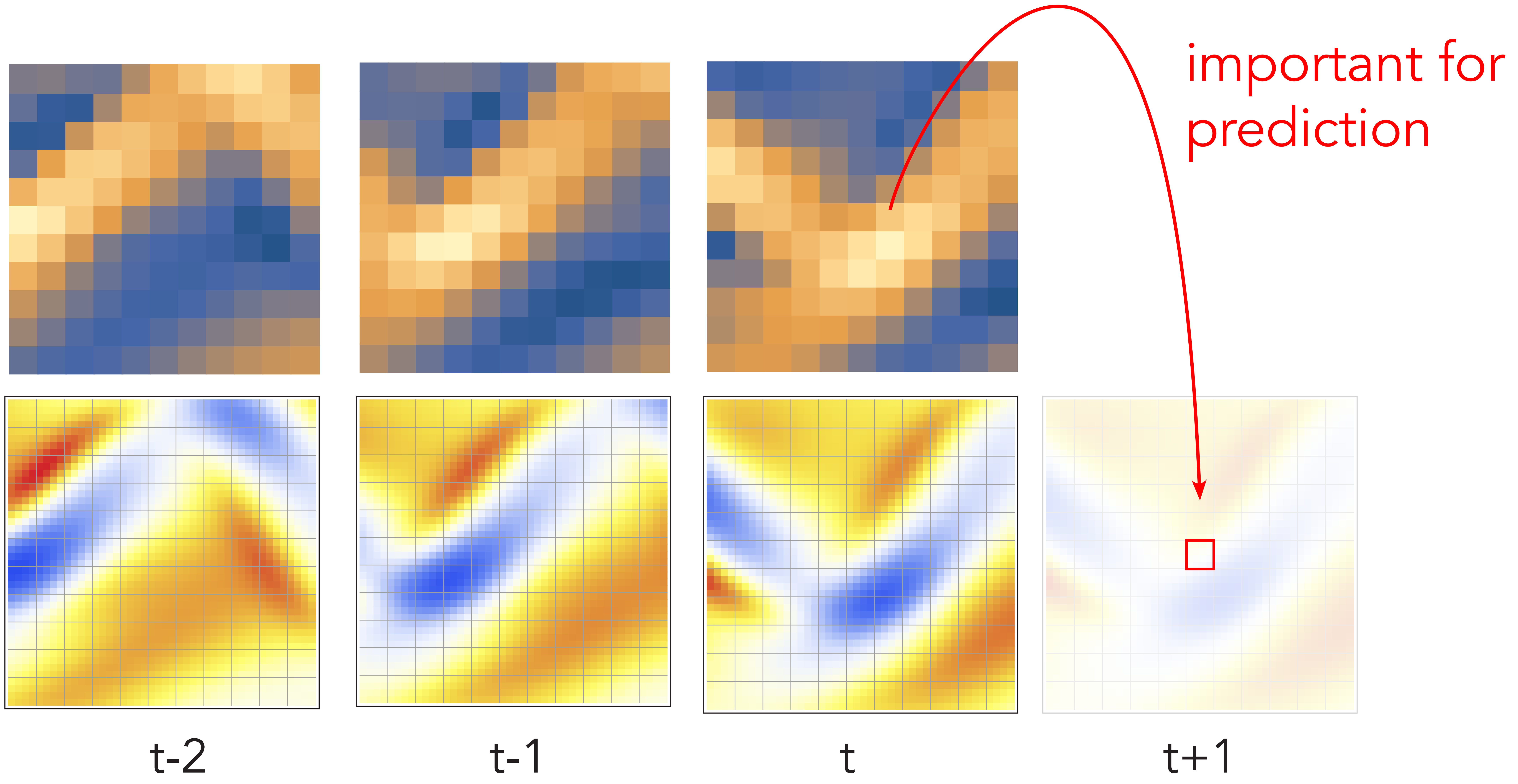

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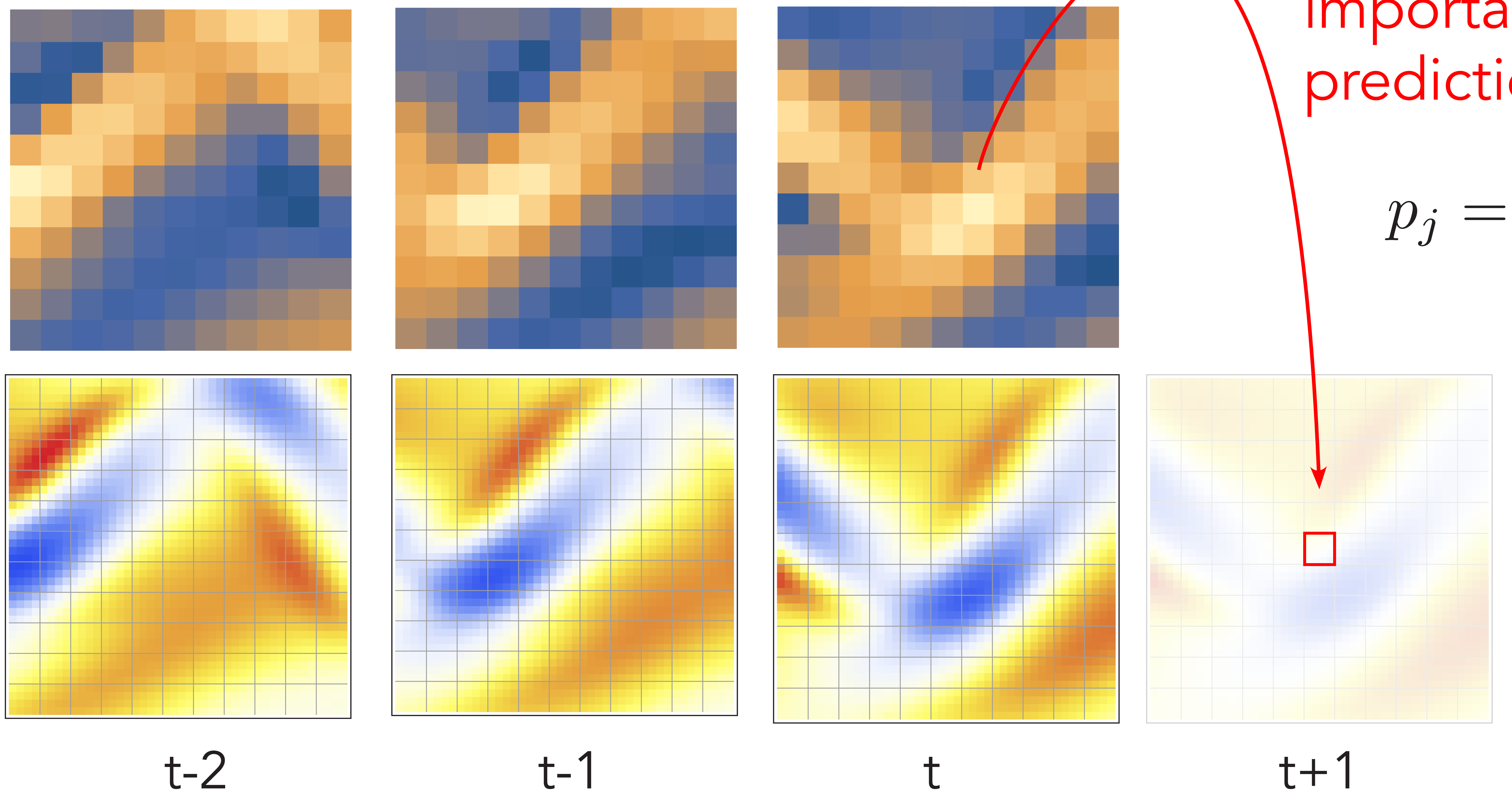
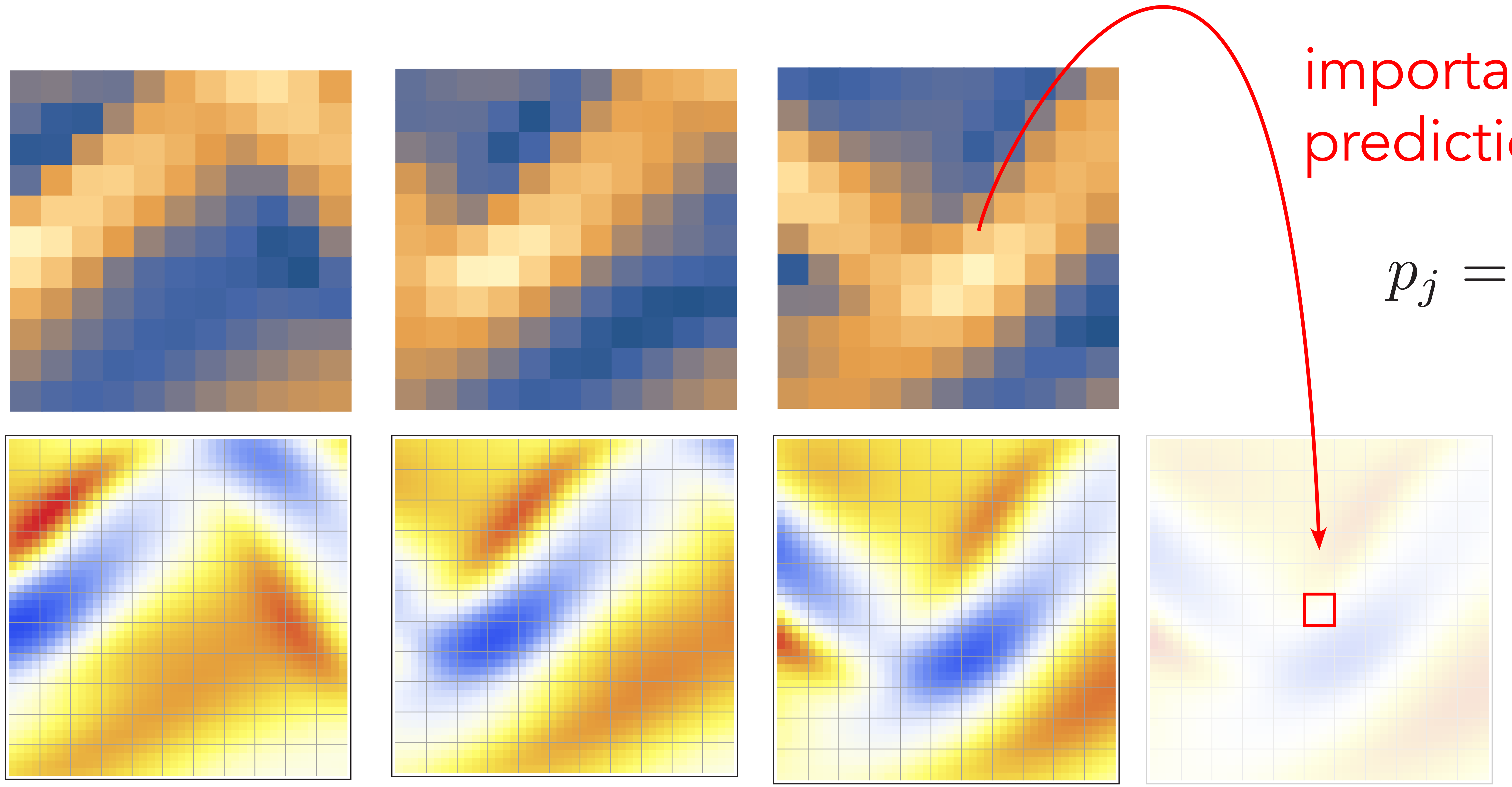


important for prediction

$$p_j = \sum_j \sigma(a_{ij})\, v_j$$

Fluid flow



t-2 t-1 t t+1

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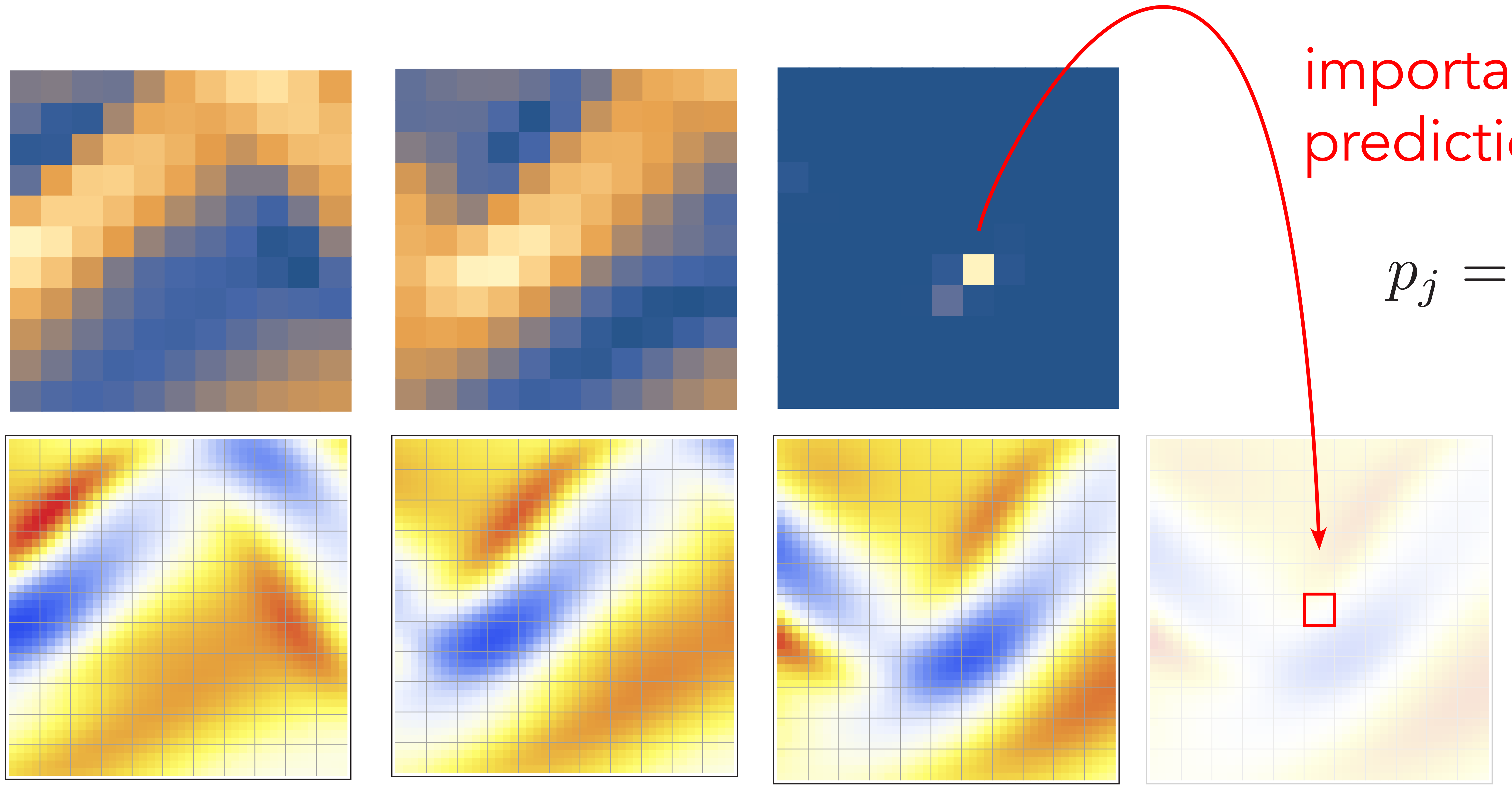
attention map values

Fluid flow



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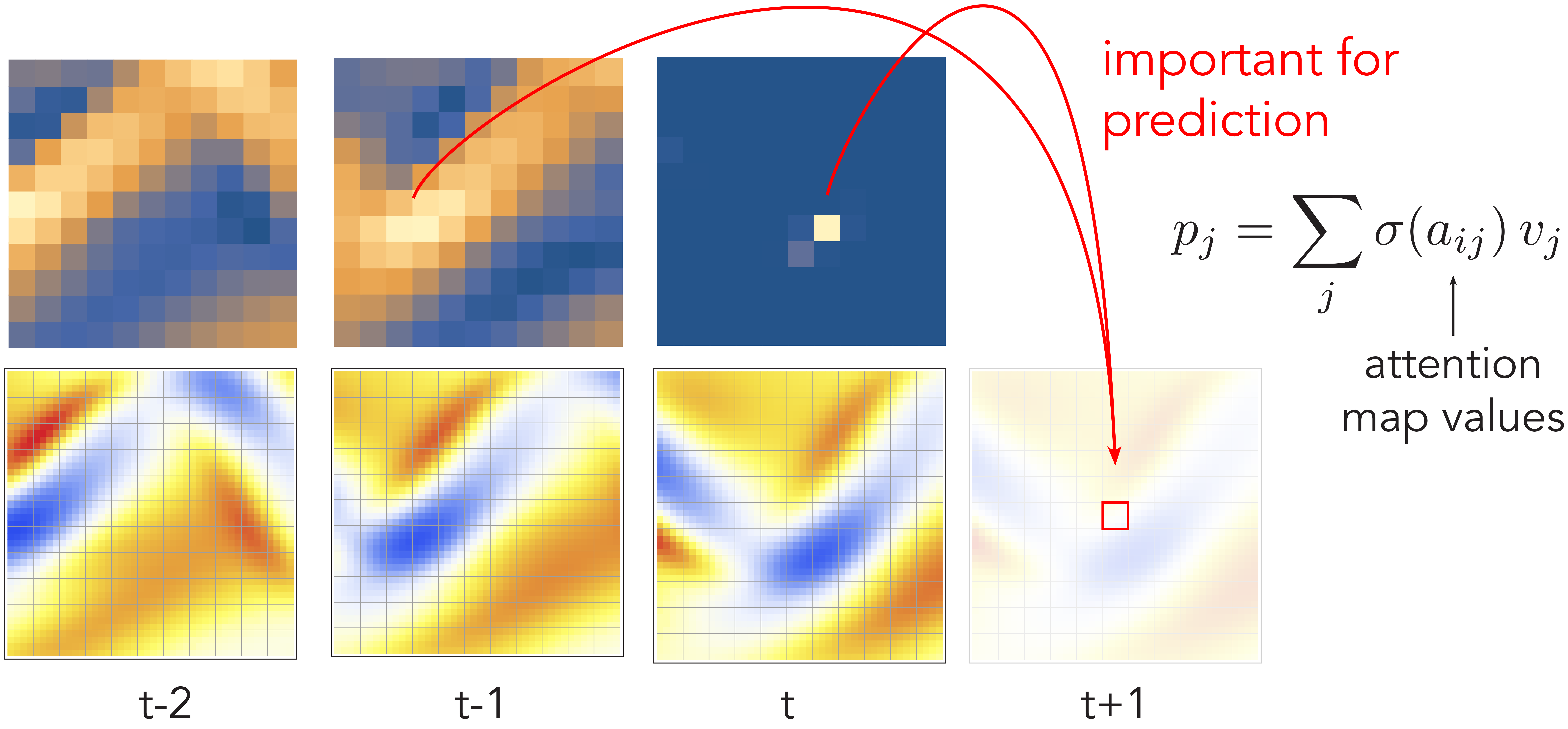

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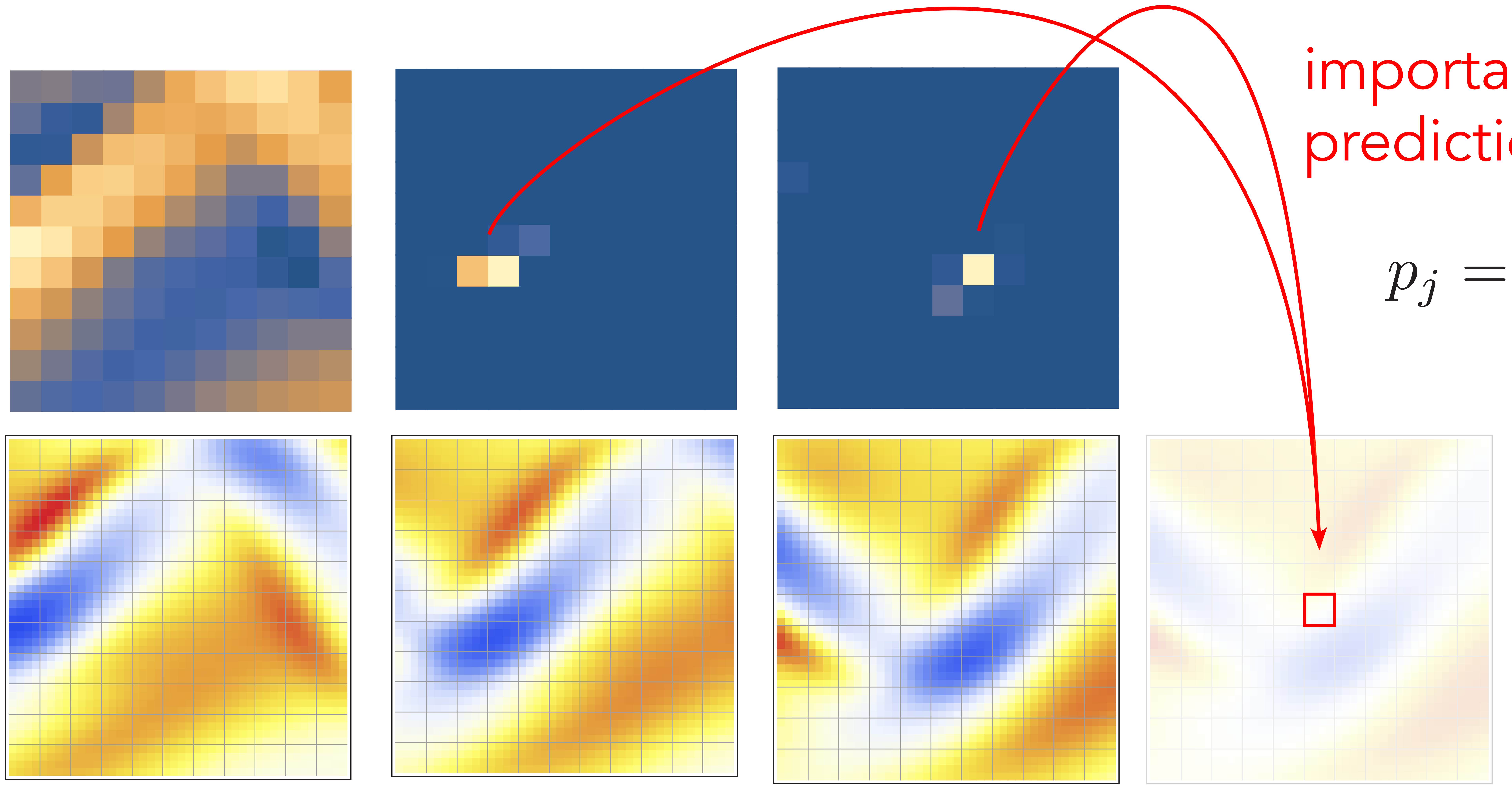

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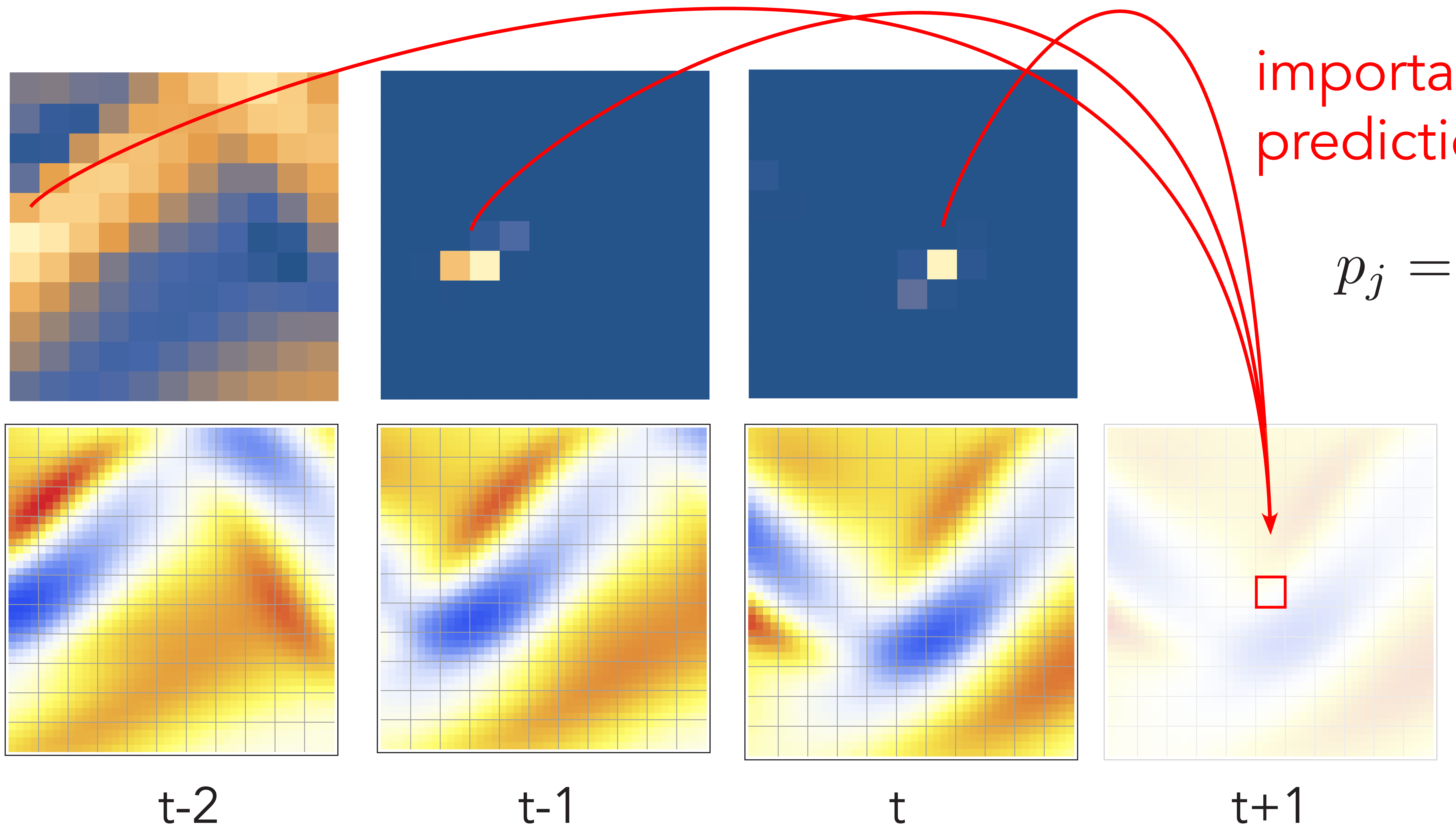

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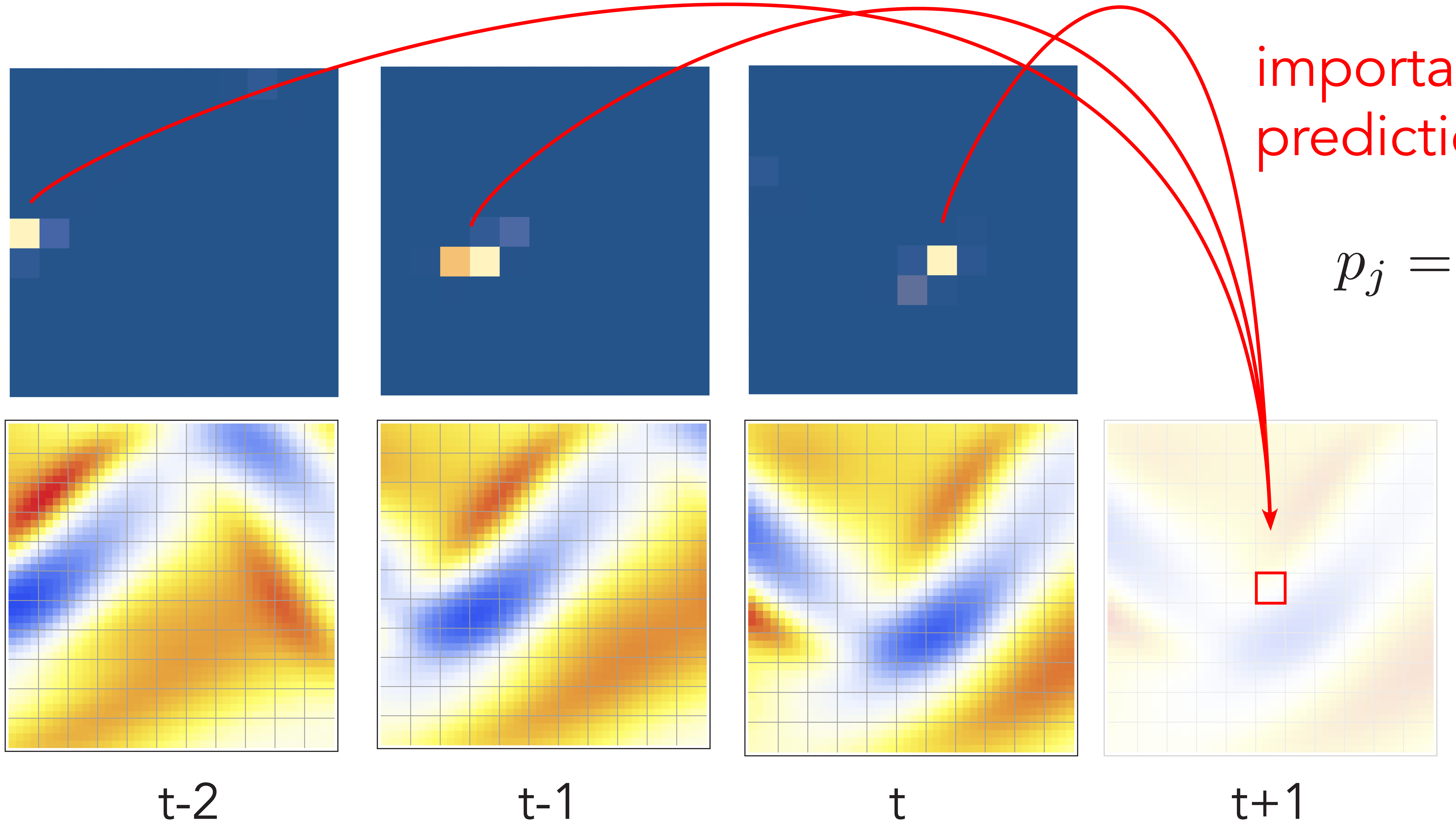

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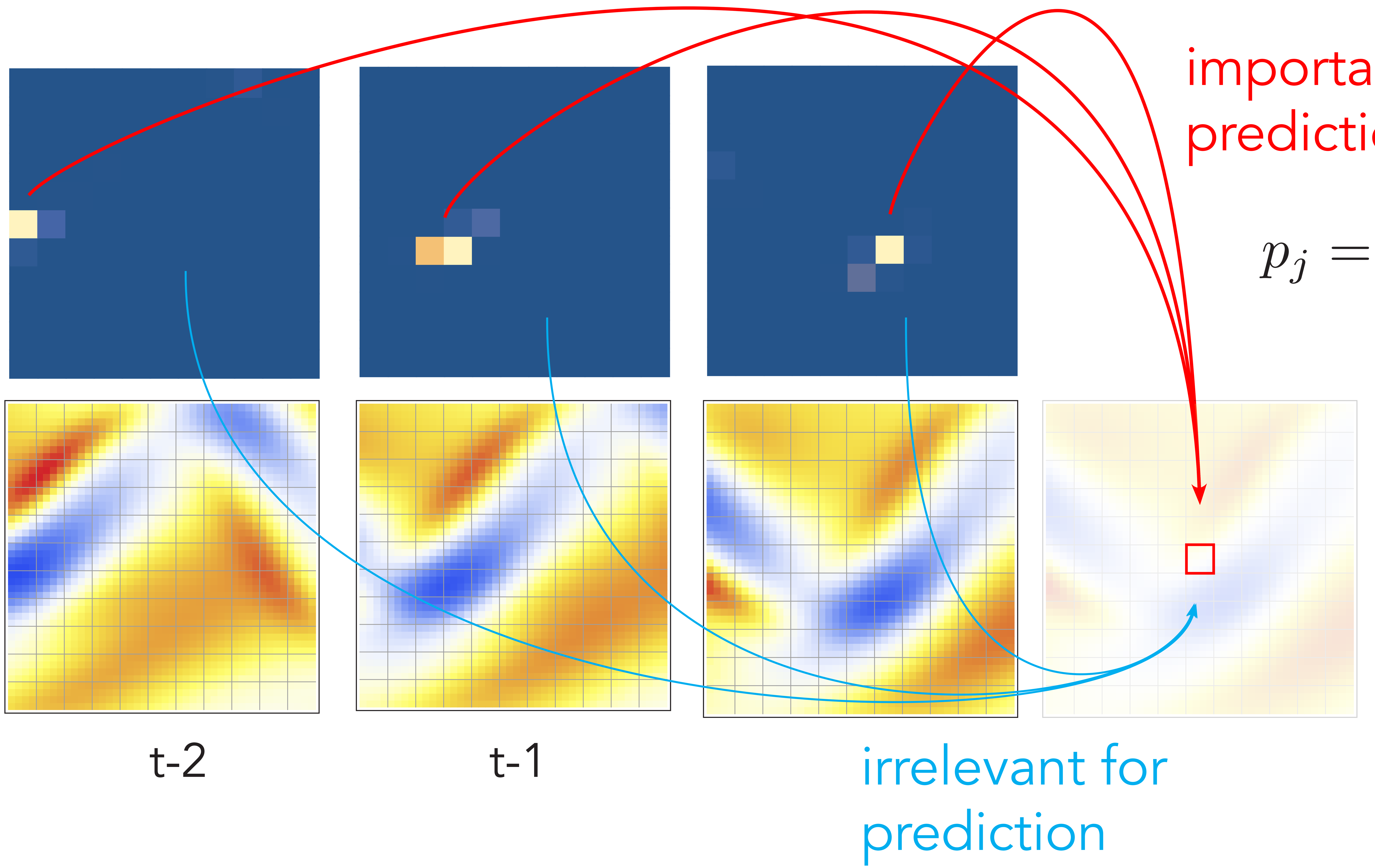

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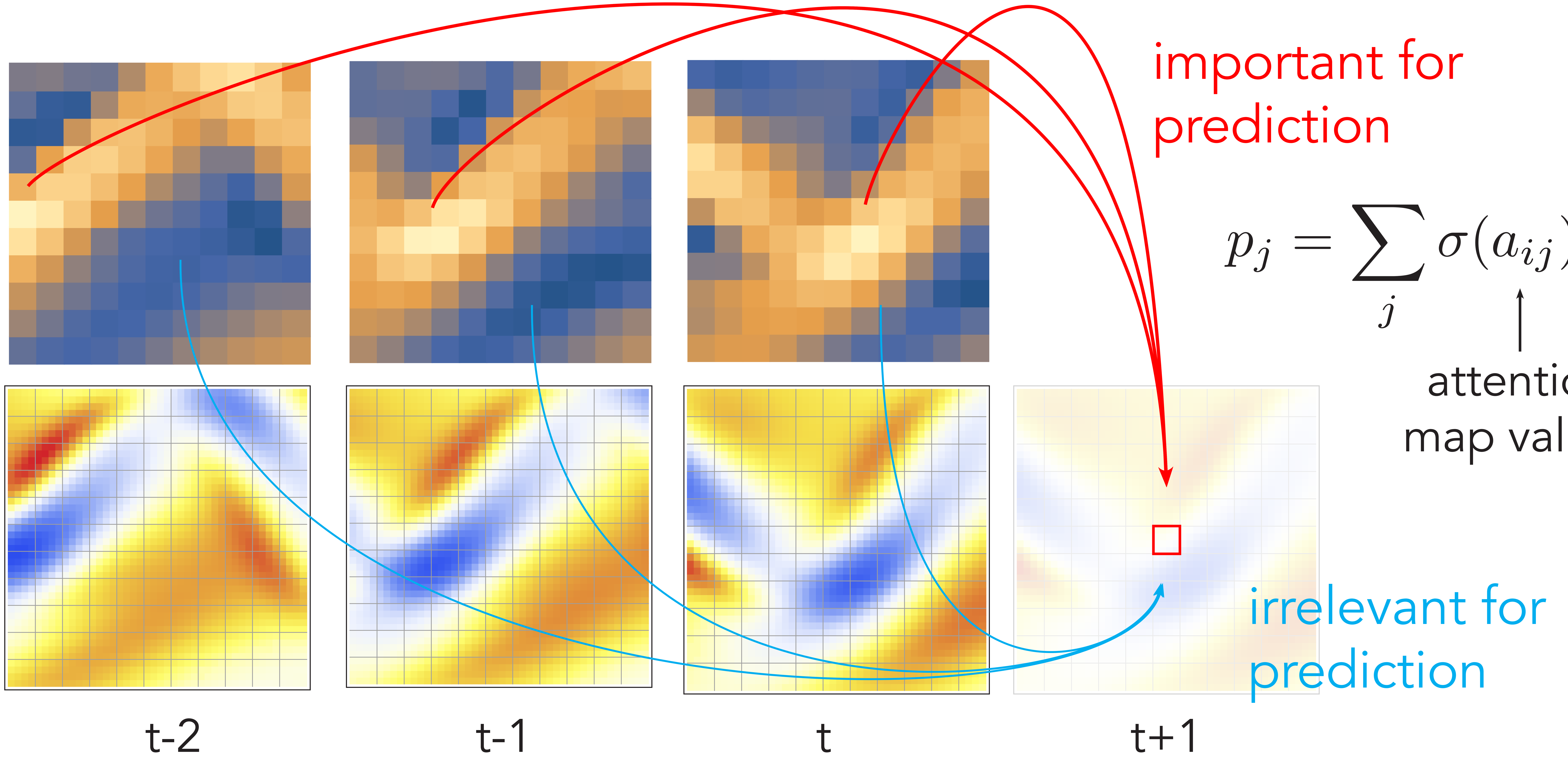

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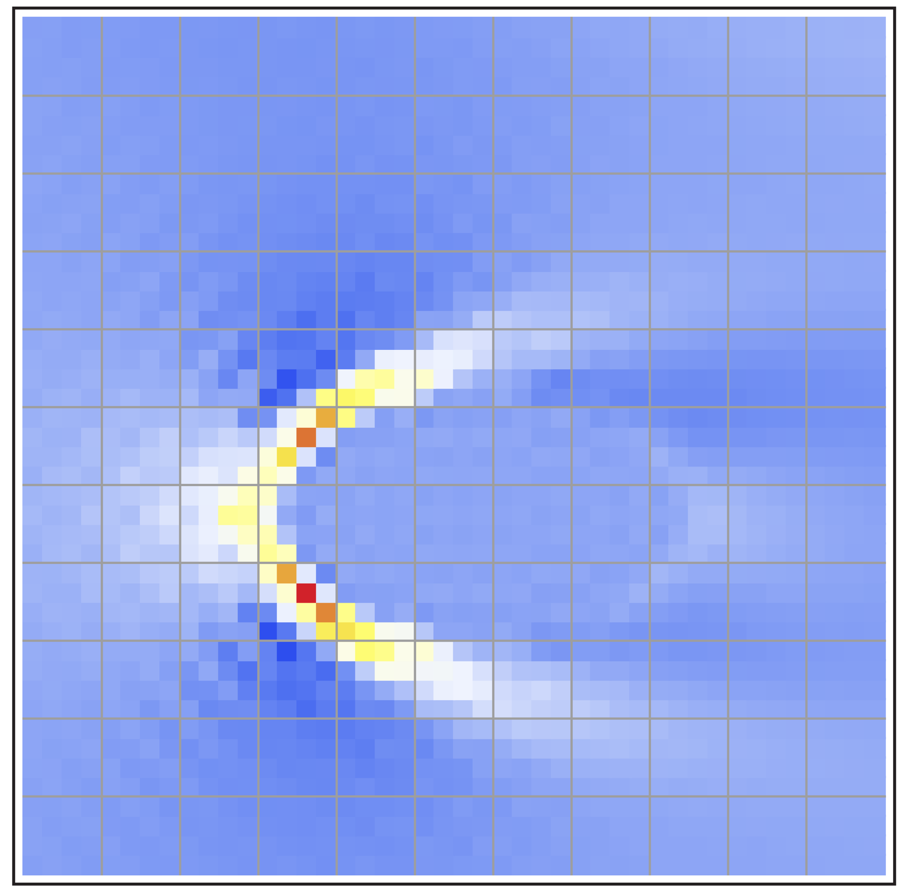
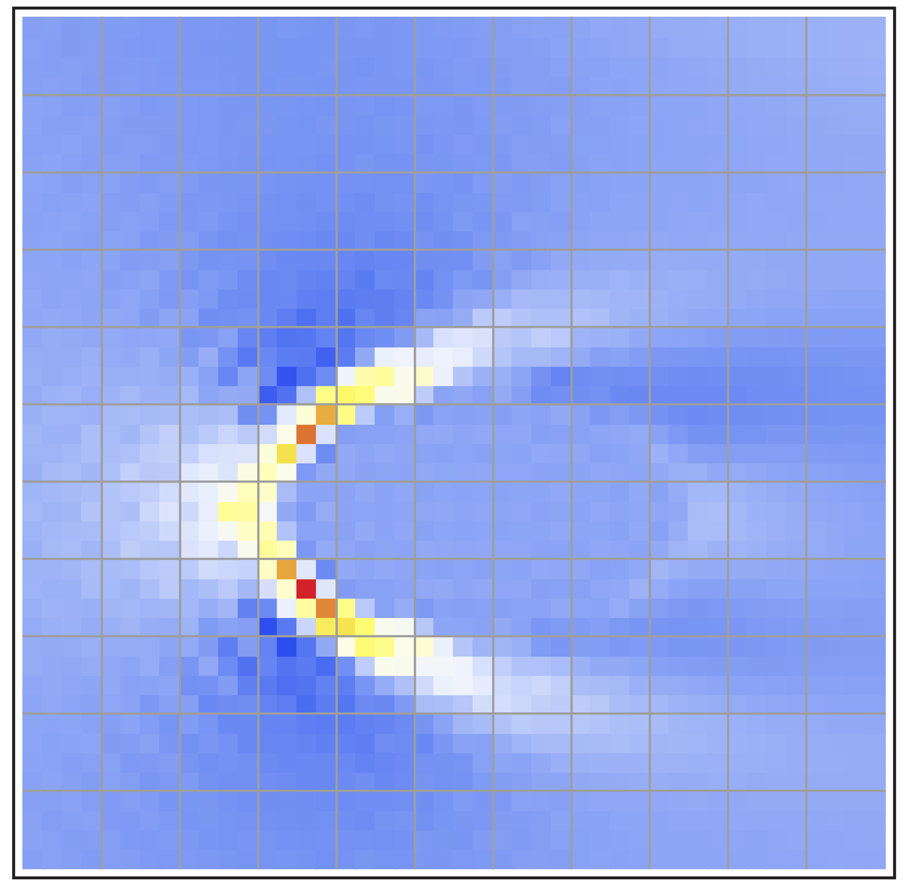
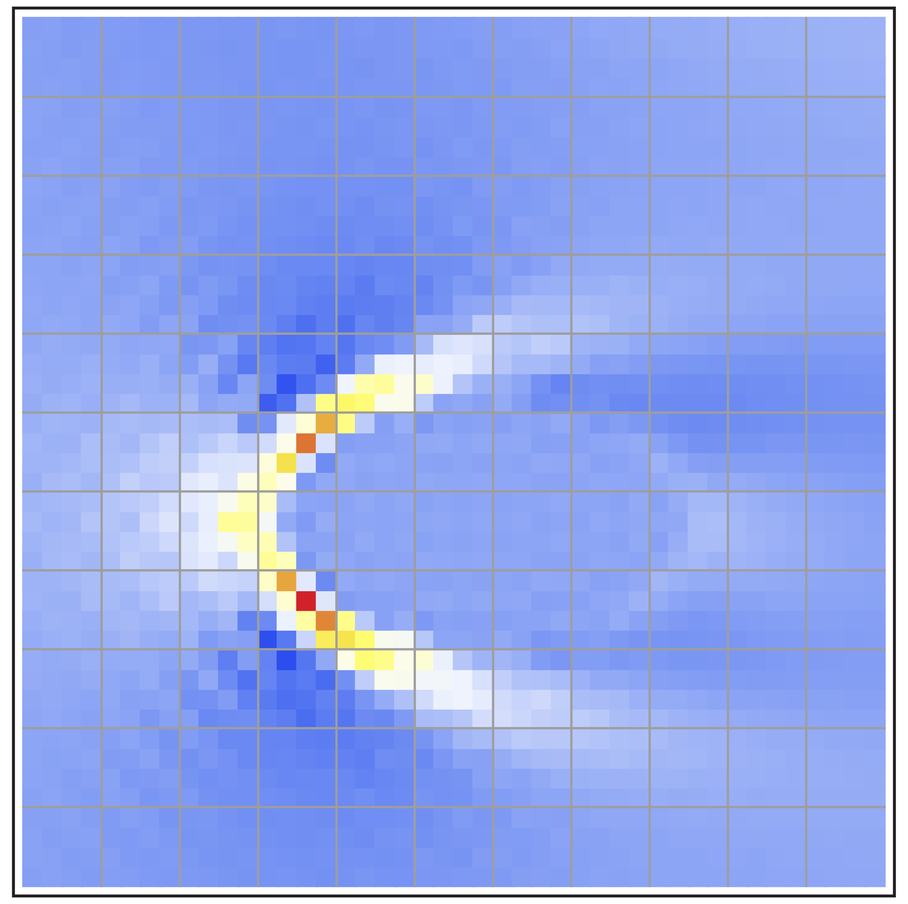


t-2

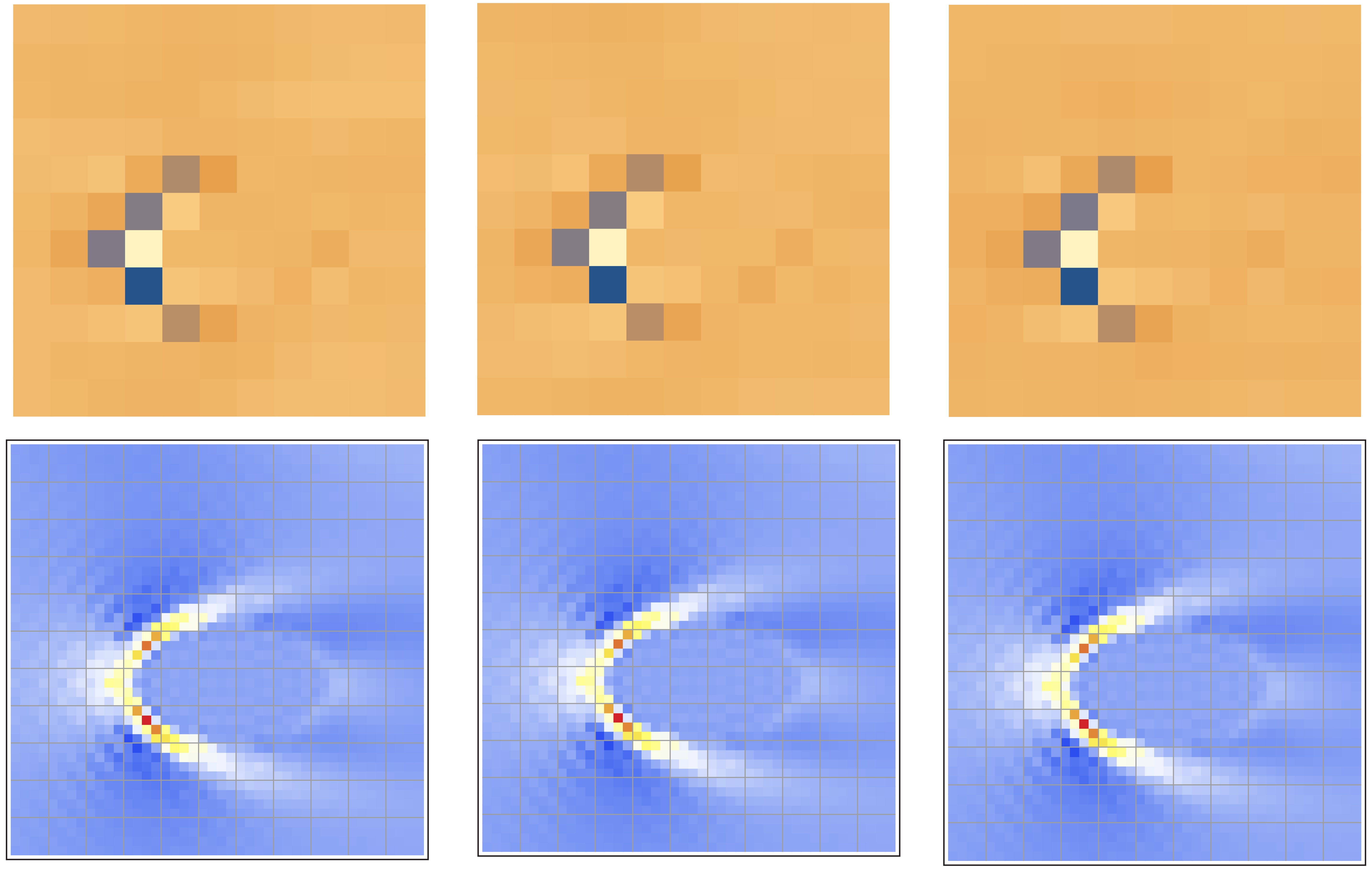


t-1



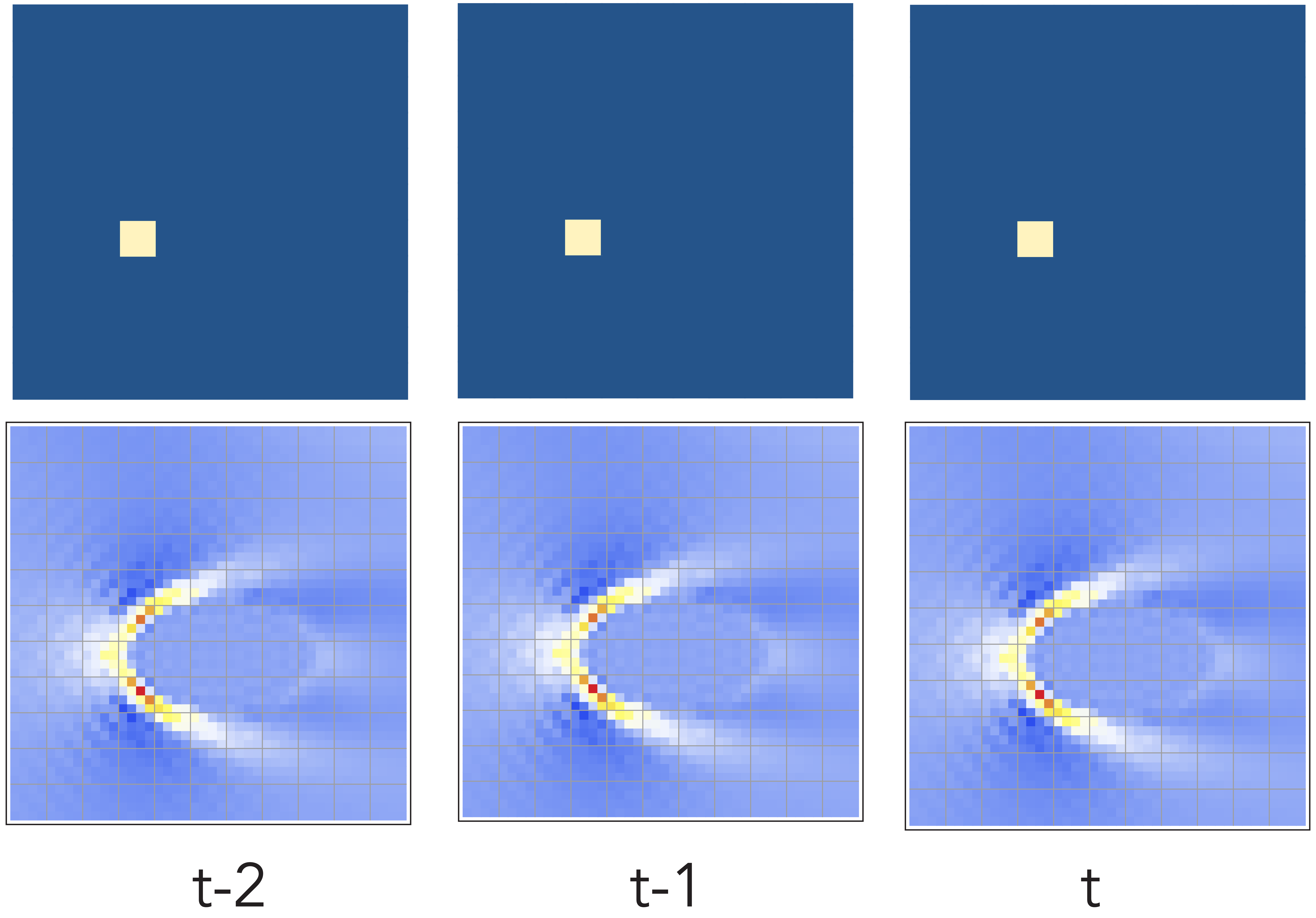
t

Fluid flow



t-2 t-1 t

Fluid flow



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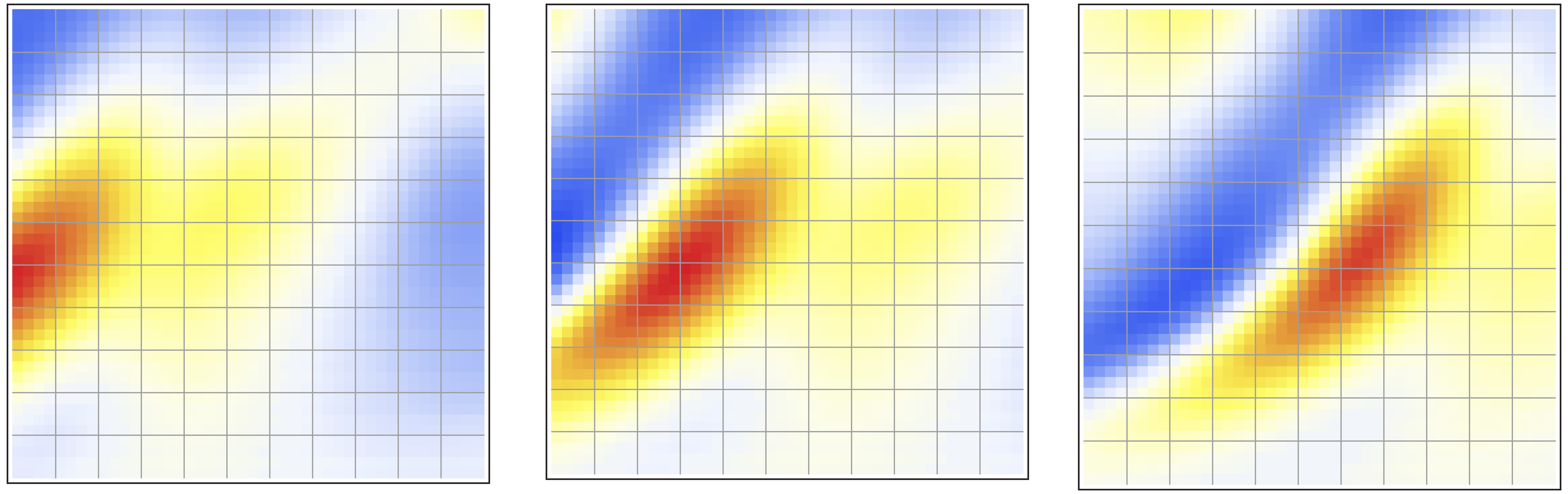

t-2 t-1 t

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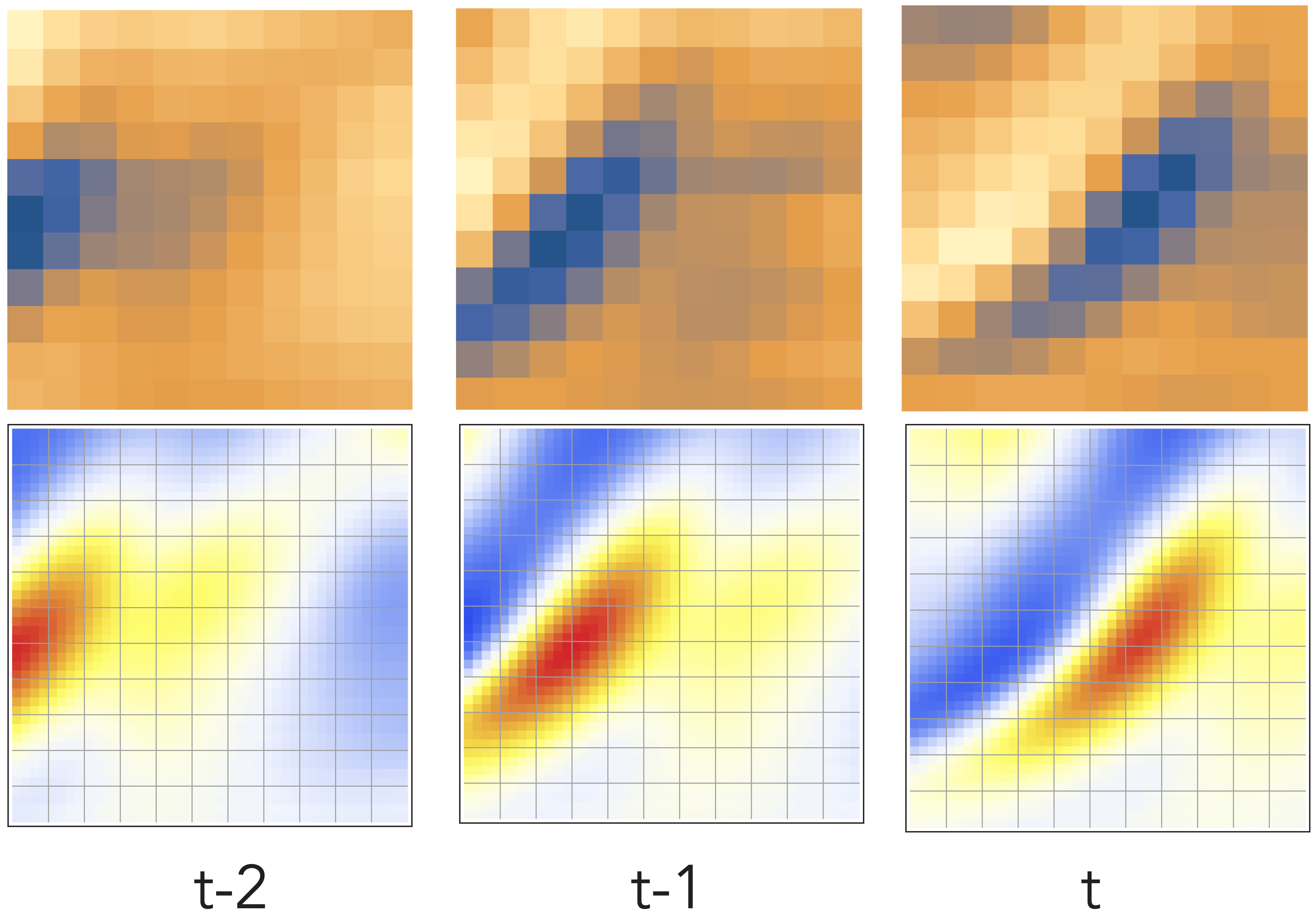

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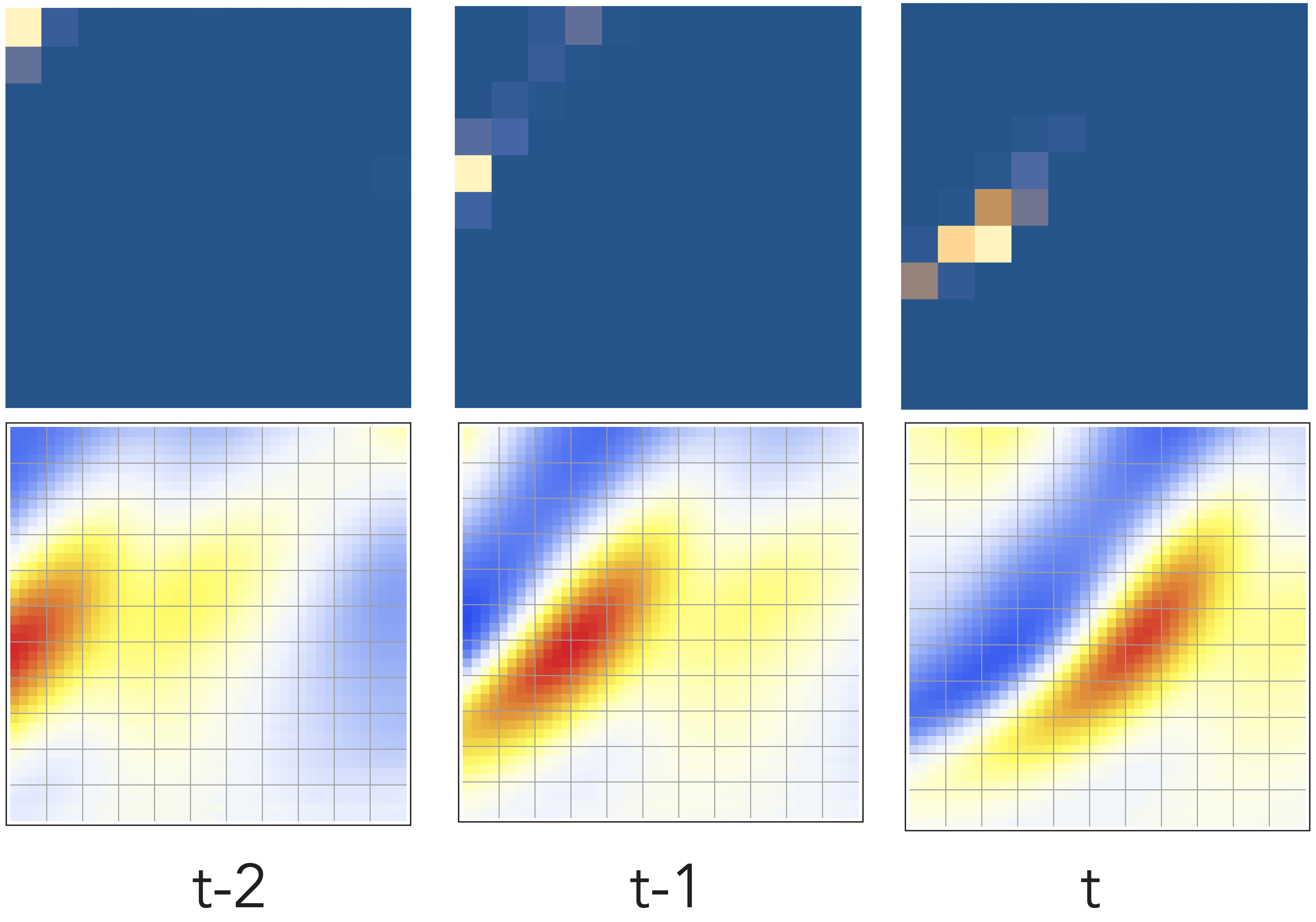
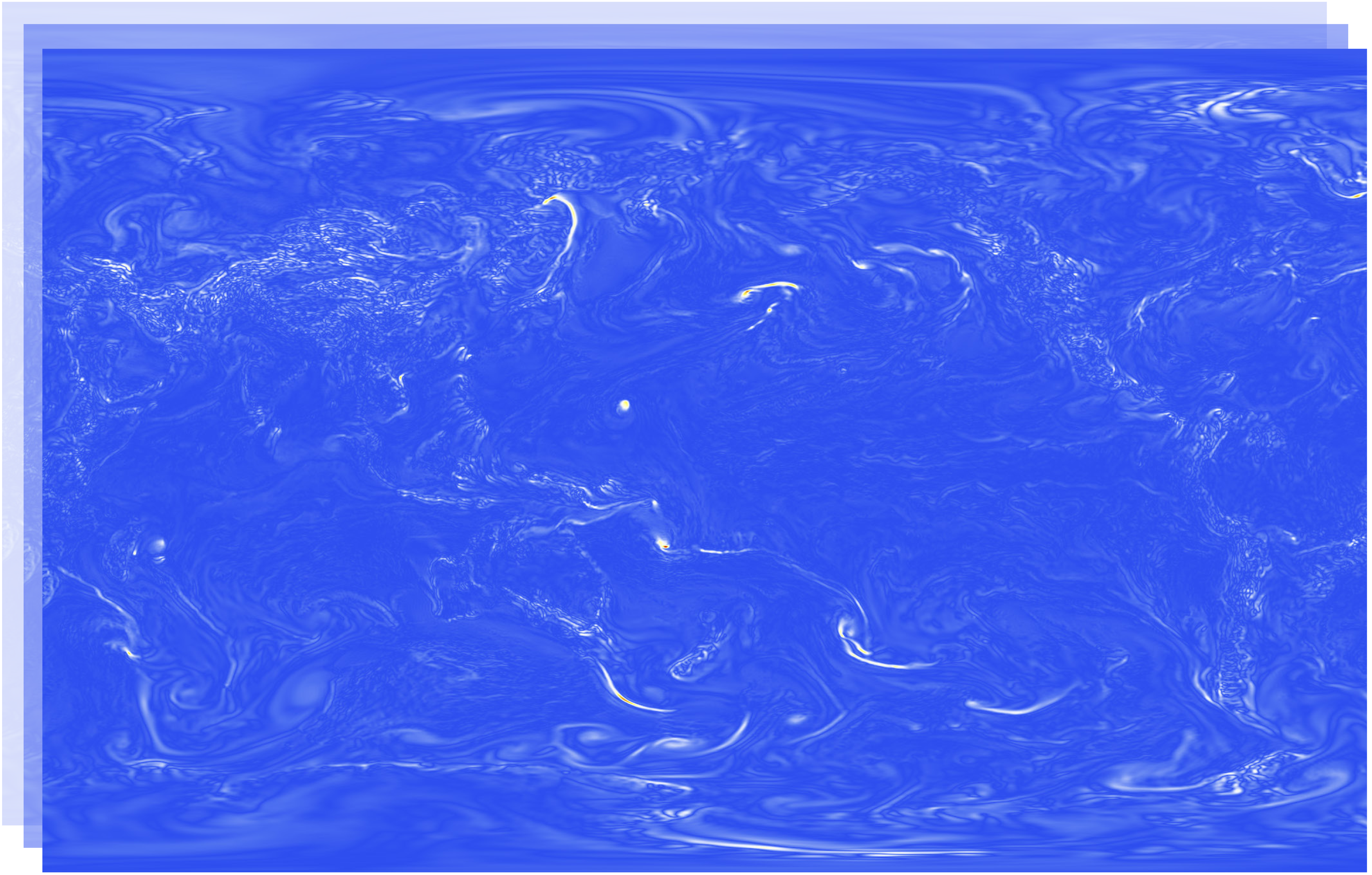


Atmospheric vorticity (ERA5)



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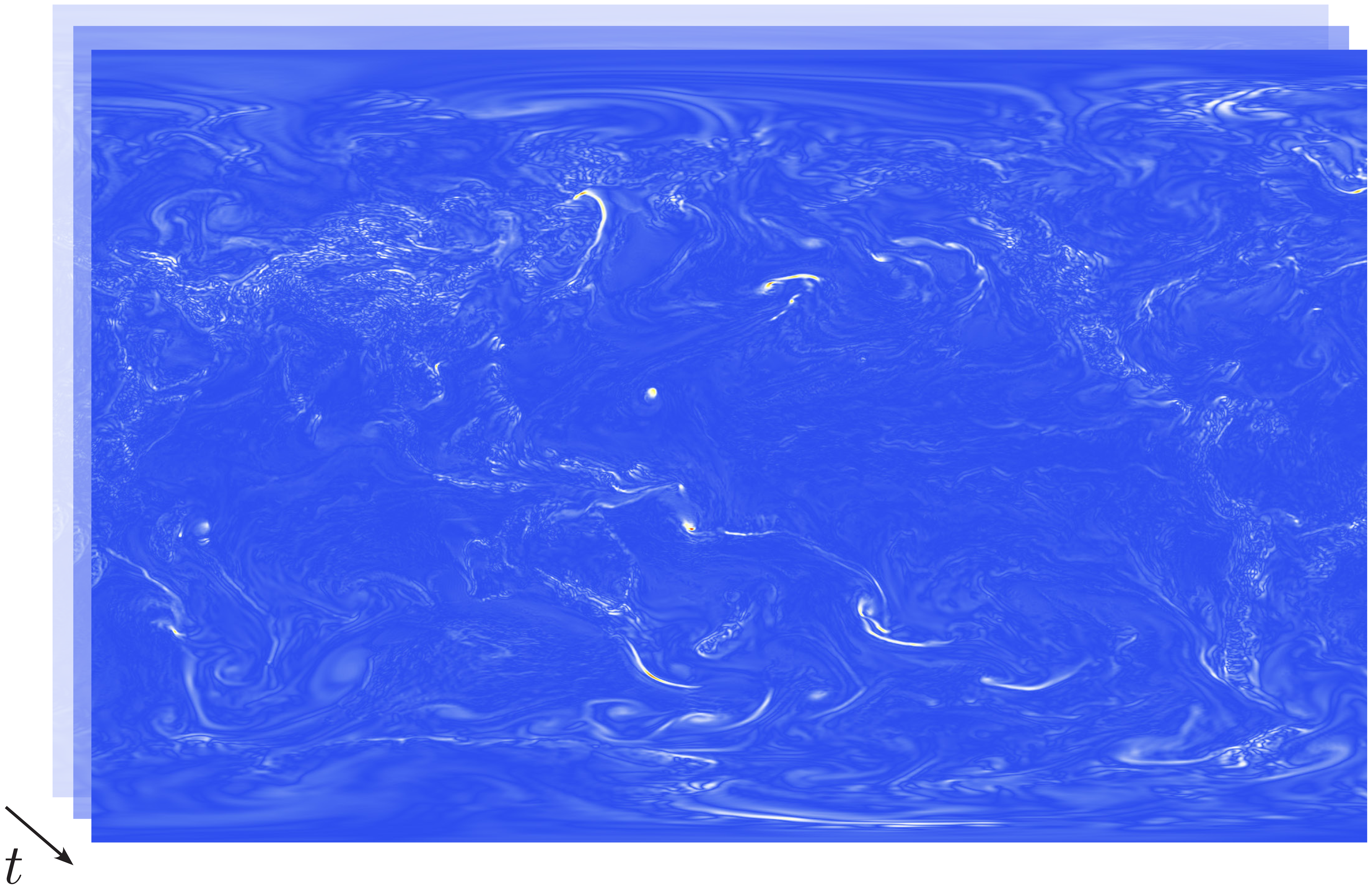

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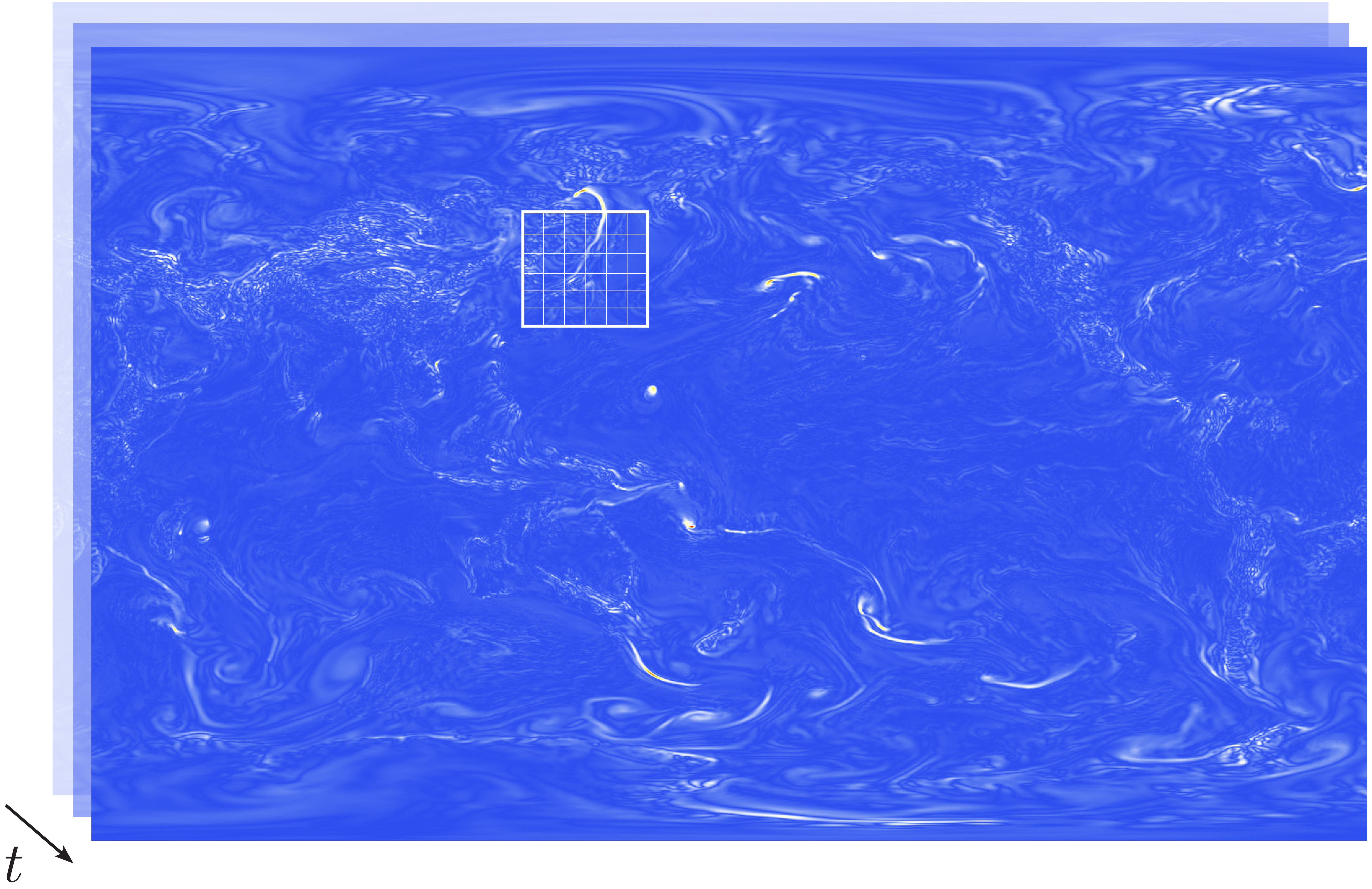

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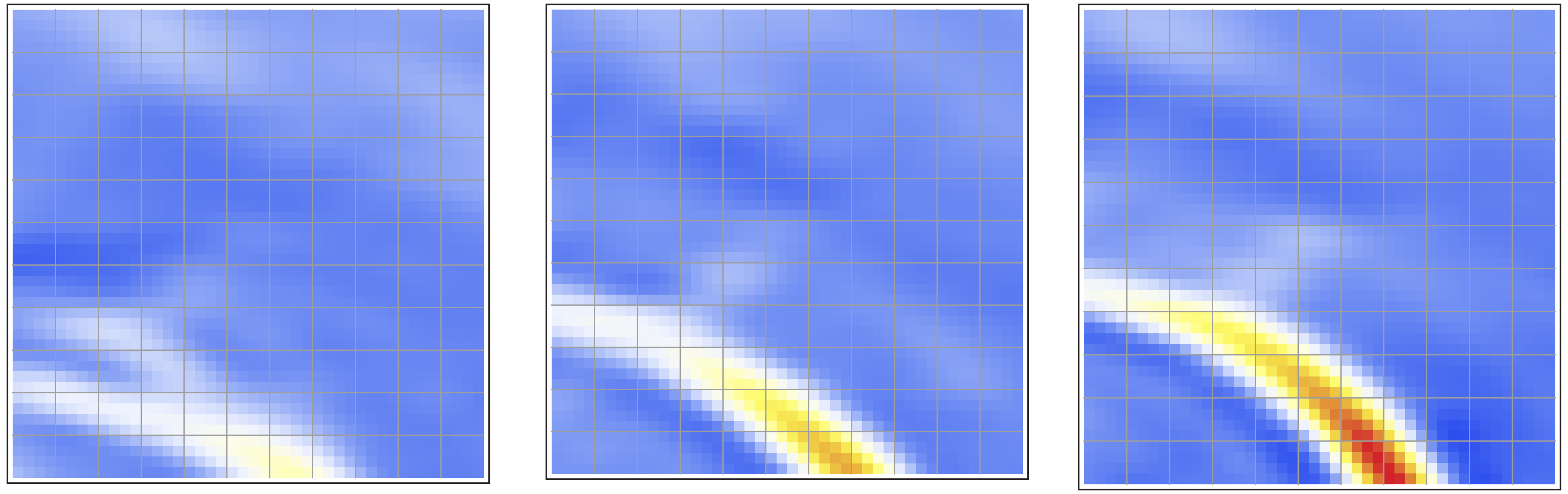

t-2 t-1 t

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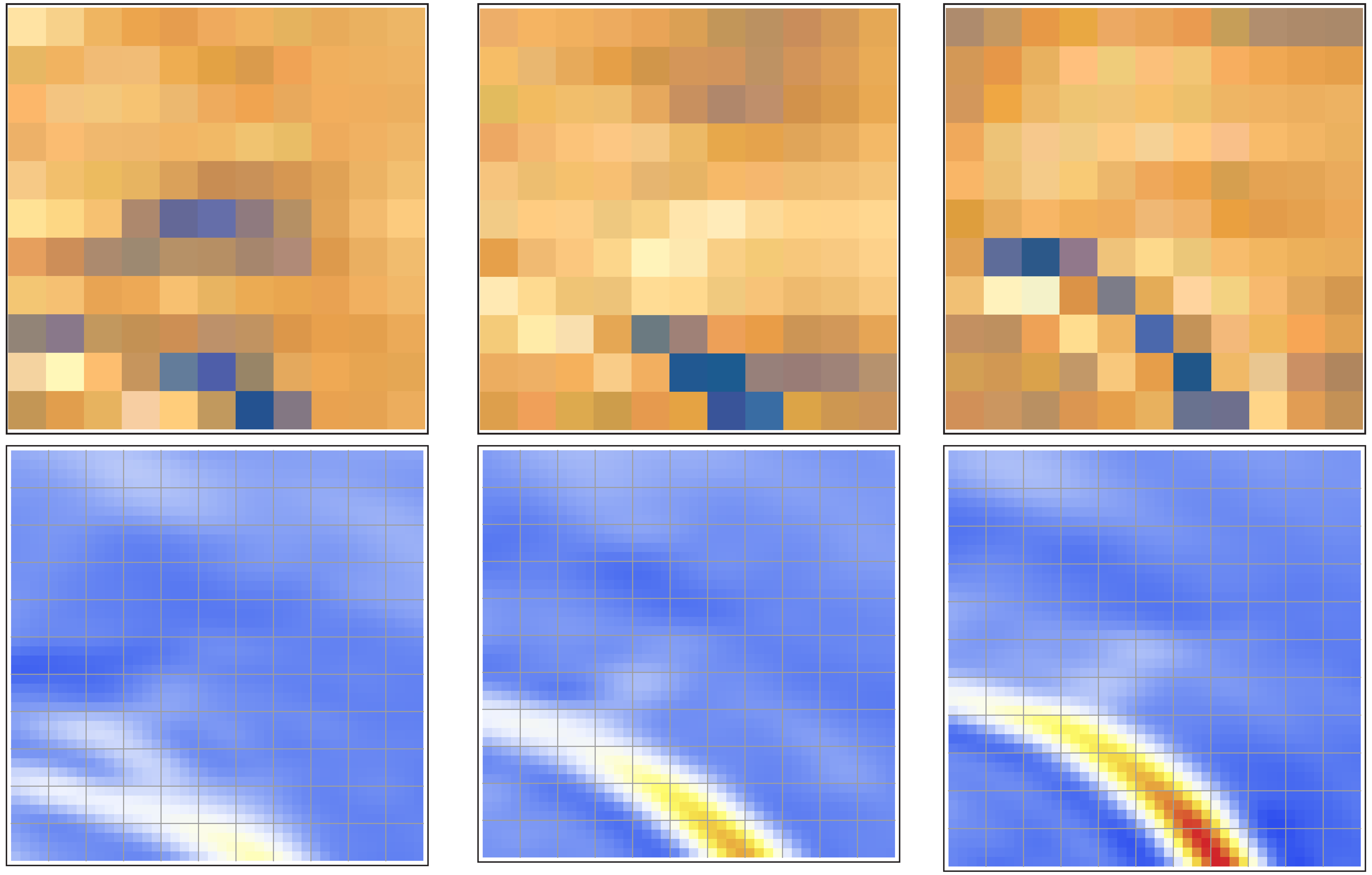

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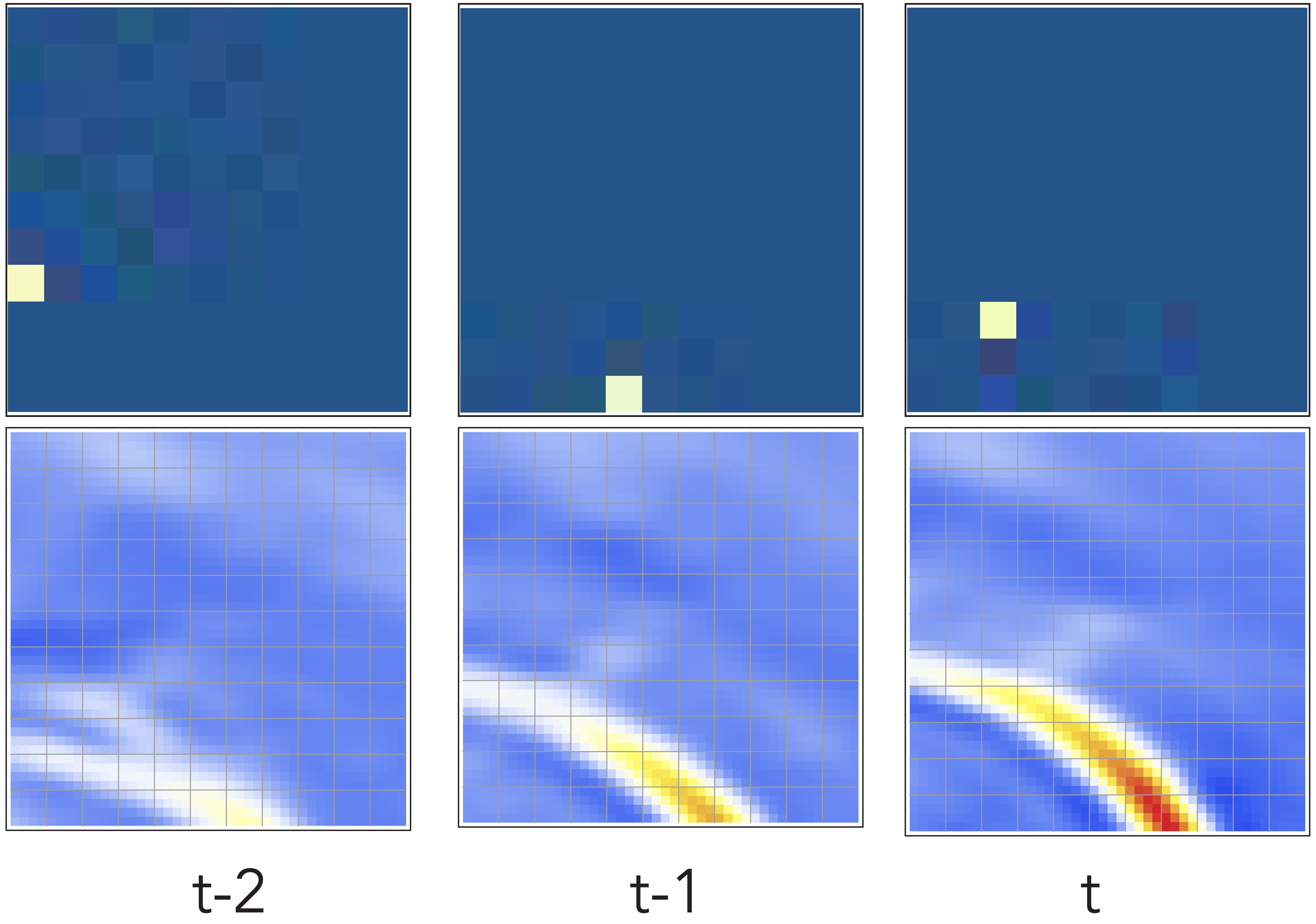

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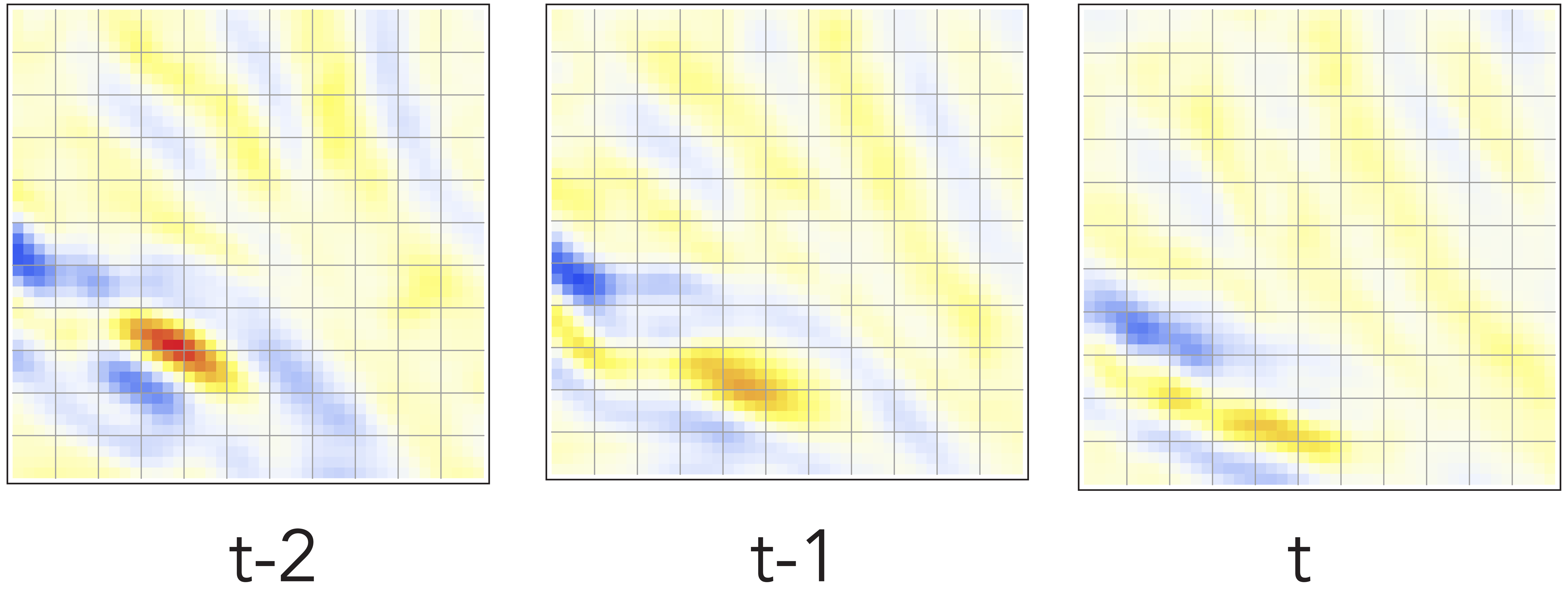

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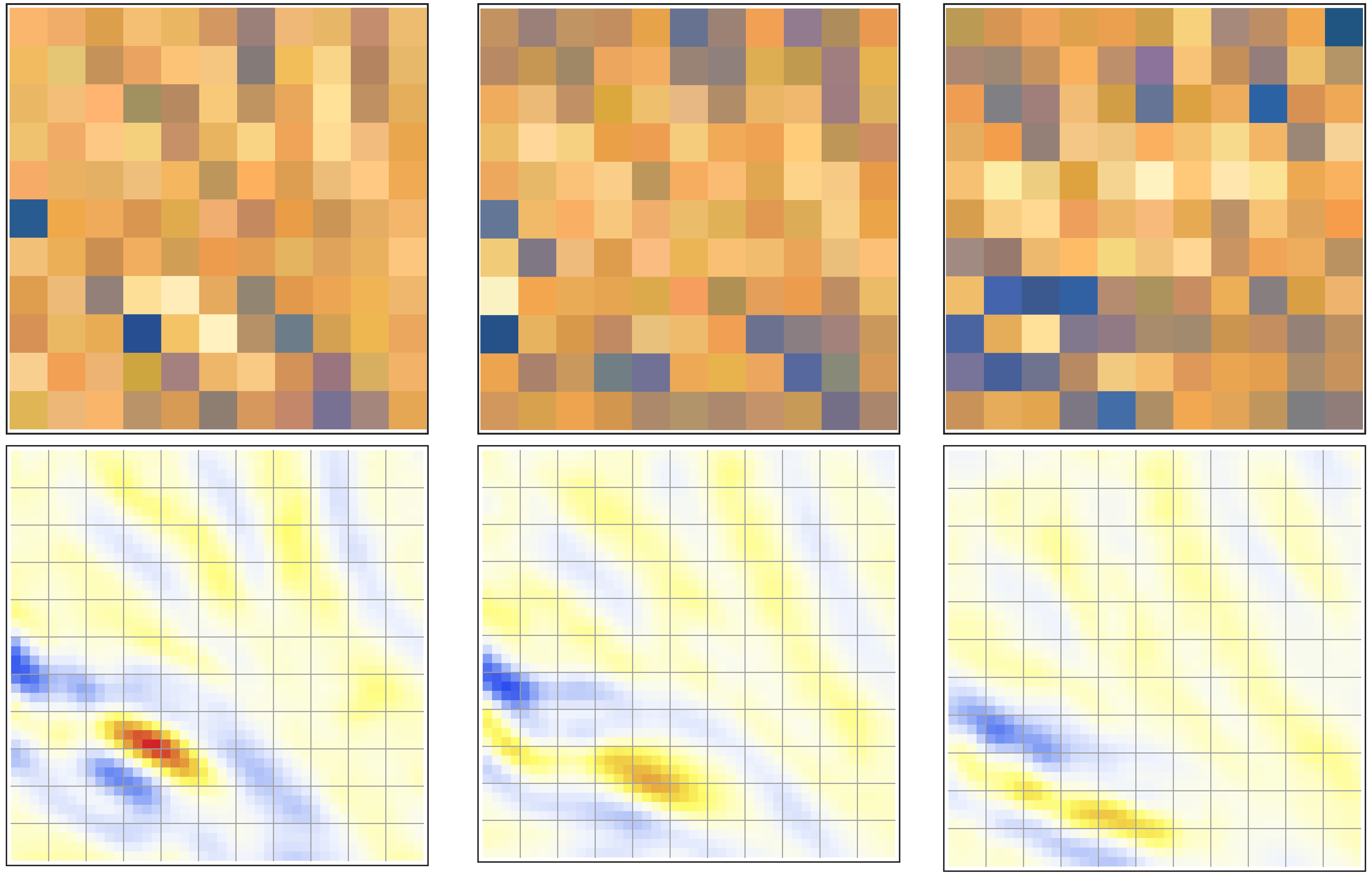

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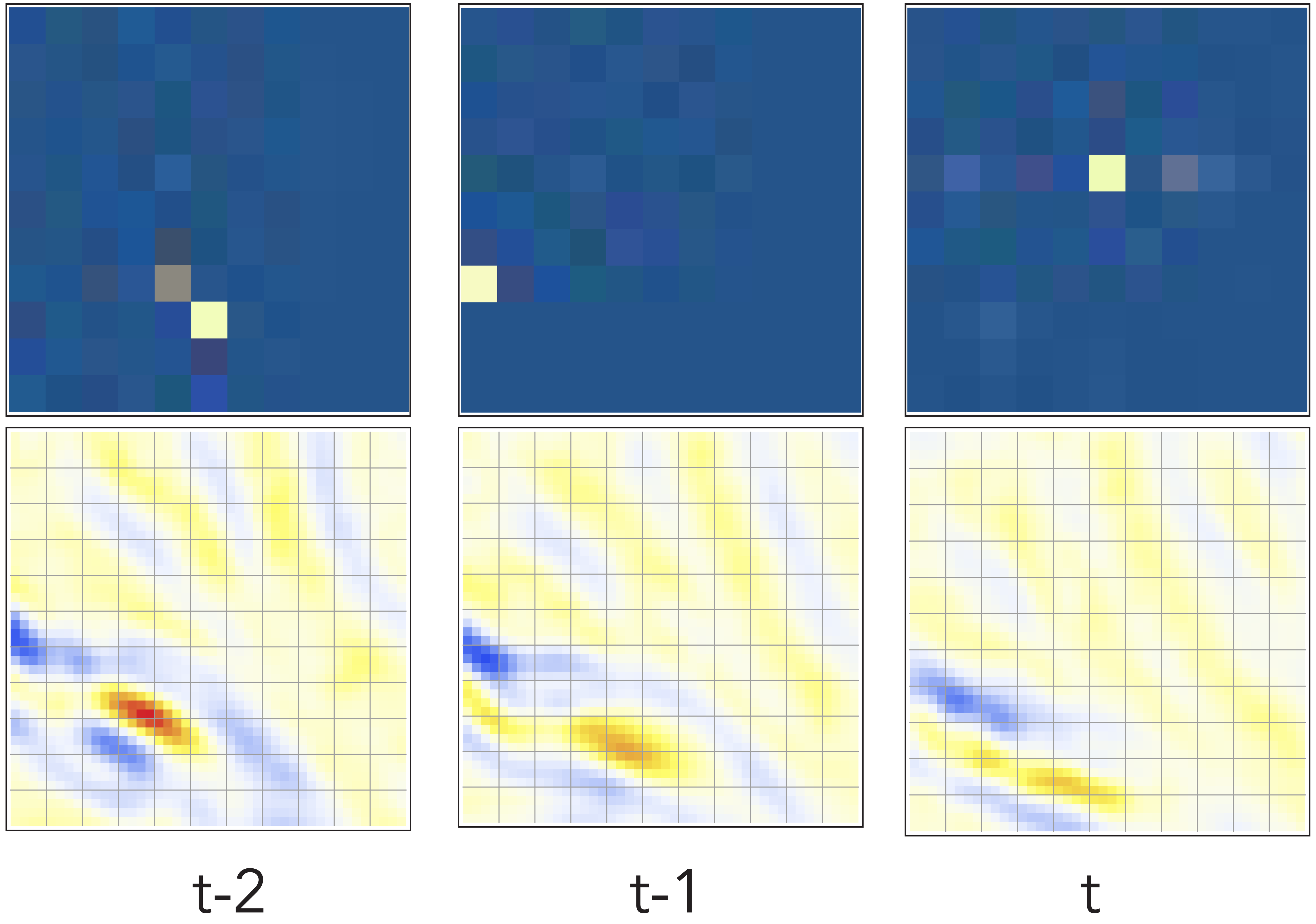

Physics and Learning?

- Scientific machine learning: use constraints from known models (e.g. symmetries) in the machine learning model

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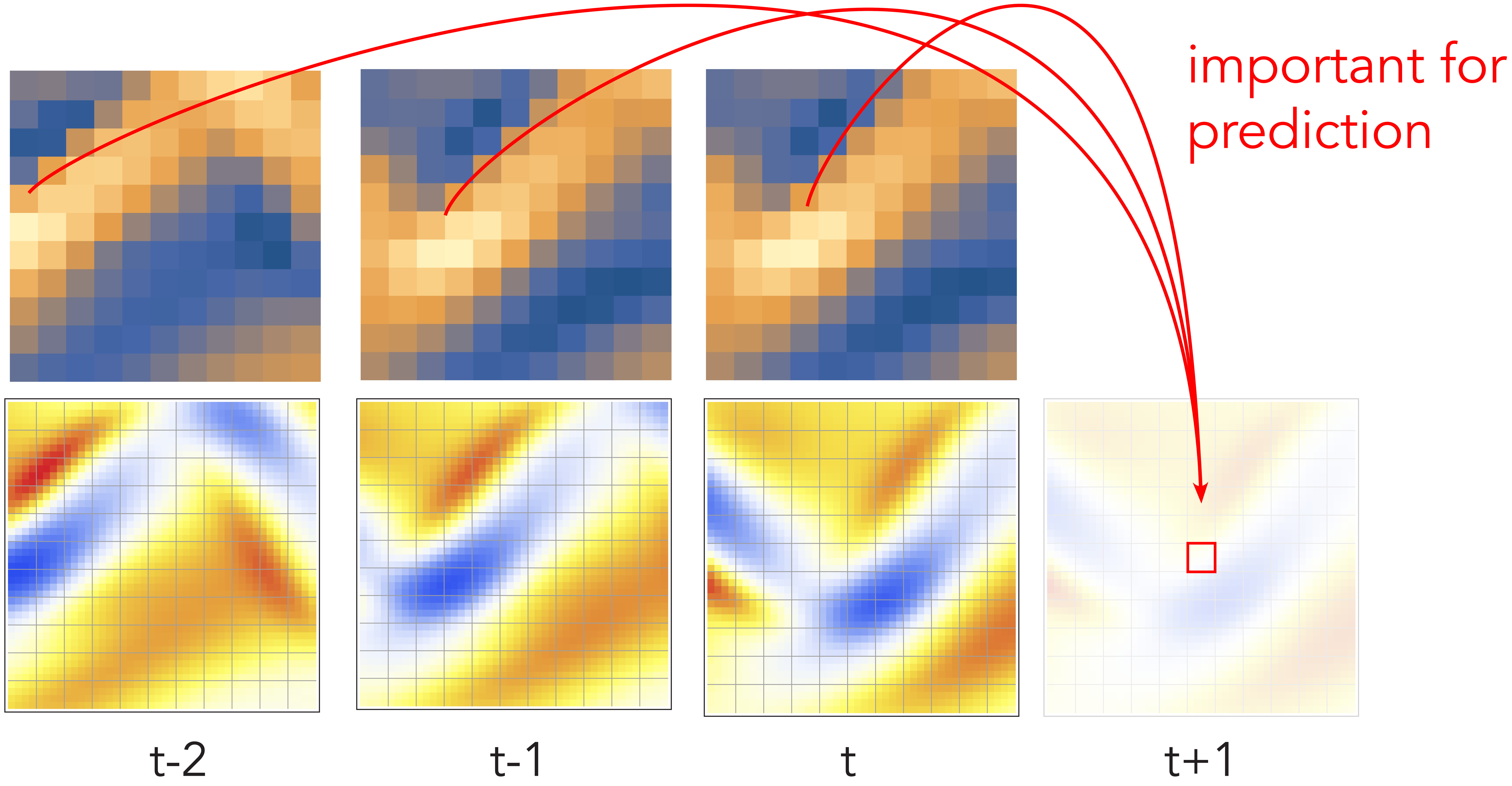
- Scientific machine learning: use constraints from known models (e.g. symmetries) in the machine learning model
- Observational data: avoid the (inductive) biases and constraints we have in our analytic models in the learning
- Use attention maps:
  - to ensure physical validity of learned models
  - to understand physical systems?

Physics and Learning?



AtmoRep

with Ilaria Luise, Maike Sonnewald, Martin Schultz, Aneesh Subramanian

Workshop of transformers in Earth sciences

- Organized with Martin Schultz, Maja Schneider, Clara Betancout, Michael Langguth
- Bring together machine learning experts and domains experts with some expertise and interest in attention-based neural networks and related concepts
- Mainly discussions, some talks
- 22/23 September, Magdeburg

Summary

- Self-supervised representation learnig offers great potential in the Earth sciences
  - Large amounts of unlabeled data (and fast growing)
  - Labeled data is scarce and difficult to obtain
- Representation learning has the potential to provide new insights into spatio-temporal interactions