Learning Similarity Metrics for Numerical Simulations

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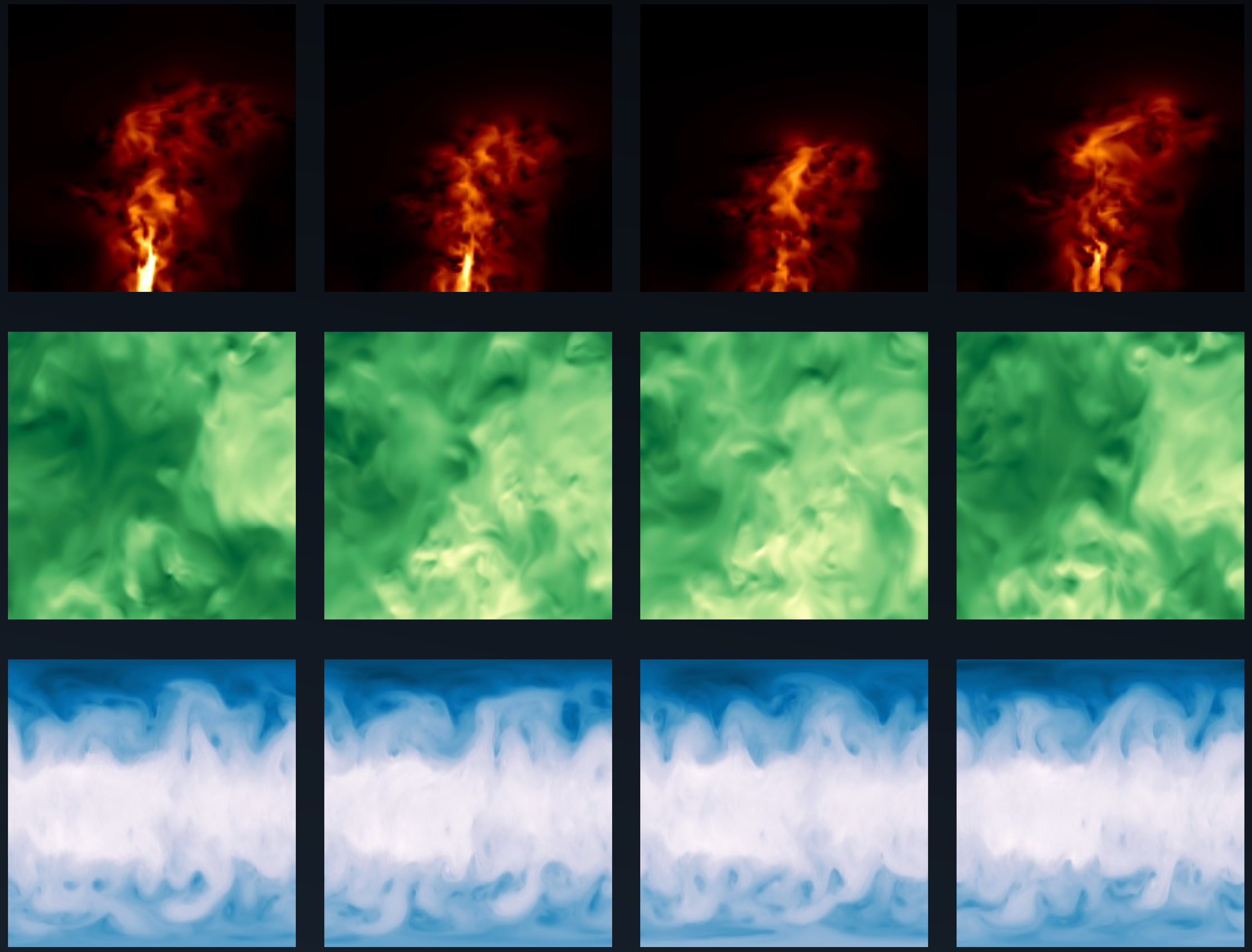
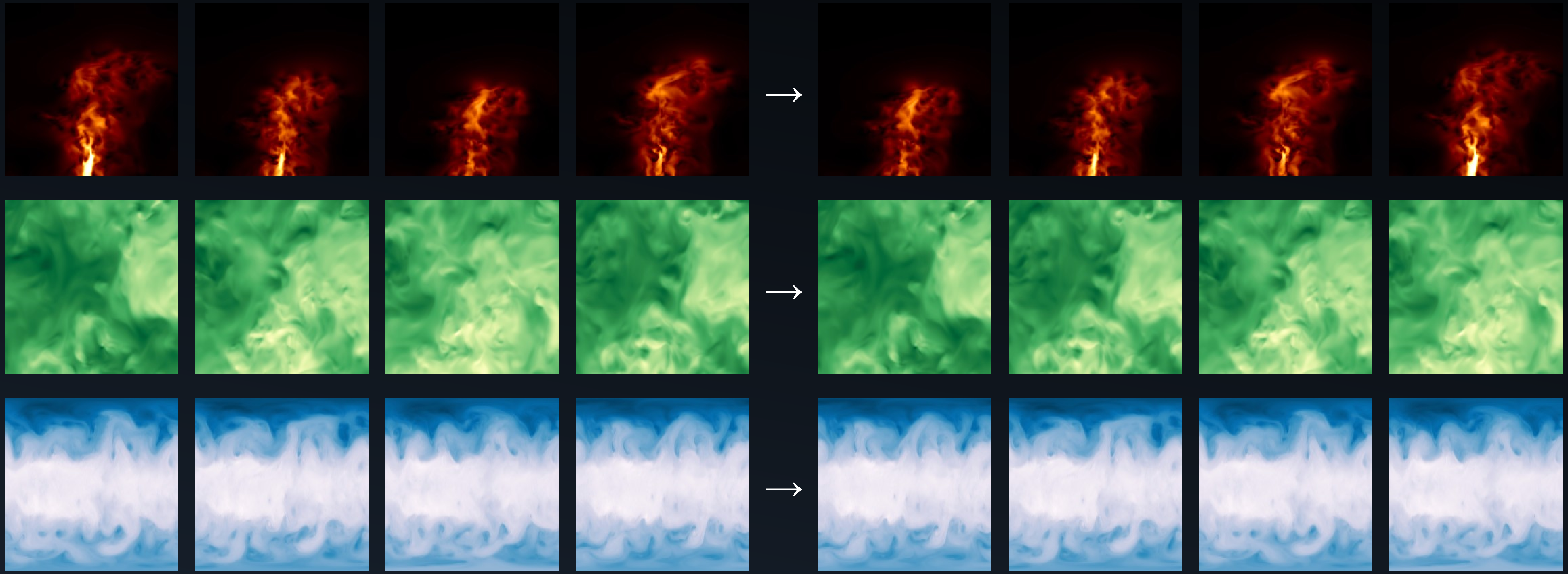
Overview – Motivation

Similarity assessment of scalar 2D simulation data from PDEs



Overview – Motivation

Similarity assessment of scalar 2D simulation data from PDEs

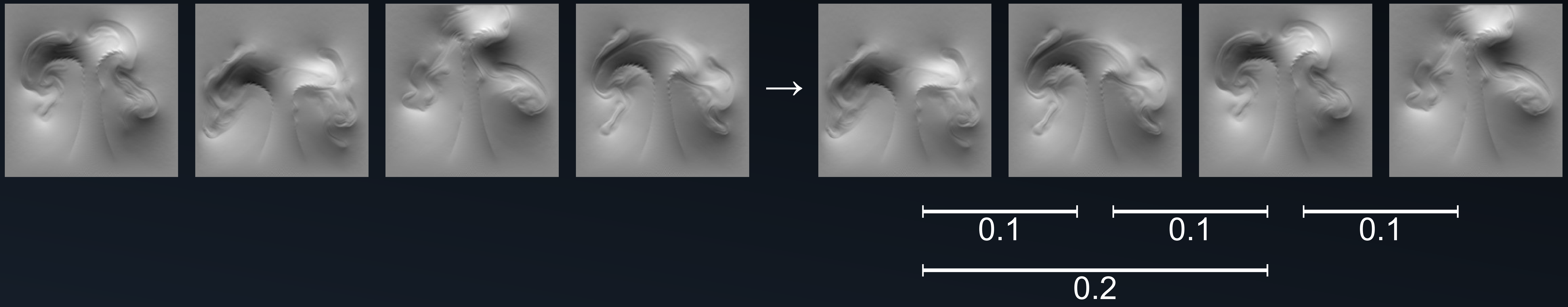


Overview – Motivation

Typical metrics like L^1 or L^2 operate locally → structures and patterns are ignored

Recognition of spatial contexts with CNNs

Mathematical metric properties should be considered



Overview – Method

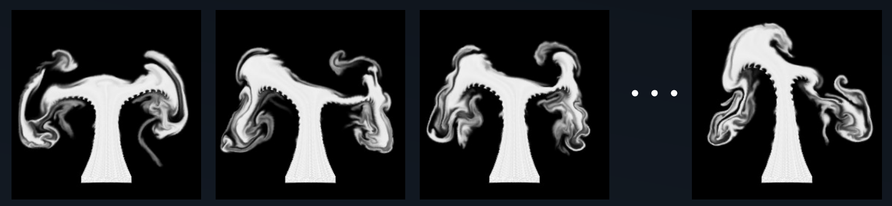
Numerical Simulation

$$\left[p_i \quad p_i{+}1\,\Delta_i \quad p_i{+}2\,\Delta_i \quad \cdots \quad p_i{+}10\,\Delta_i\right]$$

Initial condition varied in isolation

Variation defines

Simulation with PDE Solver

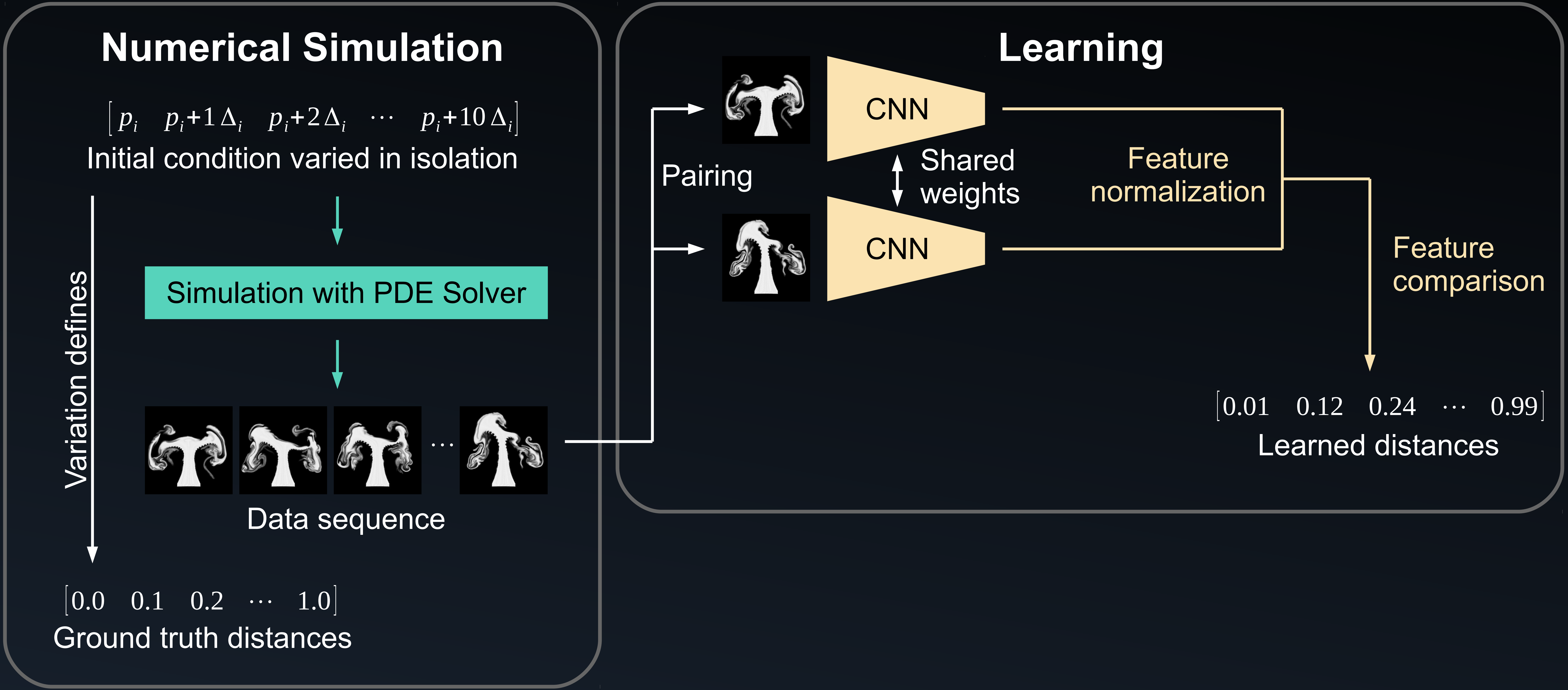


Data sequence

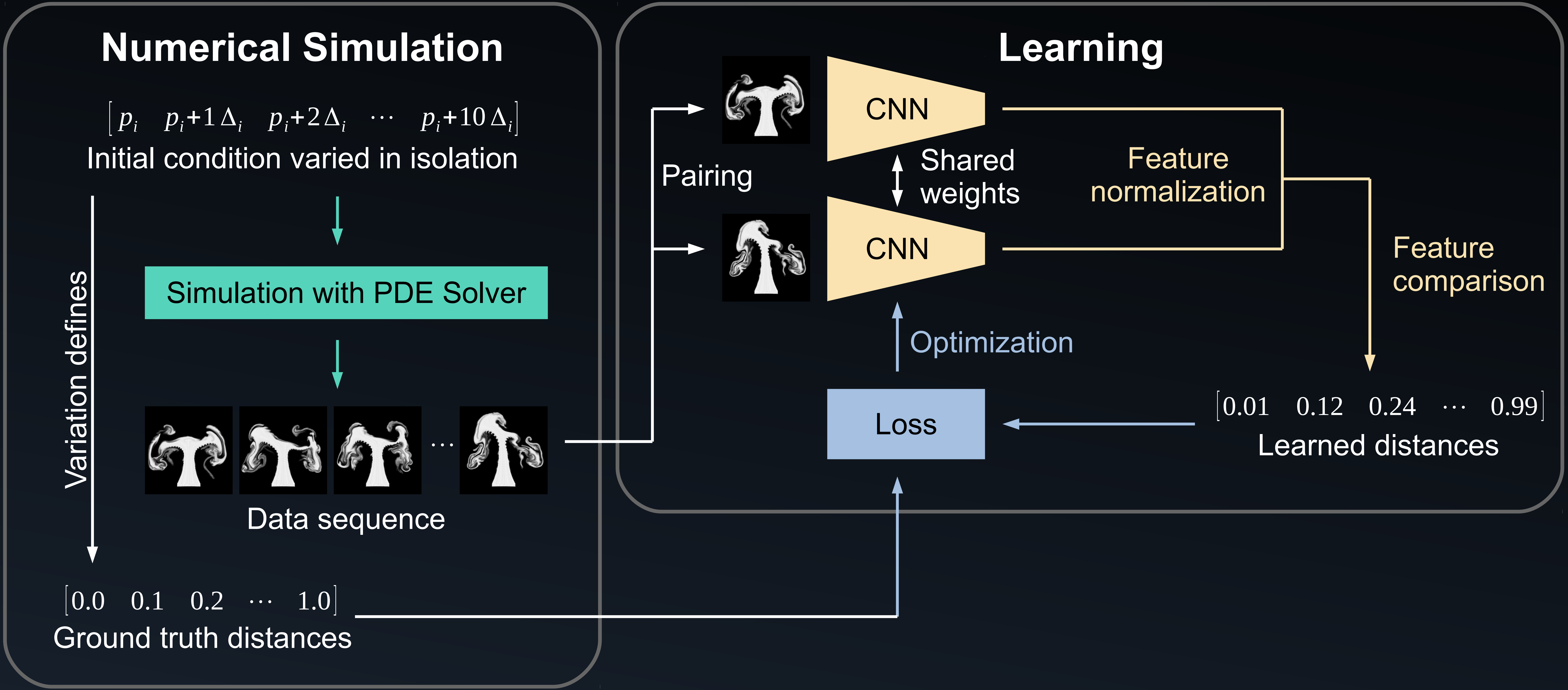
$$\left[0.0 \quad 0.1 \quad 0.2 \quad \cdots \quad 1.0\right]$$

Ground truth distances

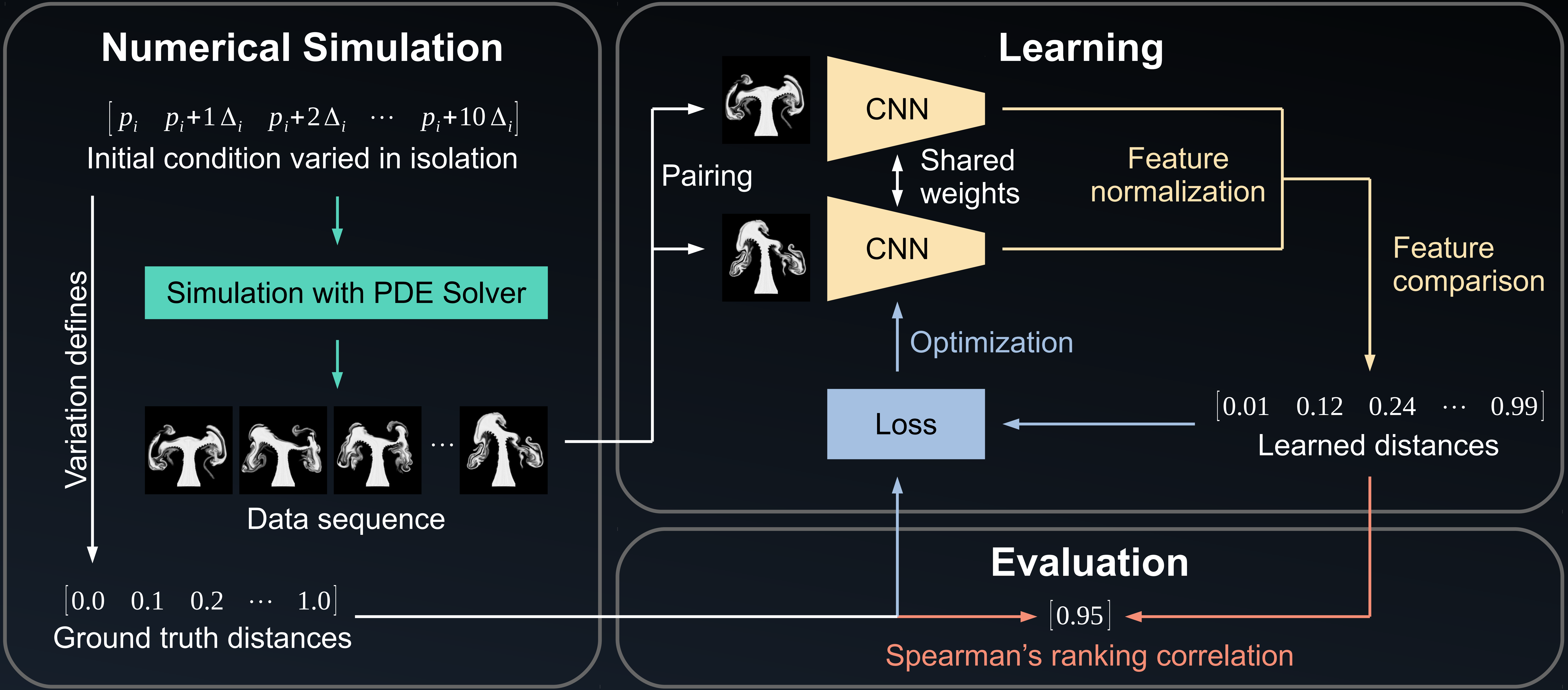
Overview – Method



Overview – Method



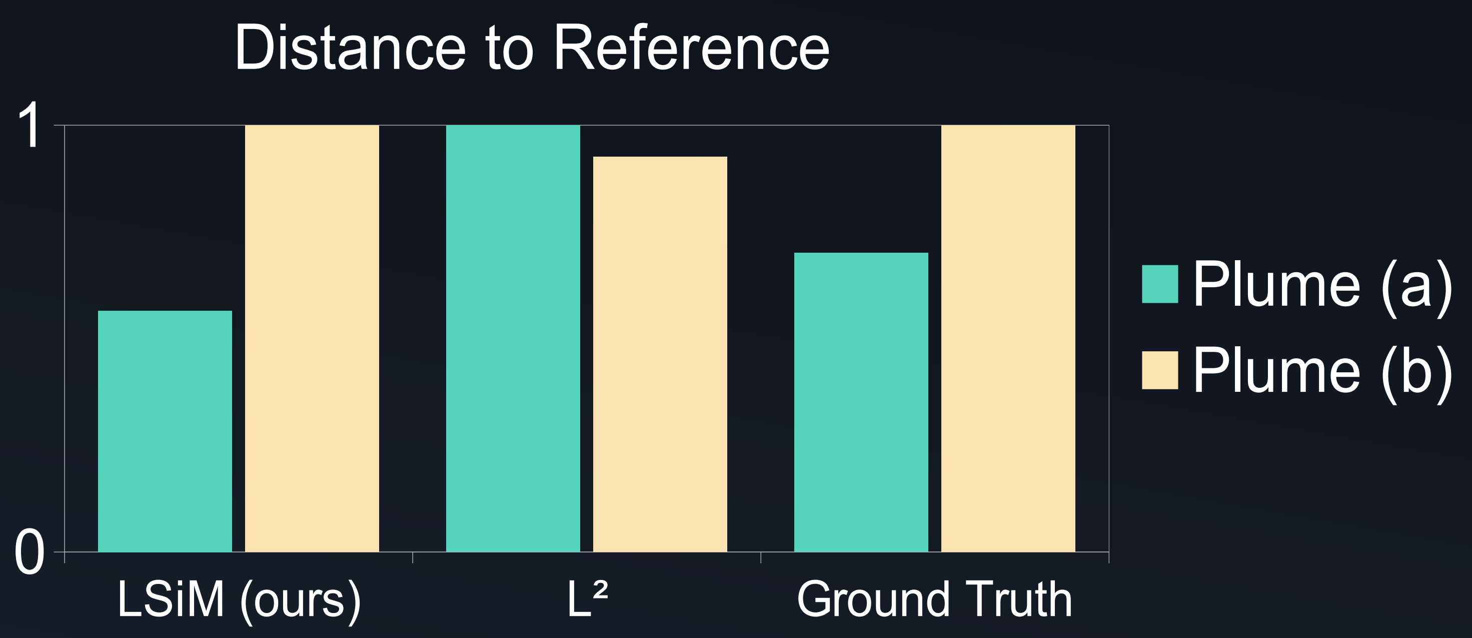
Overview – Method



Overview – Results

Single example: distance comparison

Plume (a) Reference Plume (b)



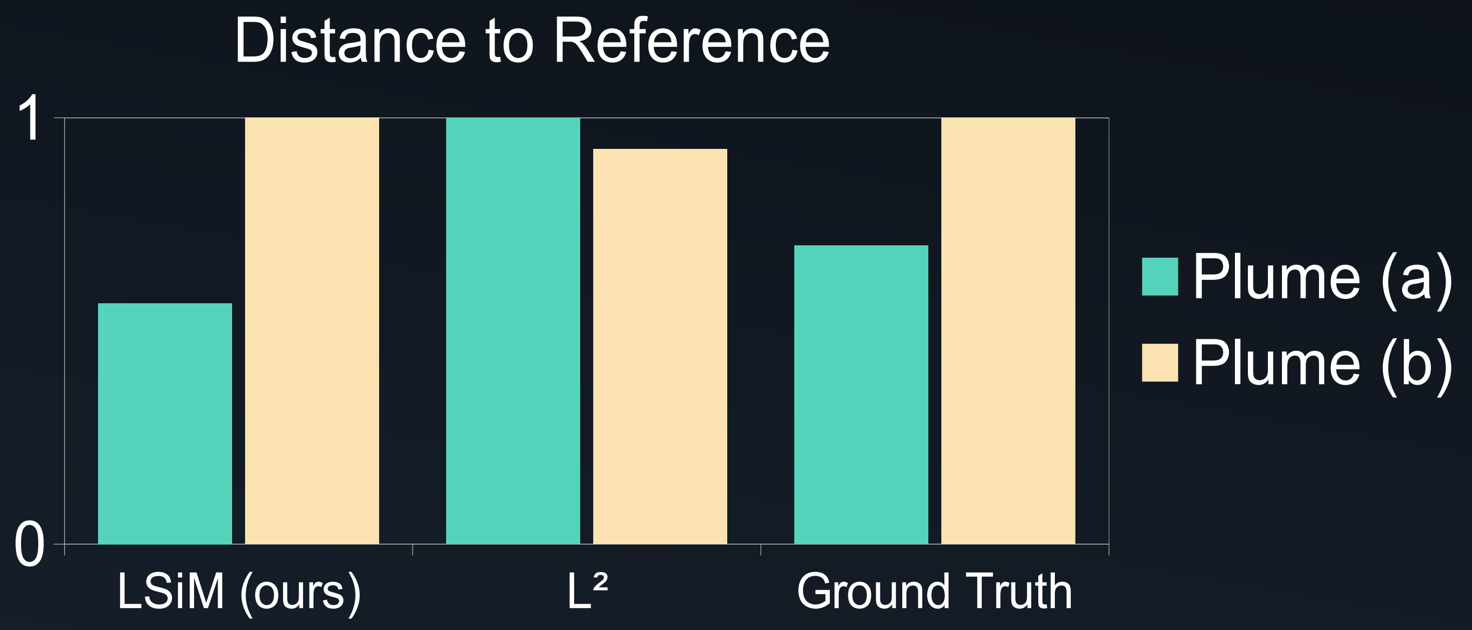
Overview – Results

Single example: distance comparison

Plume (a)

Reference

Plume (b)



Combined test data: correlation evaluation

Related Work

"Shallow" vector space metrics

- Metrics induced by L^p-norms, peak signal-to-noise ratio (PSNR)
- Structural similarity index (SSIM) [Wang04]

Evaluation with user studies for PDE data

- Liquid simulations [Um17]
- Non-oscillatory discretization schemes [Um19]

Image-based deep metrics with CNNs

- E.g. learned perceptual image patch similarity (LPIPS) [Zhang18]

[Wang04] Wang, Bovik, Sheikh, and Simoncelli. Image quality assessment: From error visibility to structural similarity. *IEEE Transactions on Image Processing*, 2004
[Um17] Um, Hu, and Thuerey. Perceptual Evaluation of Liquid Simulation Methods. *ACM Transactions on Graphics*, 2017
[Um19] Um, Hu, Wang, and Thuerey. Spot the Difference: Accuracy of Numerical Simulations via the Human Visual System. *CoRR, abs/1907.04179*, 2019
[Zhang18] Zhang, Isola, Efros, Shechtman, and Wang. The Unreasonable Effectiveness of Deep Features as a Perceptual Metric. *CVPR*, 2018

Data Generation

Time depended, motion-based PDE with one varied initial condition

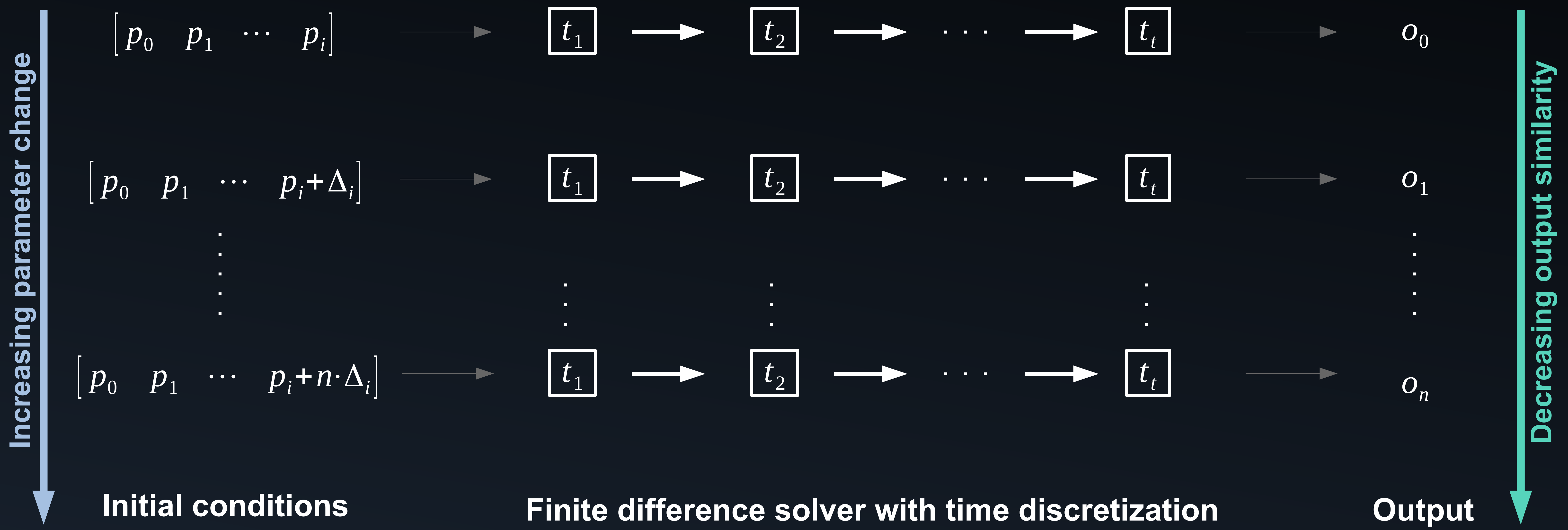
Initial conditions

Finite difference solver with time discretization

Output

Data Generation

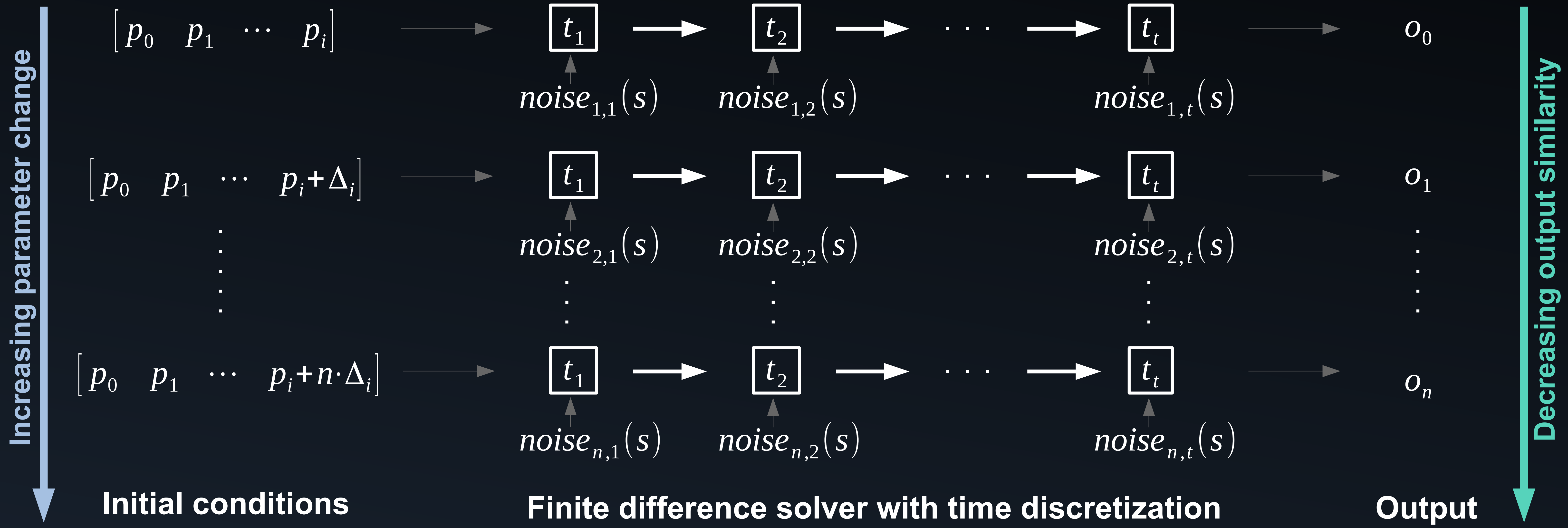
Time depended, motion-based PDE with one varied initial condition



Data Generation

Time depended, motion-based PDE with one varied initial condition

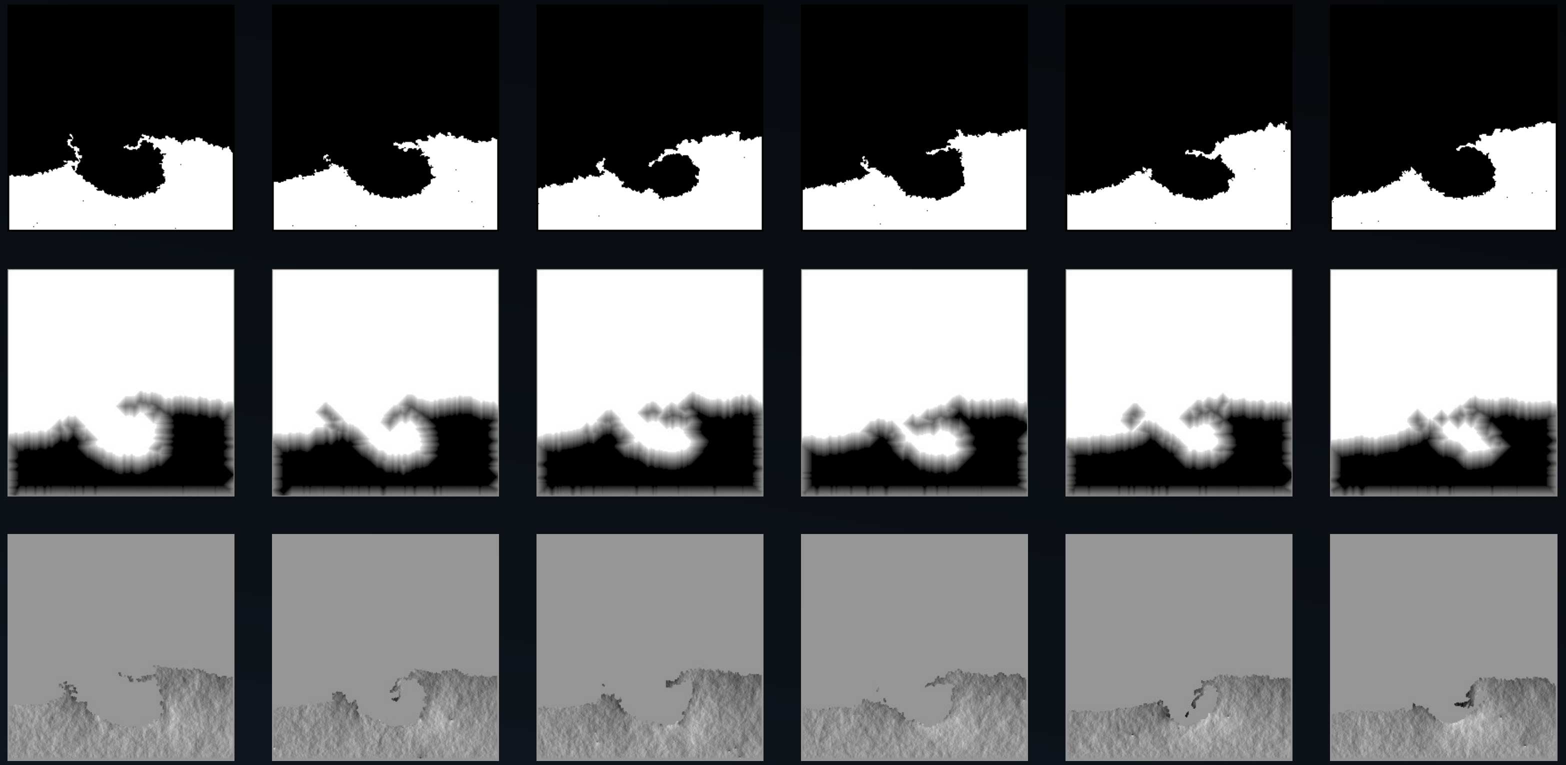
Chaotic behavior in controlled environment → added noise to adjust data difficulty



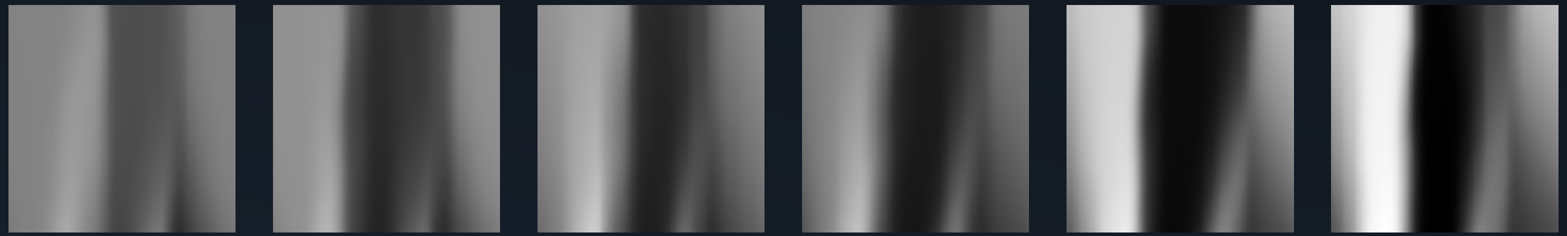
Training Data

Eulerian smoke plume

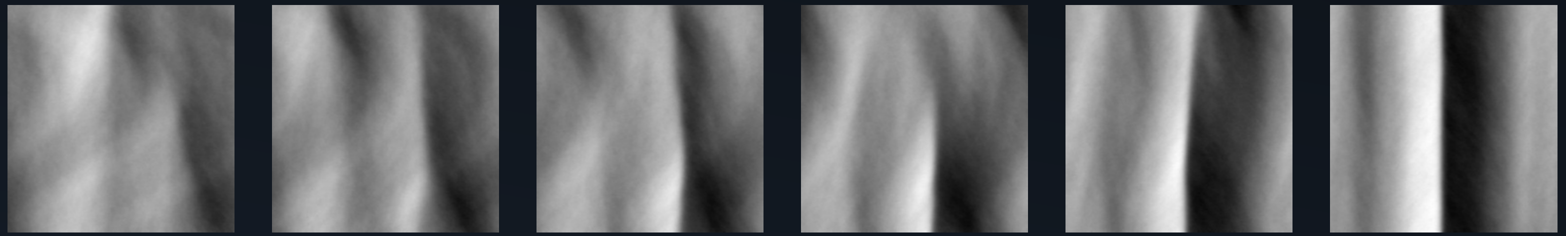
Liquid via FLIP [Zhu05]



Advection-diffusion transport



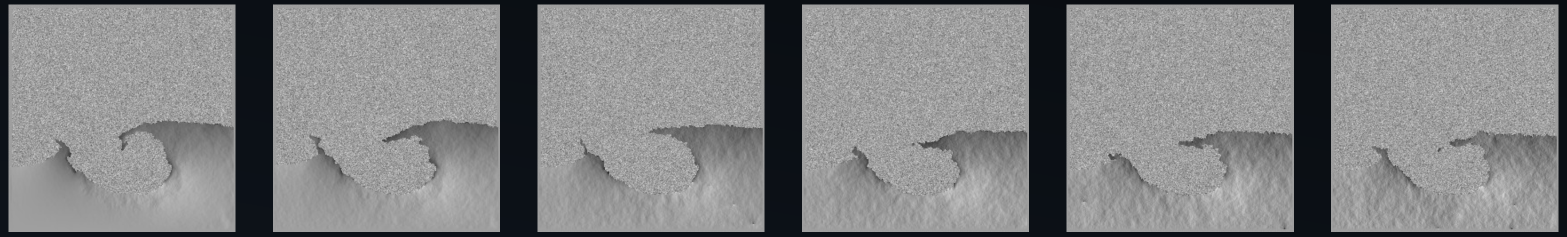
Burger’s equation



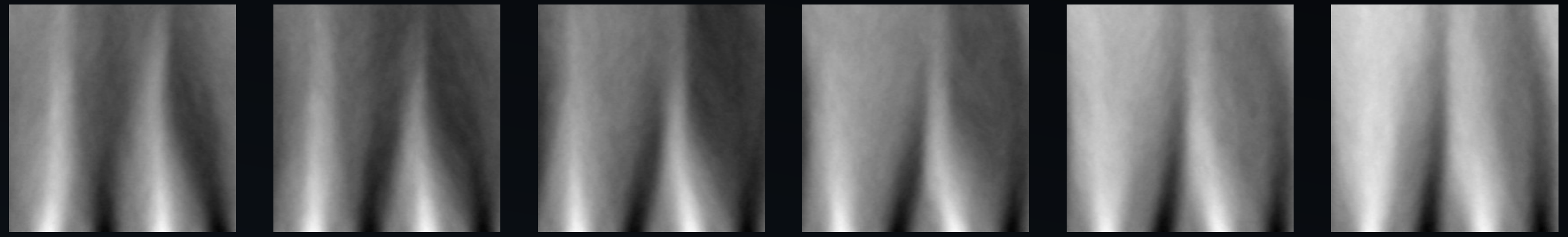
[Zhu05] Zhu and Bridson. Animating sand as a fluid. *ACM SIGGRAPH*, 2005

Test Data

Liquid (background noise)



Advection-diffusion transport (density)



Shape data

Video data

TID2013 [Ponomarenko15]

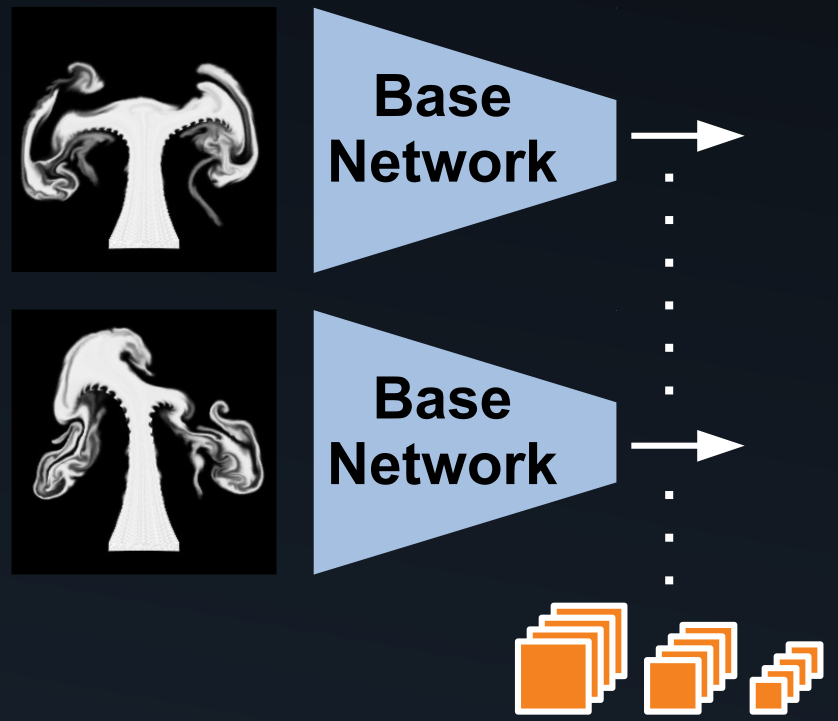
[Ponomarenko15] Ponomarenko, Jin, Ieremeiev, et al. Image database TID2013: Peculiarities, results and perspectives. *Signal Processing-Image Communication*, 2015

Method – Base Network

Siamese architecture (shared weights) → Convolution + ReLU layers

Feature extraction from both inputs

Existing network possible → specialized model works better

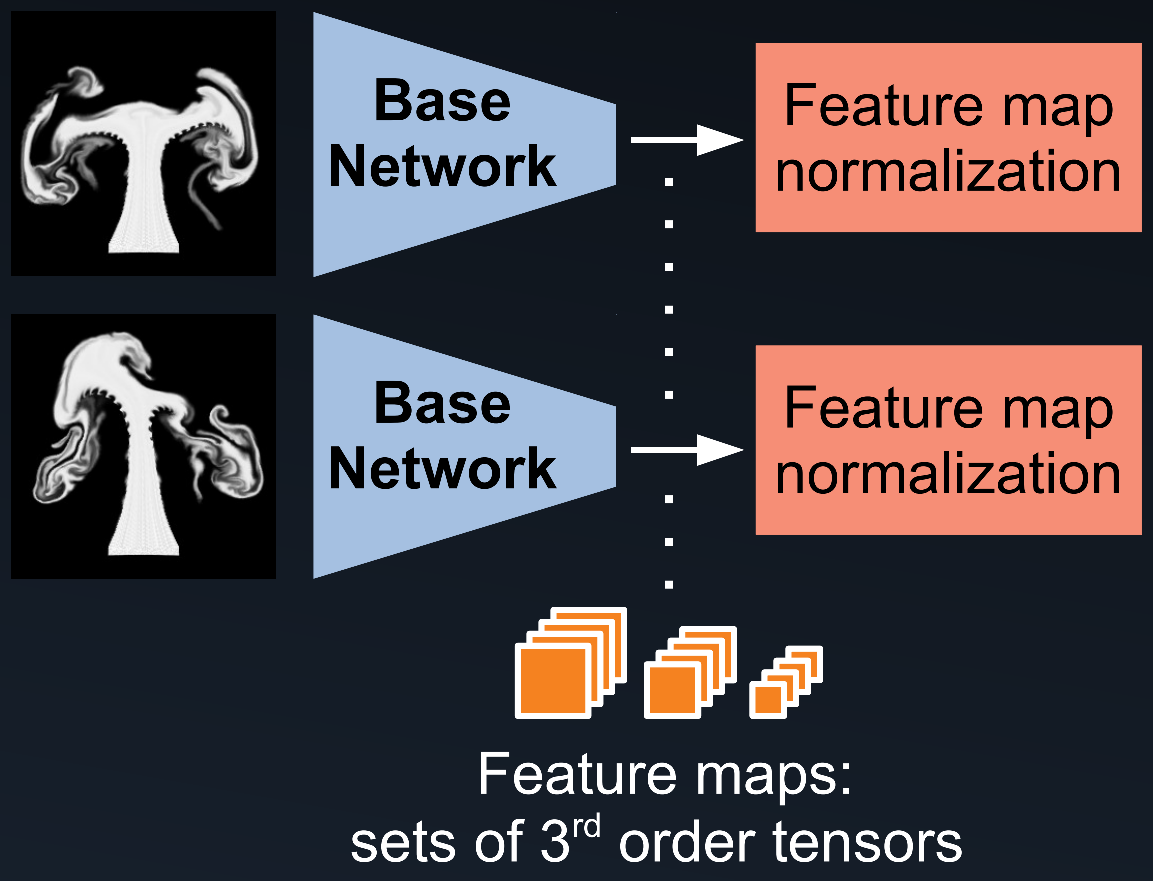


Feature maps:
sets of 3rd order tensors

Method – Feature Normalization

Adjust value range of feature vectors along channel dimension

- Unit length normalization → cosine distance (only angle comparison)
- Element-wise std. normal distribution → angle and length in global length distribution

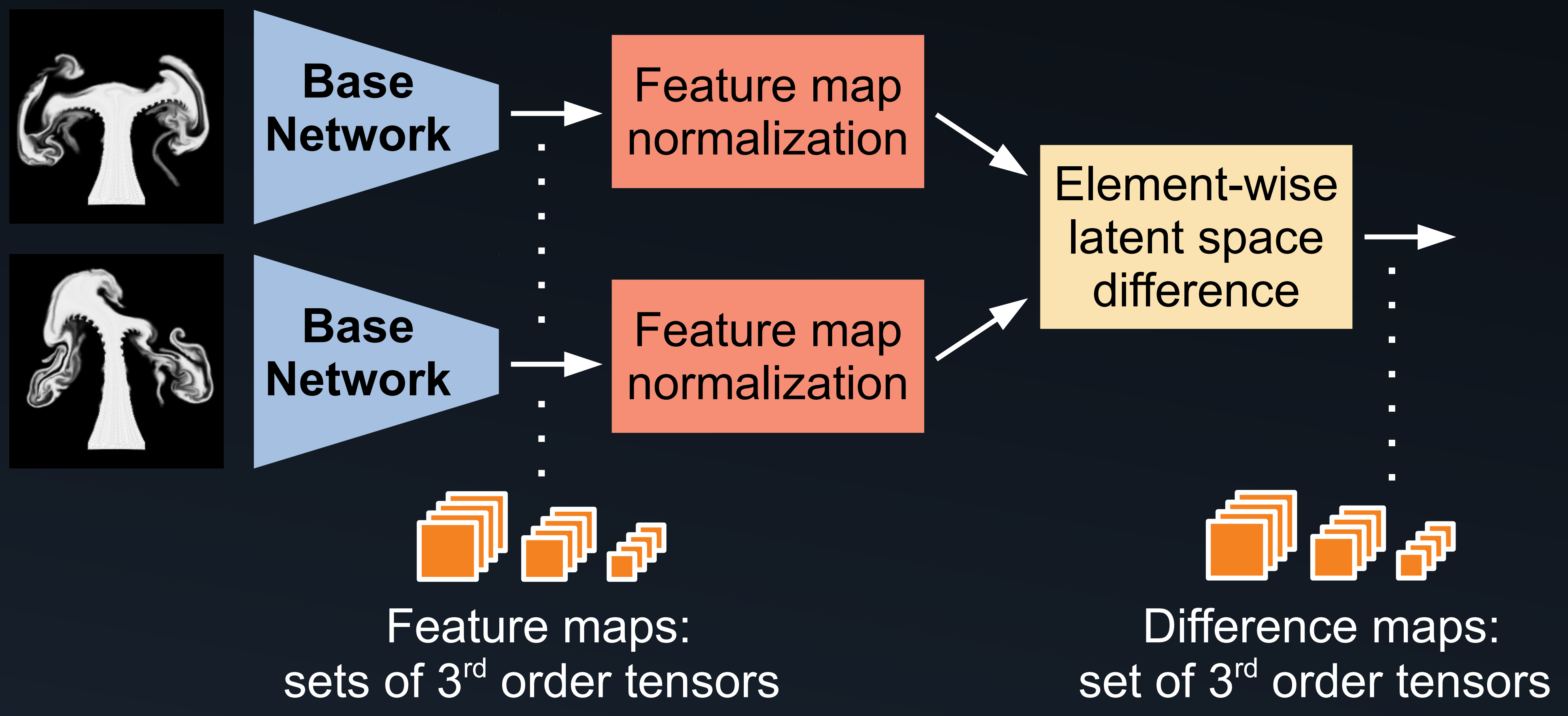


Method – Latent Space Difference

Actual comparison of feature maps → element-wise distance

Must be a metric w.r.t. the latent space → ensure metric properties

$|\tilde{x} - \tilde{y}|$ or $(\tilde{x} - \tilde{y})^2$ are useful options

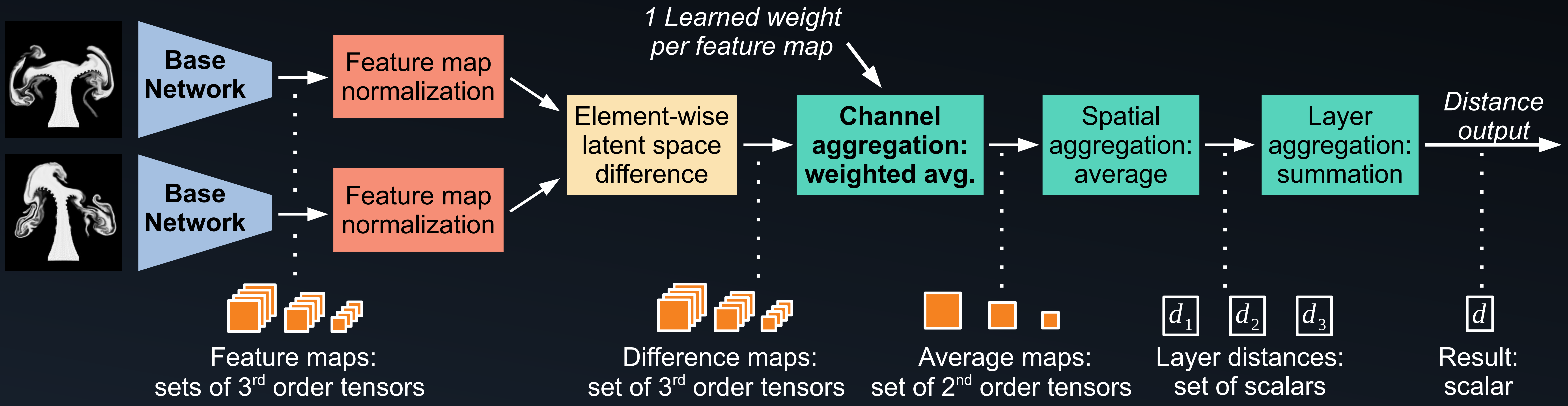


Method – Aggregations

Compression of difference maps to scalar distance prediction

Learned channel aggregation via weighted average

Simple aggregations with sum or average



Loss Function

Ground truth distances *c* and predicted distances *d*

$$L(c,d) = \lambda_1 (c-d)^2 + \lambda_2 \left(1 - \frac{(c-\bar{c})\cdot(d-\bar{d})}{\|c-\bar{c}\|_2 \, \|d-\bar{d}\|_2}\right)$$

Mean squared error term → minimize distance deviation directly

Inverted correlation term → maximize linear distance relationship

Results

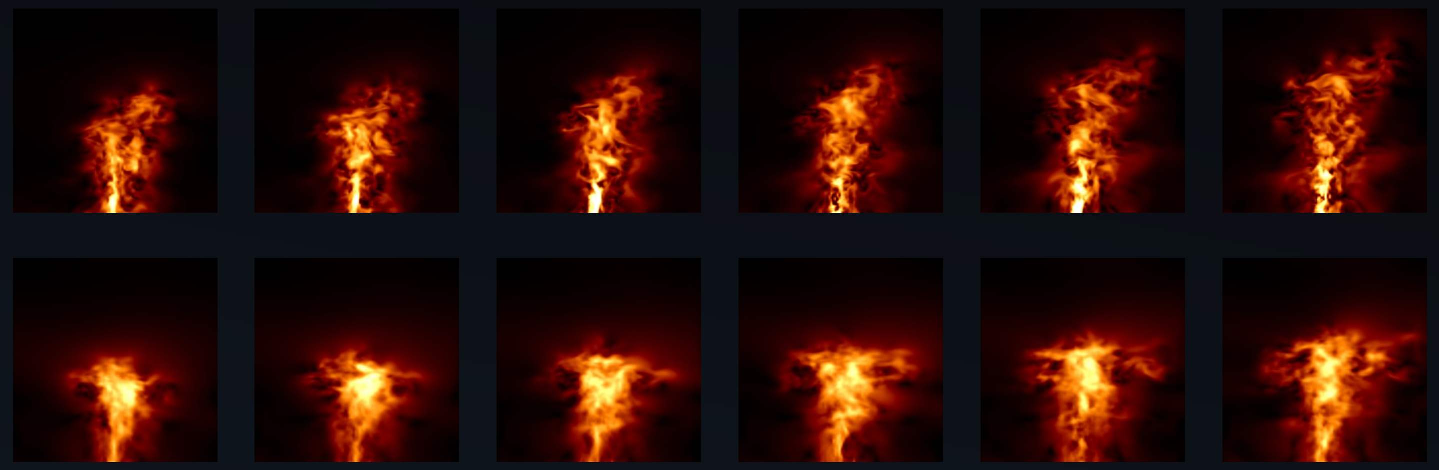
Evaluation with Spearman's rank correlation

Ground truth against predicted distances

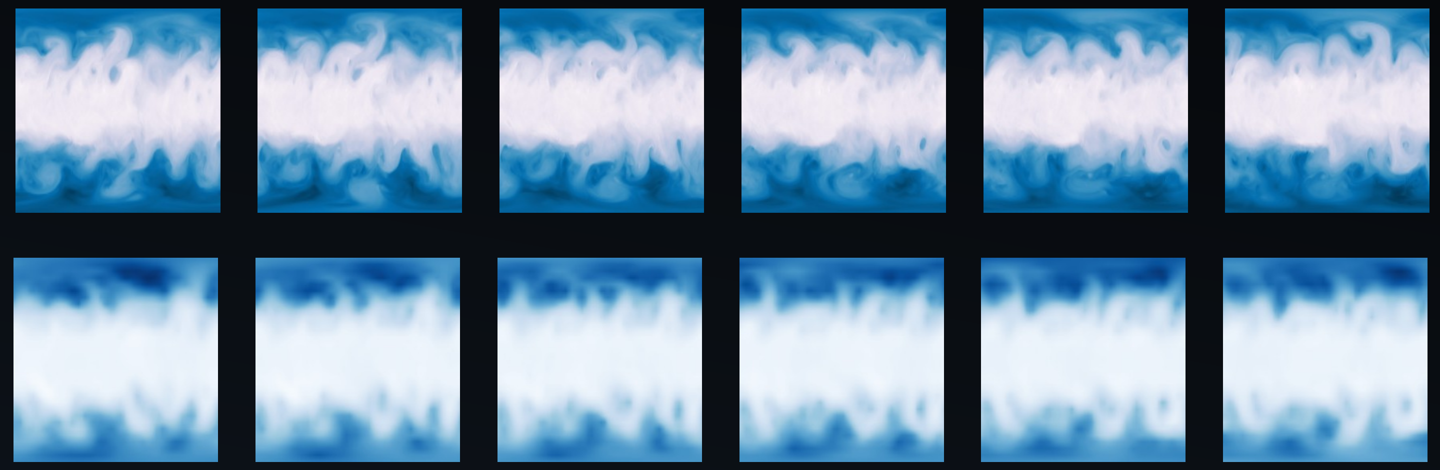
Metric	Validation data sets				Test data sets					
	Smo	*Liq*	*Adv*	*Bur*	*TID*	*LiqN*	*AdvD*	*Sha*	*Vid*	*All*
L^2	0.66	0.80	0.74	*0.62*	0.82	0.73	*0.57*	0.58	0.79	0.61
SSIM	0.69	0.74	0.77	0.71	*0.77*	*0.26*	**0.69**	*0.46*	*0.75*	*0.53*
LPIPS	*0.63*	*0.68*	*0.68*	0.72	**0.86**	0.50	0.62	0.84	**0.83**	0.66
LSiM	**0.78**	**0.82**	**0.79**	**0.75**	0.86	**0.79**	0.58	**0.88**	0.81	**0.73**

Real-world Evaluation

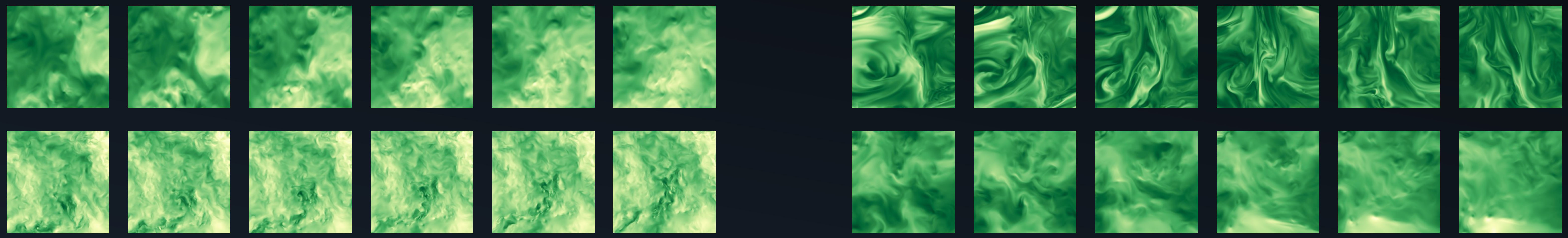
ScalarFlow [Eckert19]



WeatherBench [Rasp20]



Johns Hopkins Turbulence Database (JHTDB) [Perlman07]



[Eckert19] Eckert, Um, and Thuerey. Scalarflow: A large-scale volumetric data set of real-world scalar transport flows [...]. *ACM Transactions on Graphics*, 2019
[Rasp20] Rasp, Dueben, Scher, Weyn, Mouatadid, and Thuerey. Weatherbench: A benchmark dataset for data-driven weather forecasting. *CoRR, abs/2002.00469, 2020*
[Perlman07] Perlman, Burns, Li, and Meneveau. Data exploration of turbulence simulations using a database cluster. *ACM/IEEE Conference on Supercomputing*, 2007

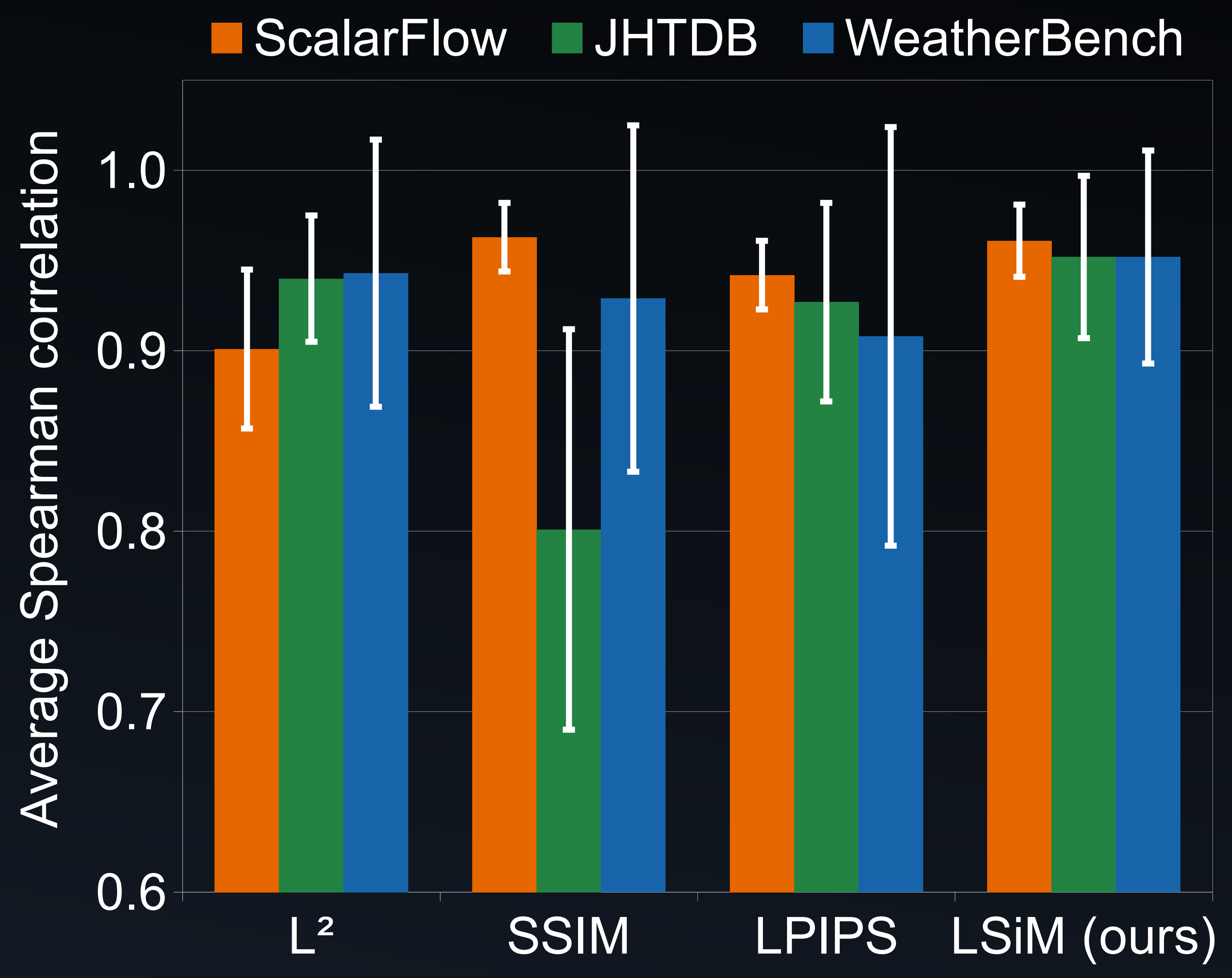
Real-world Evaluation

Retrieve order of spatial and temporal frame translations

Six interval spacings per data repository

180-240 sequences each

Mean and standard deviation over correlation of each spacing



Future Work

Accuracy assessment of new simulation methods

Parameter reconstructions of observed behavior

Guiding generative models of physical systems

Extensions to other data

- 3D flows and further PDEs
- Multi-channel turbulence data

Thank you for your attention!

Join the live-sessions for questions and discussion

Source code available at https://github.com/tum-pbs/LSIM