

 **ATLAS**
EXPERIMENT
Candidate Event:
 $pp \rightarrow H(\rightarrow bb) + W(\rightarrow \mu\nu)$
Run: 338712 Event: 335908183
2017-10-19 23:31:18 CEST

Advanced Topics: Quantum computing & ML in other scientific domains

Lecture 5

Sofia Vallecorsa | Ilaria Luise

Thematic CERN School of Computing on Machine Learning
18th October 2024

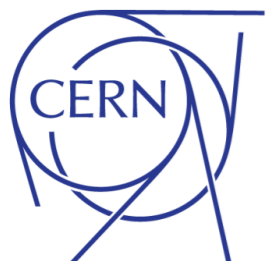


Table of Content

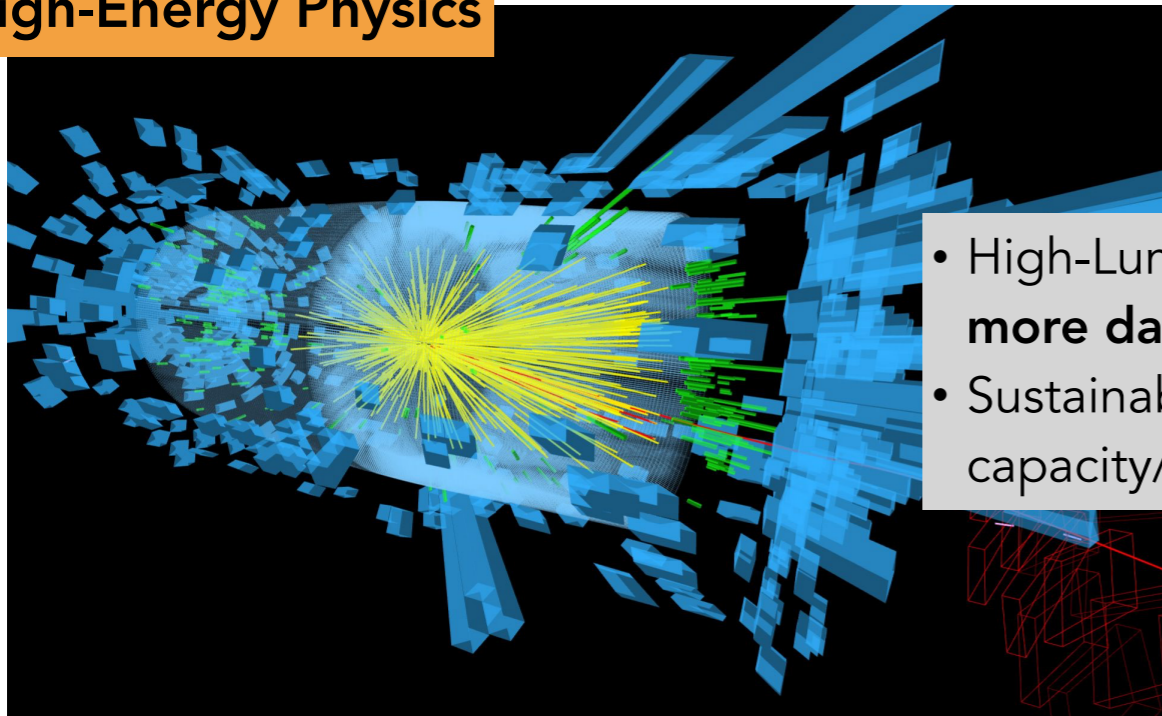
Foundation models for science: AtmoRep
Quantum Machine Learning

Weather and climate

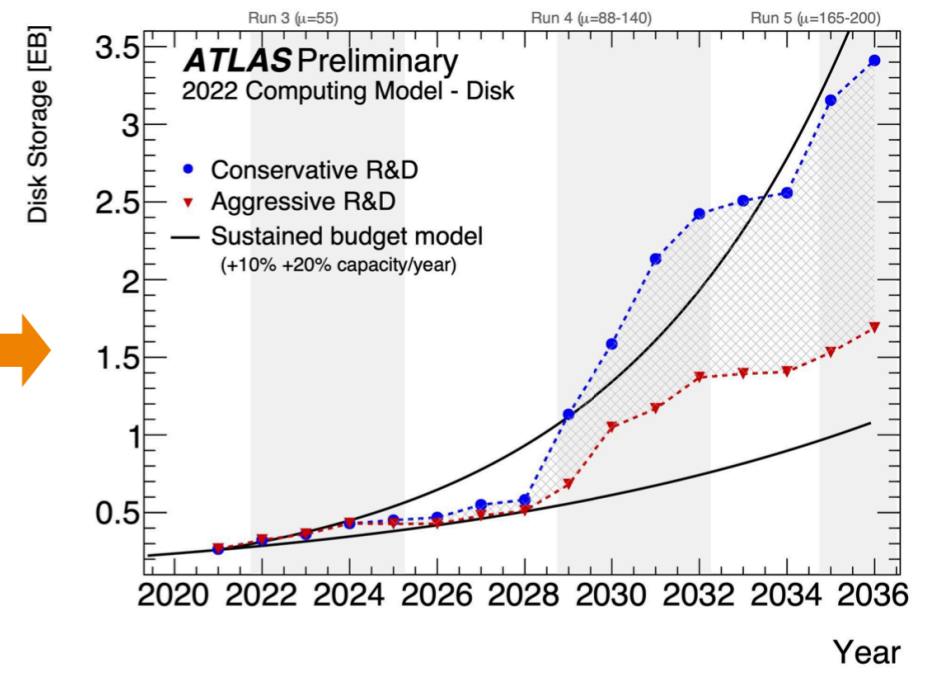
The AI revolution in weather and climate

The future of observational data

High-Energy Physics



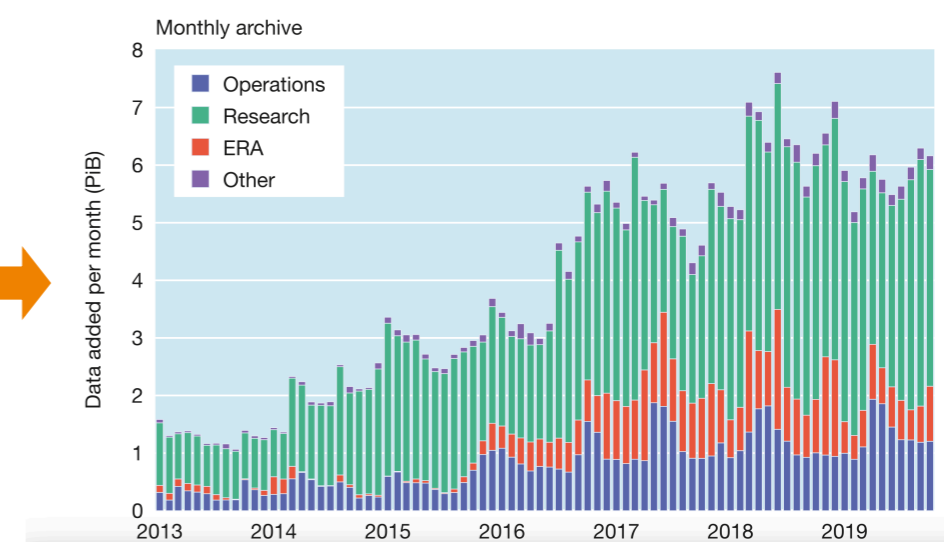
- High-Lumi LHC: **6 times more data by 2030**
- Sustainable model +20% capacity/year



Earth System science



- ESA's MetOp-SG satellite: **864 GB/day**
- ERA5: **6+ PB**



Need to find sustainable ways to store all these data

The first breakthrough: weather & climate

Large datasets:

First time that an AI-model trained on TBs of pre-processed observations outperforms the numerical models for a 10 day forecasts

Review Article | Published: 02 September 2015

The quiet revolution of numerical weather prediction

Peter Bauer, Alan Thorpe & Gilbert Brunet

Nature 525, 47–55 (2015) | Cite this article

48k Accesses | 1239 Citations | 1116 Altmetric | Metrics

Perspective | Published: 22 February 2021

The digital revolution of Earth-system science

Peter Bauer, Peter D. Dueben, Torsten Hoefler, Tiago Quintino, Thomas C. Schulthess & Nils P. Wedi

Nature Computational Science 1, 104–113 (2021) | Cite this article

18k Accesses | 94 Citations | 300 Altmetric | Metrics

Forecasting Global Weather

The AI revolution in weather and climate modeling

Abstract

We present a data-driven approach for forecasting global weather using graph neural networks. The system learns to step forward the current 3D atmospheric state by six hours, and multiple steps are chained together to produce skillful forecasts going out several days into the future. The underlying model is trained on reanalysis data from ERA5 or forecast data from GFS. Test performance on metrics such as Z500 (geopotential height) and T850 (temperature) improves upon previous data-driven approaches and is comparable to operational, full-resolution, physical models from GFS and ECMWF, at least when evaluated on 1-degree scales and when using reanalysis initial conditions. We also show results from connecting this data-driven model to live, operational forecasts from GFS.

DATA-DRIVEN HIGH-RESOLUTION 3D ADAPTIVE FOURIER NEURAL NETWORKS FOR WEATHER FORECASTING

medium-range solution System weather Forecast

Thorsten Kurth, NVIDIA Corporation, Santa Clara, CA 95051

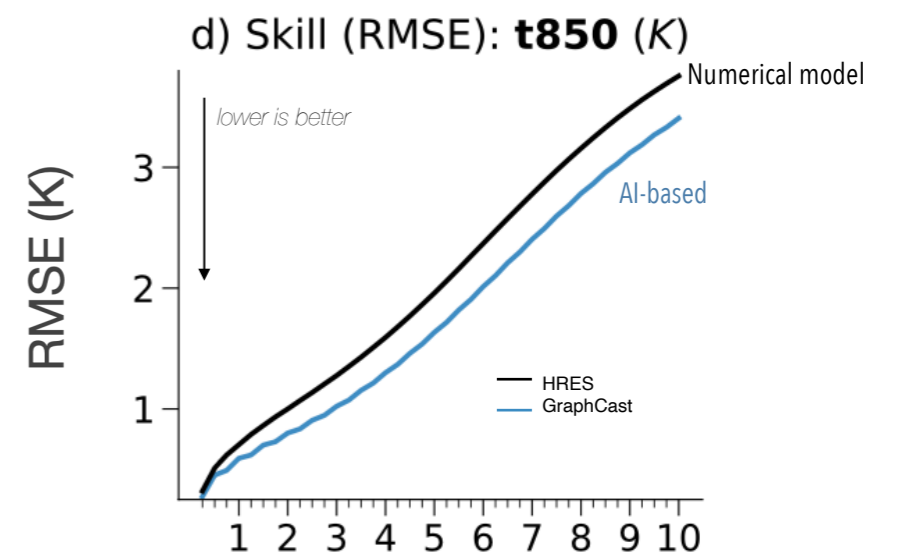
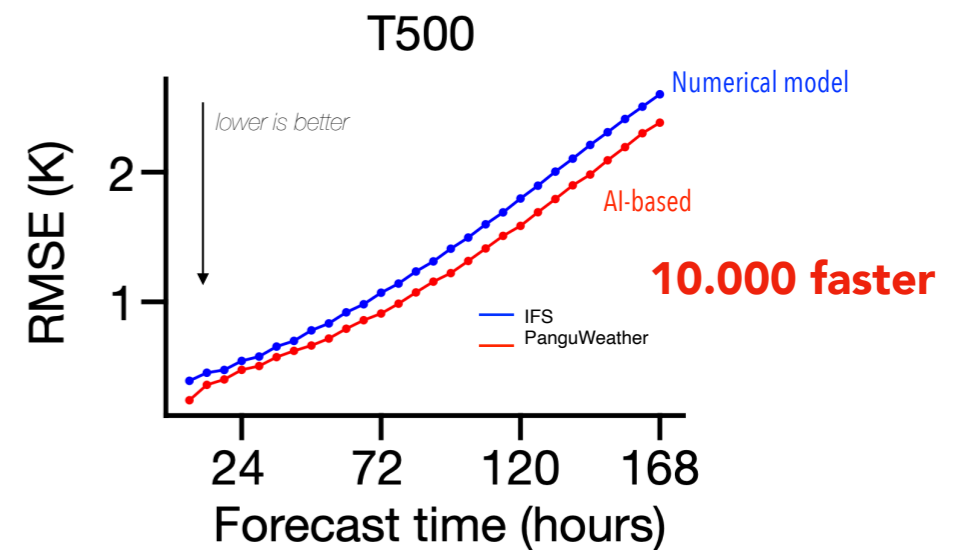
Kanyar Arizadoneshelli, Purdue University, West Lafayette, IN 47907

Animashree Anandkumar, California Institute of Technology, Pasadena, CA 91125, NVIDIA Corporation, Santa Clara, CA 95051

1960-2010

2005-2025

2022-



All these models have been trained on a single task: weather forecasting

State of the art - numerical models: IFS

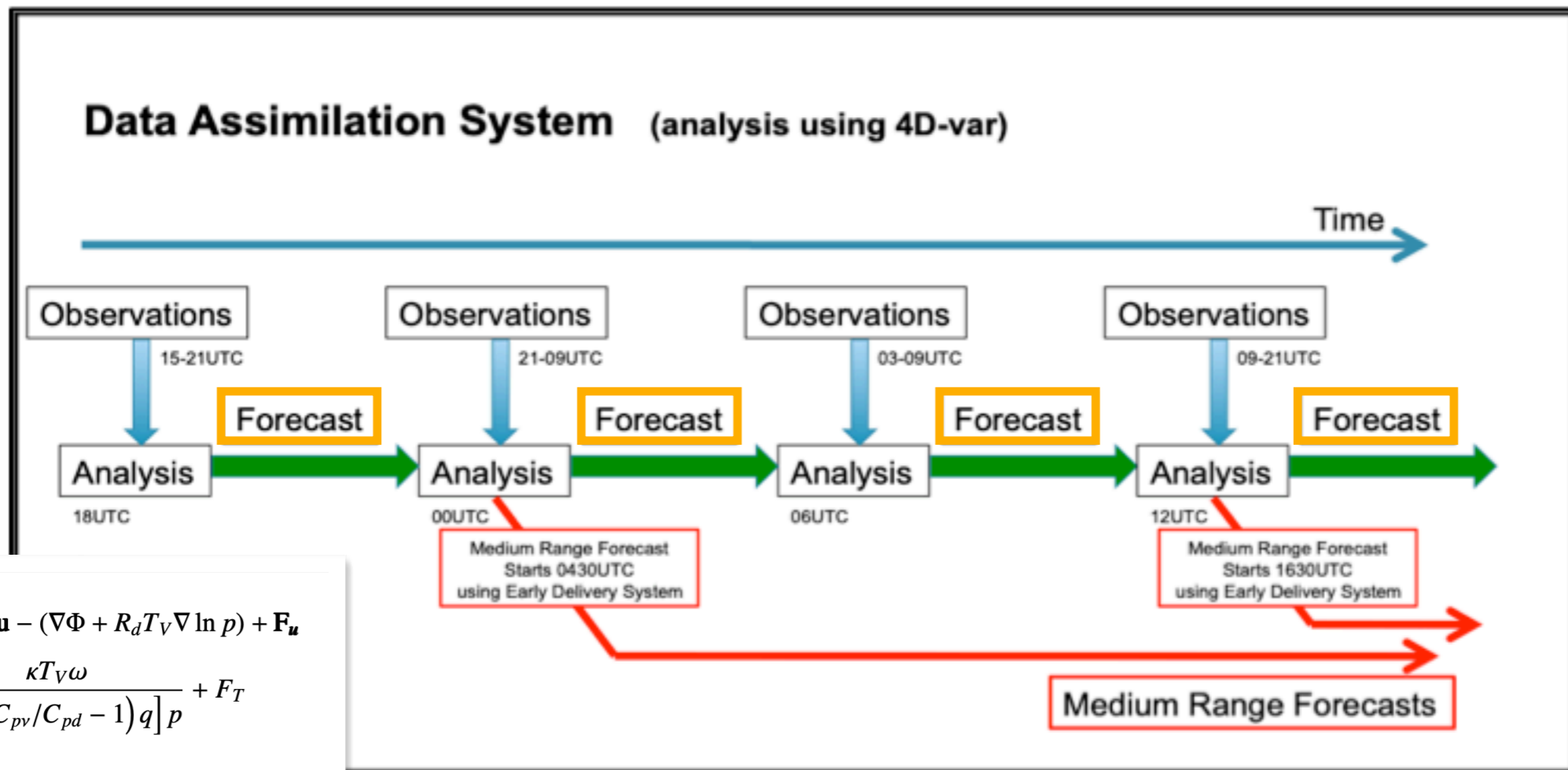
Europe: Integrated Forecasting System (IFS)

Language: **Fortran-based**

Length: **over 2 million lines**

US: Global Forecast System (GFS)

Japan: Global Spectral Model (GSM2303) ...



$$\frac{d\mathbf{u}}{dt} = -f\mathbf{z} \times \mathbf{u} - (\nabla\Phi + R_d T_V \nabla \ln p) + \mathbf{F}_u$$

$$\frac{dT}{dt} = \frac{\kappa T_V \omega}{[1 + (C_{pv}/C_{pd} - 1)q]} + F_T$$

$$\frac{dq}{dt} = F_q$$

$$\frac{dq_c}{dt} = F_c$$

$$\frac{\partial}{\partial t} \left(\frac{\partial p}{\partial \eta} \right) + \nabla \cdot \left(\mathbf{u} \frac{\partial p}{\partial \eta} \right) + \frac{\partial}{\partial \eta} \left(\dot{\eta} \frac{\partial p}{\partial \eta} \right) = 0$$

Machine Learning approaches

Language: python + torch

Length: a few thousands lines

Who? What? Where?

- PanguWeather



- GraphCast
- NeuralGCM
- MetNet3



- FourCastNet



- ClimaX
- Aurora

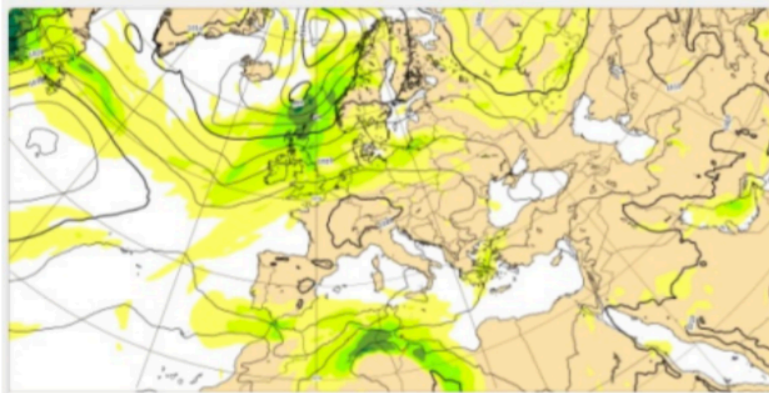
Microsoft Research



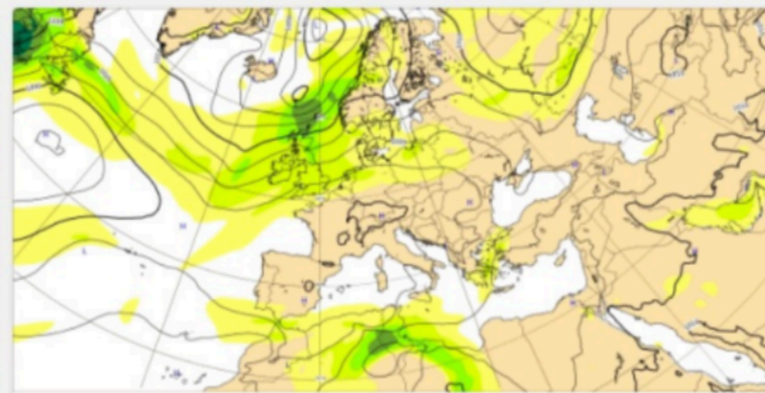
- Prithvi (earth observations)

... but what about academia?
Are the research centres following the trend?

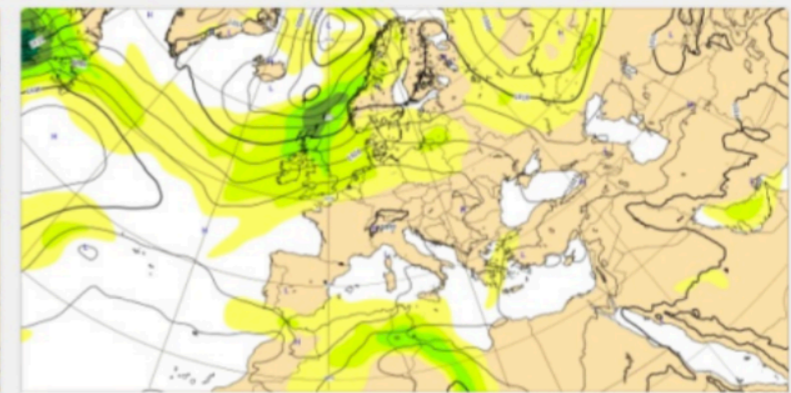
Real time AI-based forecasts @ ECMWF



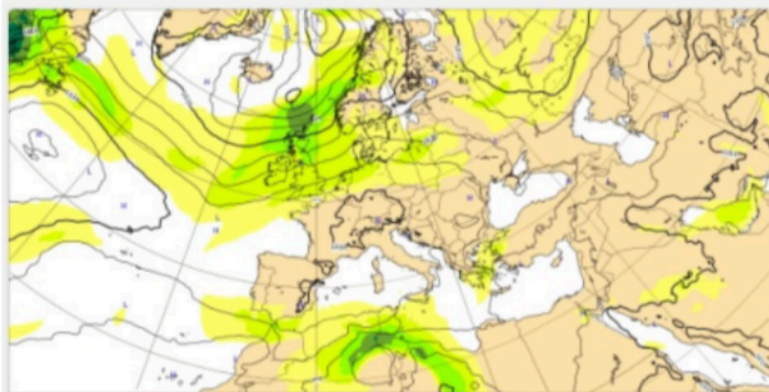
Mean sea level pressure and 850 hPa wind speed



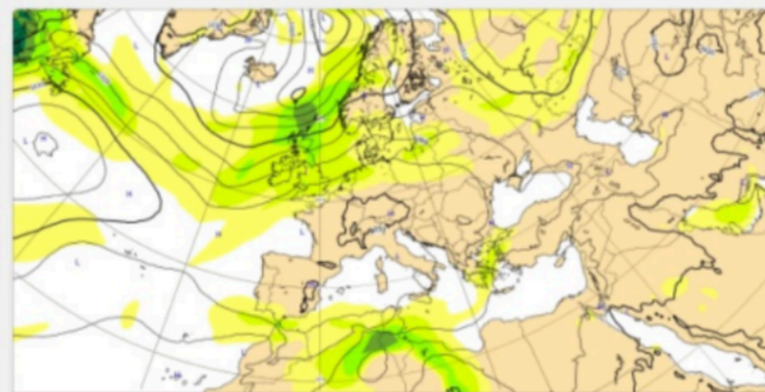
Experimental: AIFS (ECMWF) ML model: Mean sea level pressure and 850 hPa wind speed



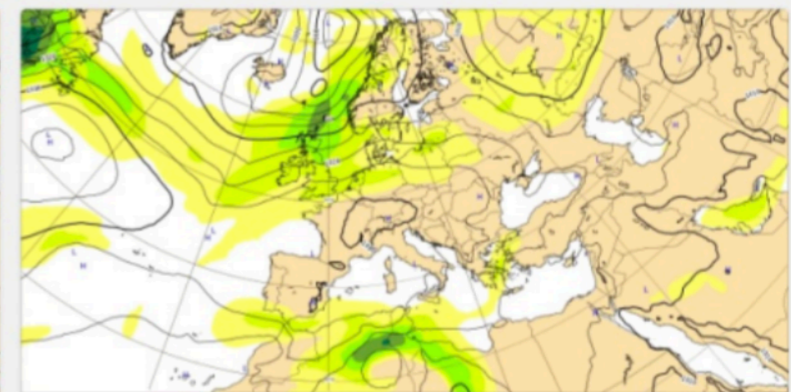
Experimental: FourCastNet ML model: Mean sea level pressure and 850 hPa wind speed



Experimental: FuXi ML model: Mean sea level pressure and 850 hPa wind speed



Experimental: GraphCast ML model: Mean sea level pressure and 850 hPa wind speed

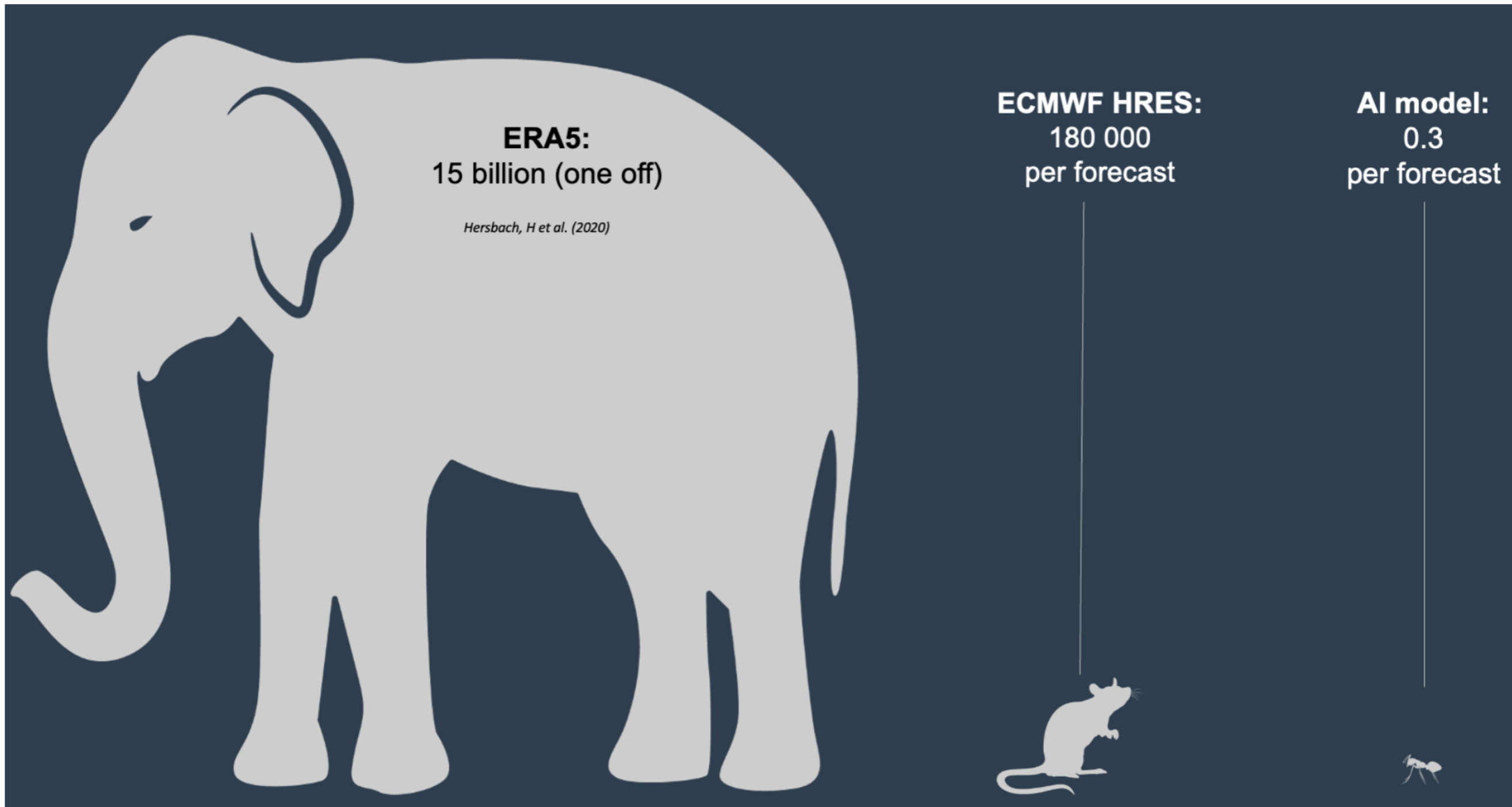


Experimental: Pangu-Weather ML model: Mean sea level pressure and 850 hPa wind speed

THE RISE OF DATA-DRIVEN WEATHER FORECASTING
A FIRST STATISTICAL ASSESSMENT OF MACHINE LEARNING-BASED WEATHER FORECASTS
IN AN OPERATIONAL-LIKE CONTEXT

A PREPRINT V2

Evaluation costs



Numerical model - processing time: hour(s)

AI-based model inference time: 1 A100 for 2 min for a 10 day forecast → Ensemble: 50x

Can we go beyond?

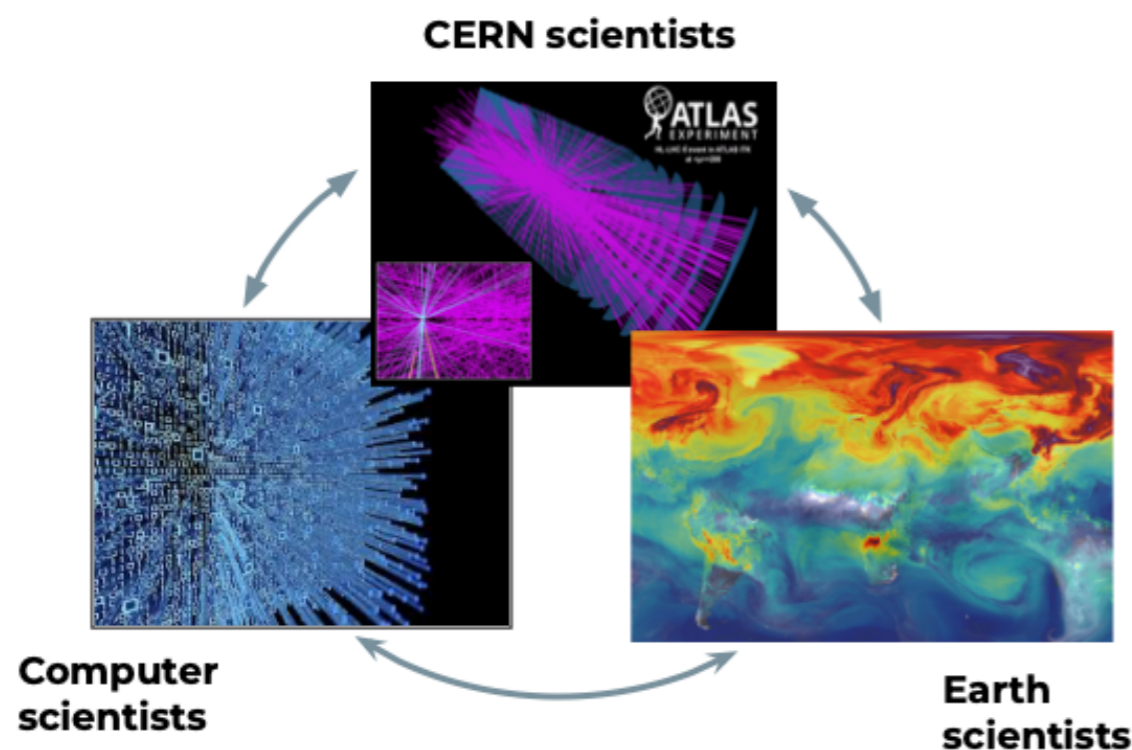
Building foundation models for science

AtmoRep: Introduction



Atmosphere:

- Set of **complex non-linearly coupled phenomena** involving a **wide range of scales**
- Very large amounts of **observational data available in a format suitable for large scale ML**



Common challenges:

Model complex, nonlinear phenomena and improve current simulations

Earth science: eg. better understand convection phenomena
CERN: eg. particle-jet showers reconstruction

Explore potential of unsupervised learning for scientific applications

Earth science: eg. early detection of extreme events
CERN: eg. anomaly detection

Condense dataset information in a compact representation

eg. condense the info in a few GB rather than TB

Common Goal:

Use unsupervised learning to build a task-independent data-driven model to encapsulate complex physics phenomena

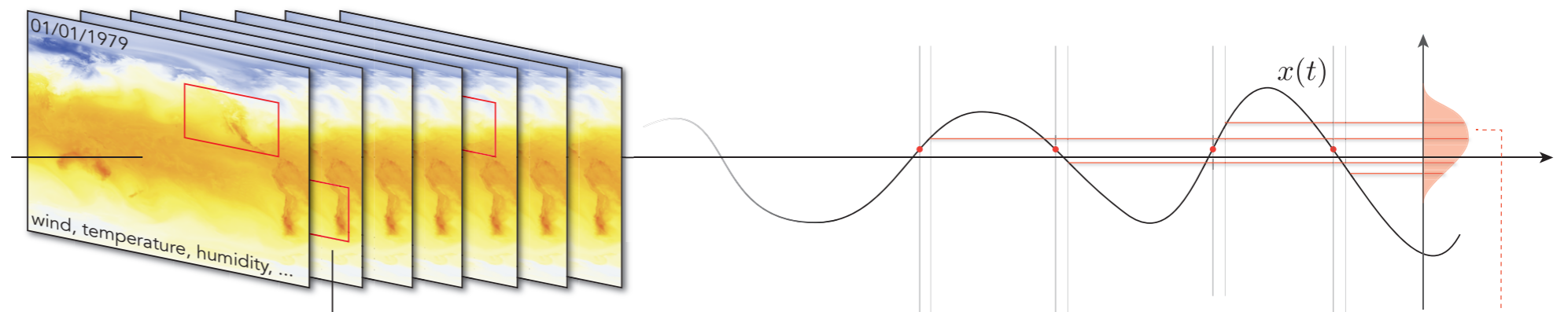
What is a task-independent model for us?

Encapsulate the spatio-temporal evolution of a dynamical system

Probability of getting the state y given the initial state x and the auxiliary info α

$$p(y | x, \alpha)$$

Auxiliary info: position, absolute time etc..



Training

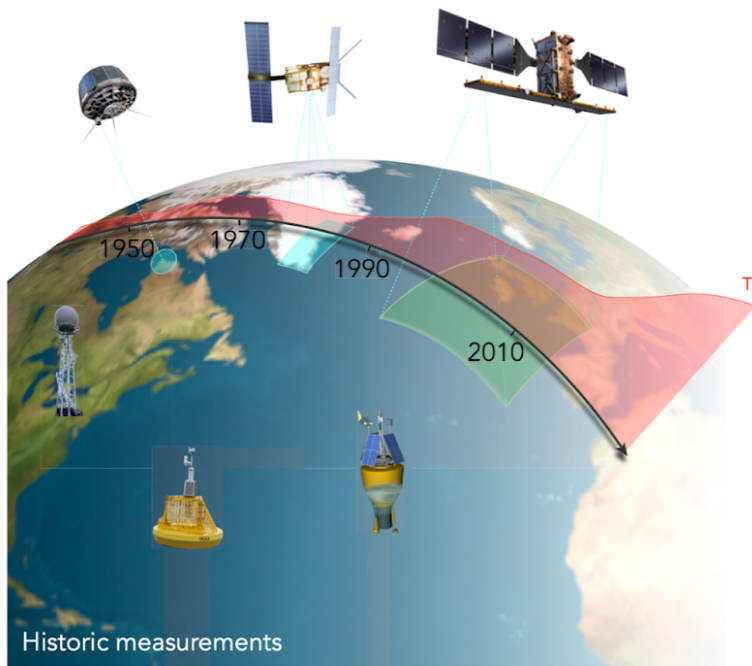
The distribution can be approximated by a large neural network

$$p(y | x, \alpha) \approx p_{\theta}(y | x, \alpha)$$

foundation model:

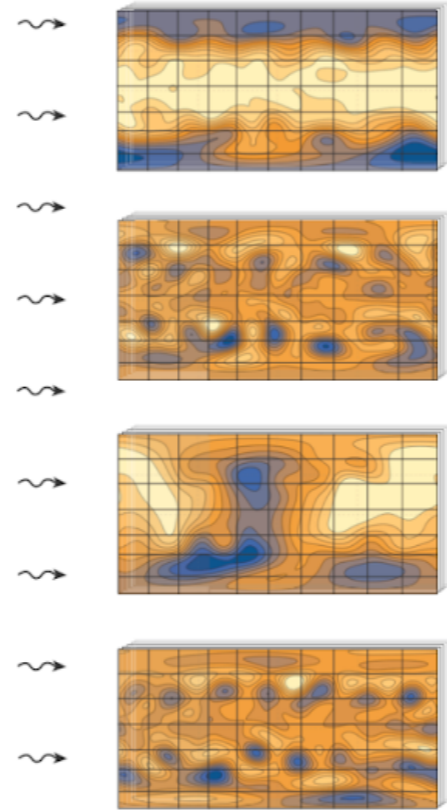
neural network that models data distribution for a specific domain

The project in a nutshell



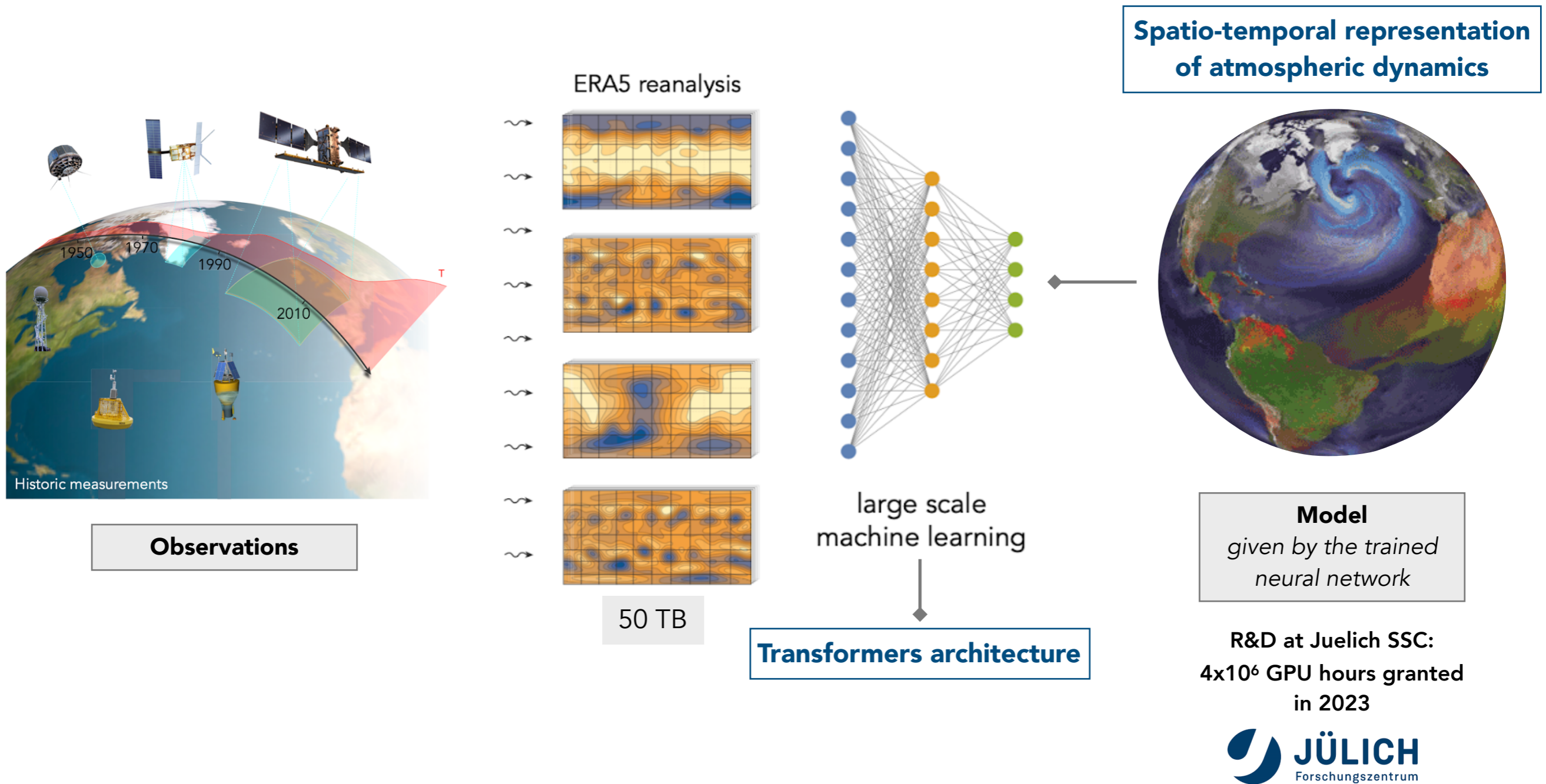
Observations

ERA5 reanalysis



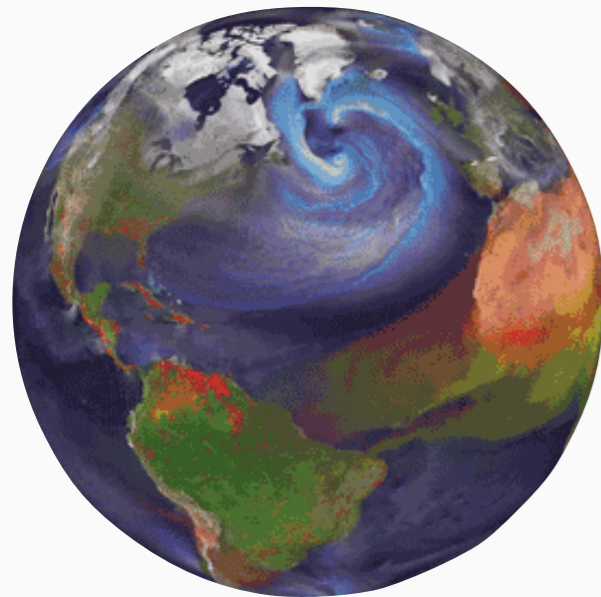
50 TB

The project in a nutshell



Applications: one model for multiple purposes

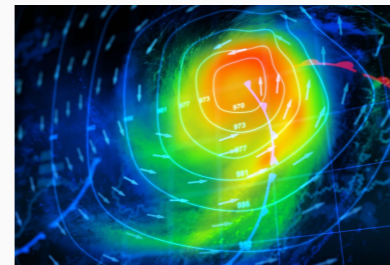
Spatio-temporal representation of atmospheric dynamics



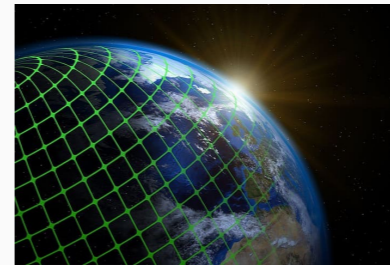
Model
given by the trained neural network

Task-dependent adaptable smaller networks

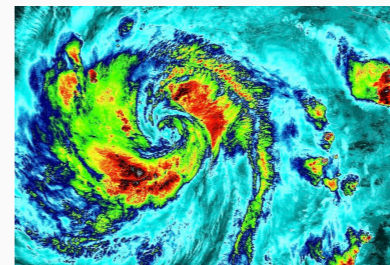
Adaptation



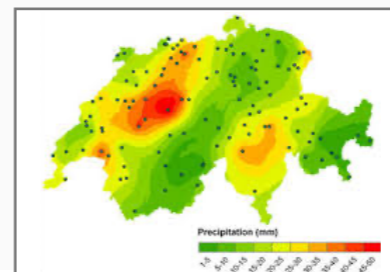
Weather predictions ✓



Downscaling ✓



Bias corrections ✓



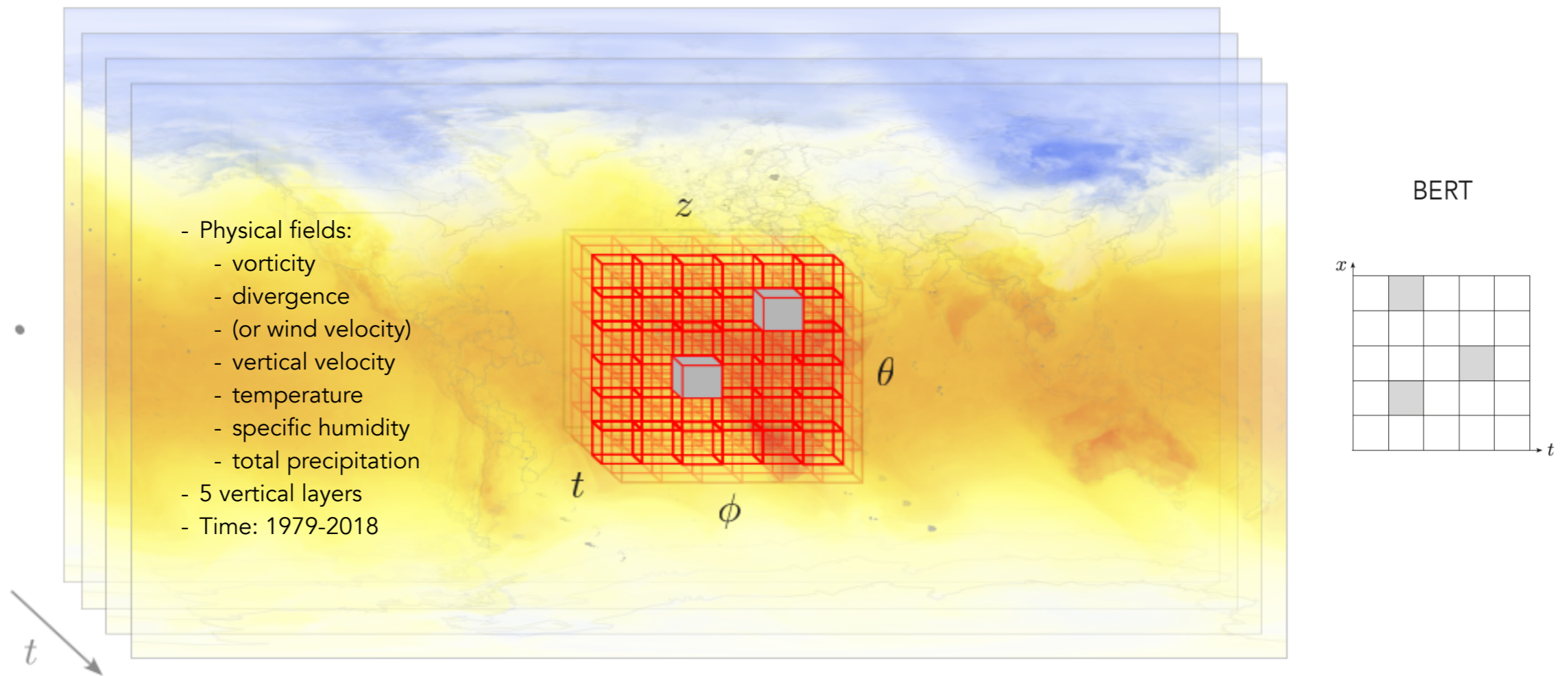
Spatio-temporal Interpolations (WIP) 🔄

Physics-related applications = uncertainties
Need for a **stochastic approach**

Key Ingredient: The training protocol

Use an extension of BERT masked language modelling from self-supervised trainings in NLP

Random sampling of neighbourhoods for training



Split cube in small space-time regions (3D cubes) → tokens

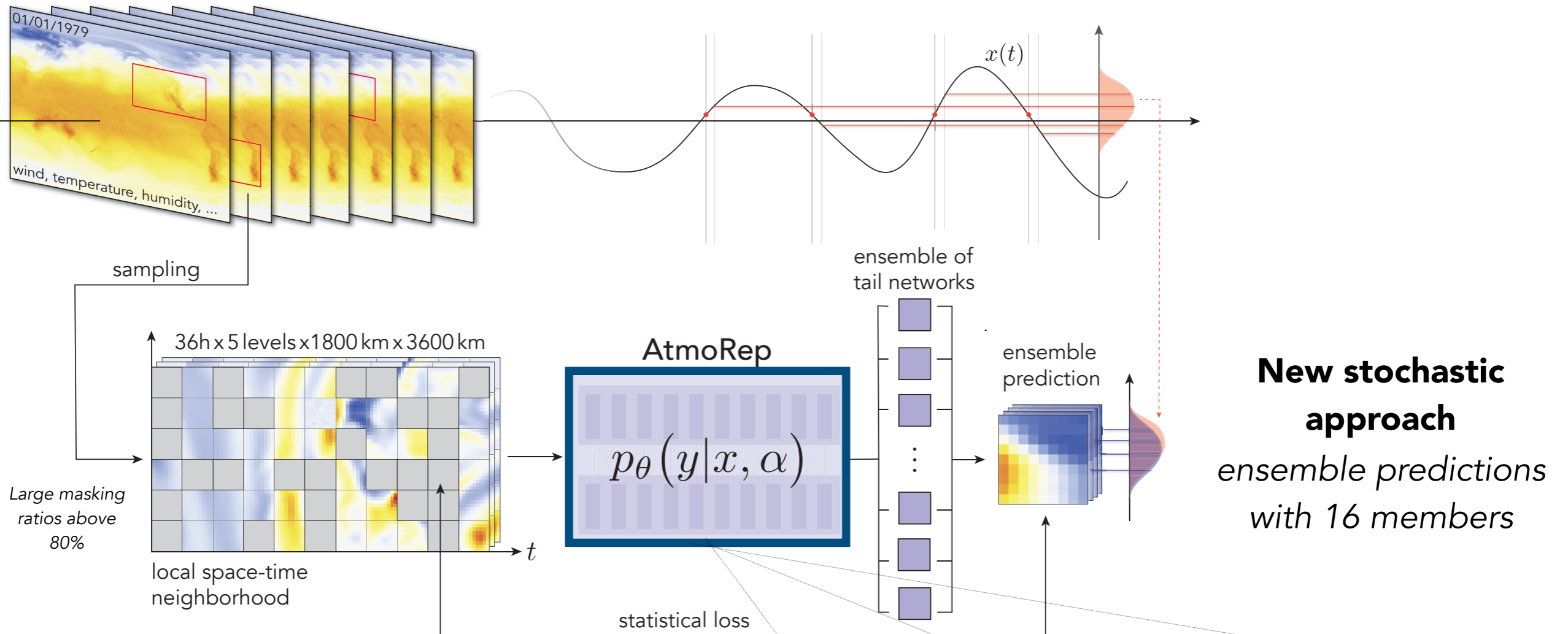
Mask random tokens within the hyper-cube and predict them

Large masking ratios above 80% using full masking, noise and climatology

Default: 12 x 6 x 12 tokens with 3 x 9 x 9 grid points

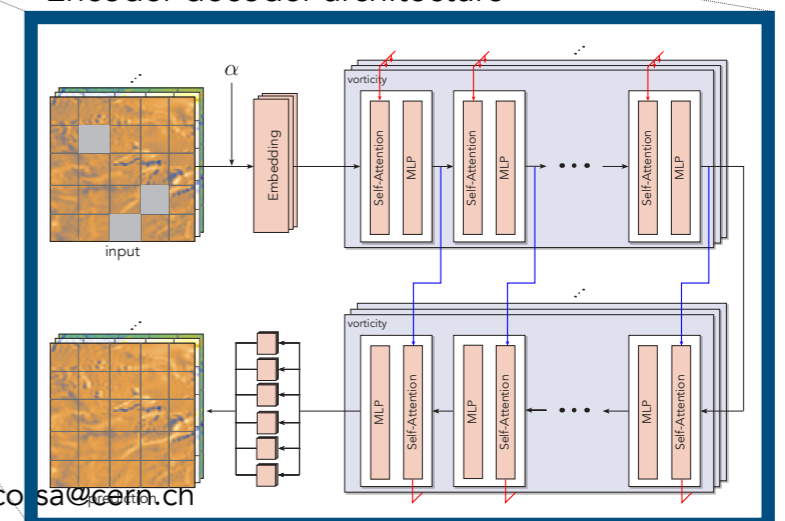
The AtmoRep workflow

pre-processed historical observational record $x(t)$ (ERA5 reanalysis)



Approximate the 4-Dim PDF of the process using a Transformers-based network with 3.5 billion parameters

Encoder decoder architecture

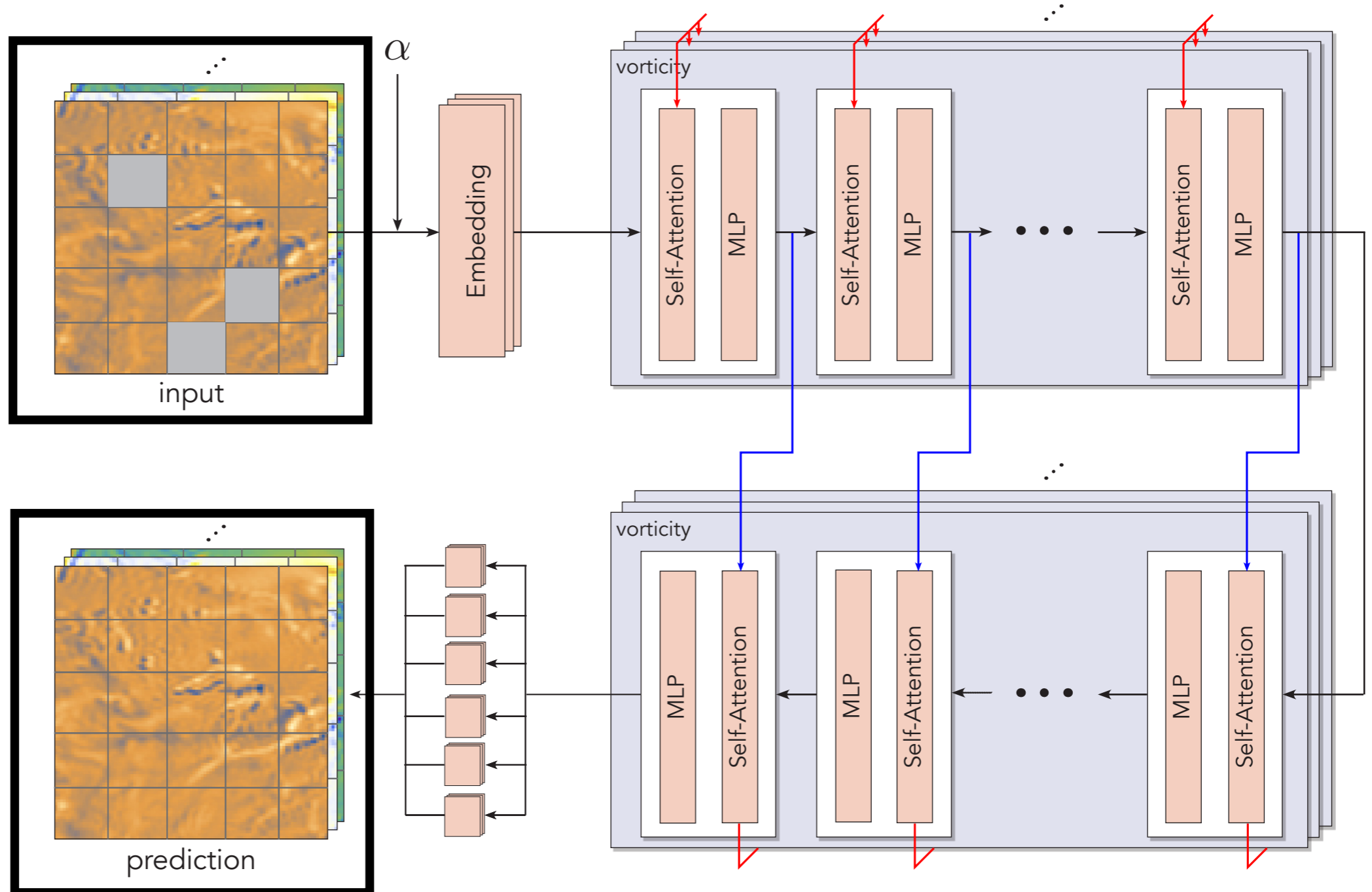


Task-specific fine-tuning

Goal: improve model performance for a specific task
e.g. forecasting, downscaling...

Examples:

e.g. fix masking scheme



OR

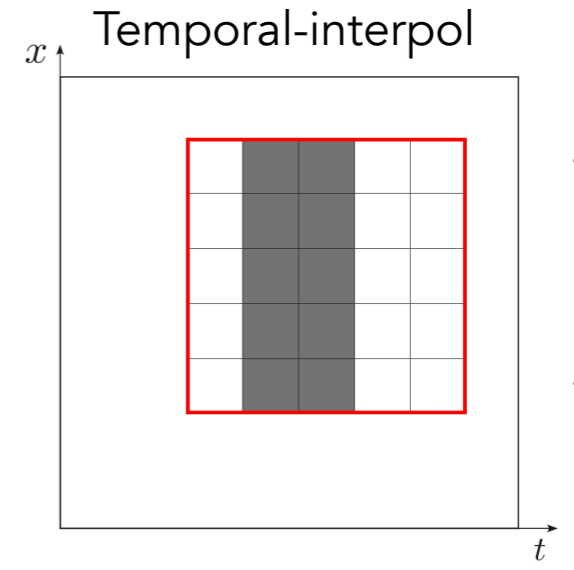
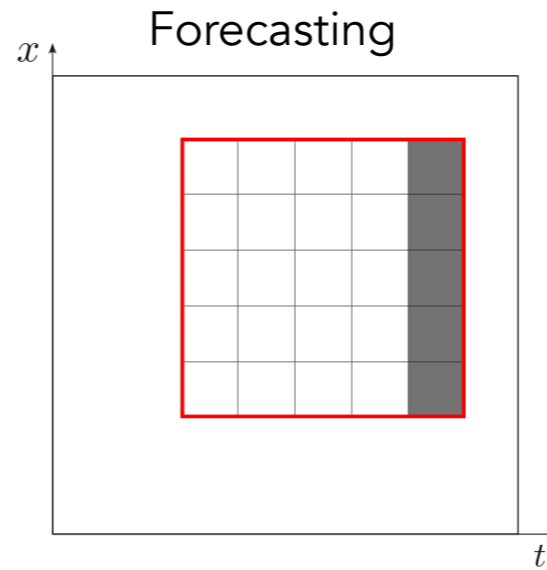
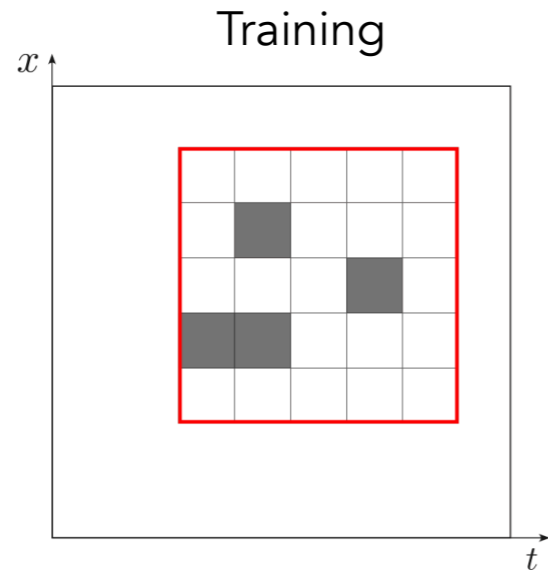
Change target dataset

Task-specific fine-tuning

Goal: improve model performance for a specific task
e.g. forecasting, downscaling...

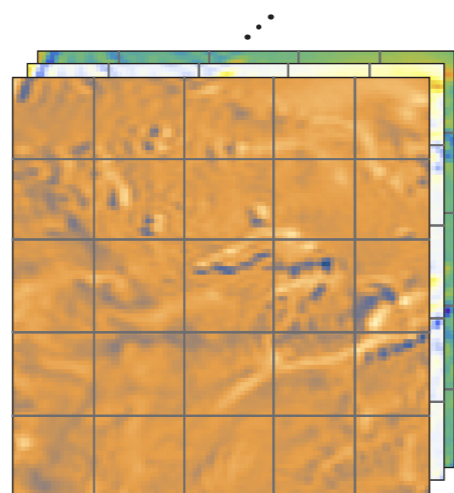
Examples:

e.g. fix masking scheme



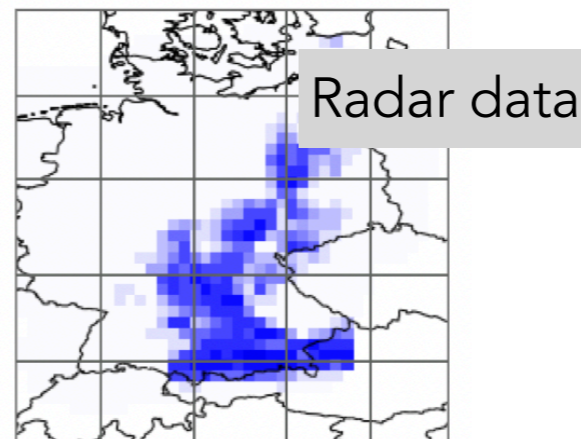
OR

Change target dataset



ERA5

Radklim data



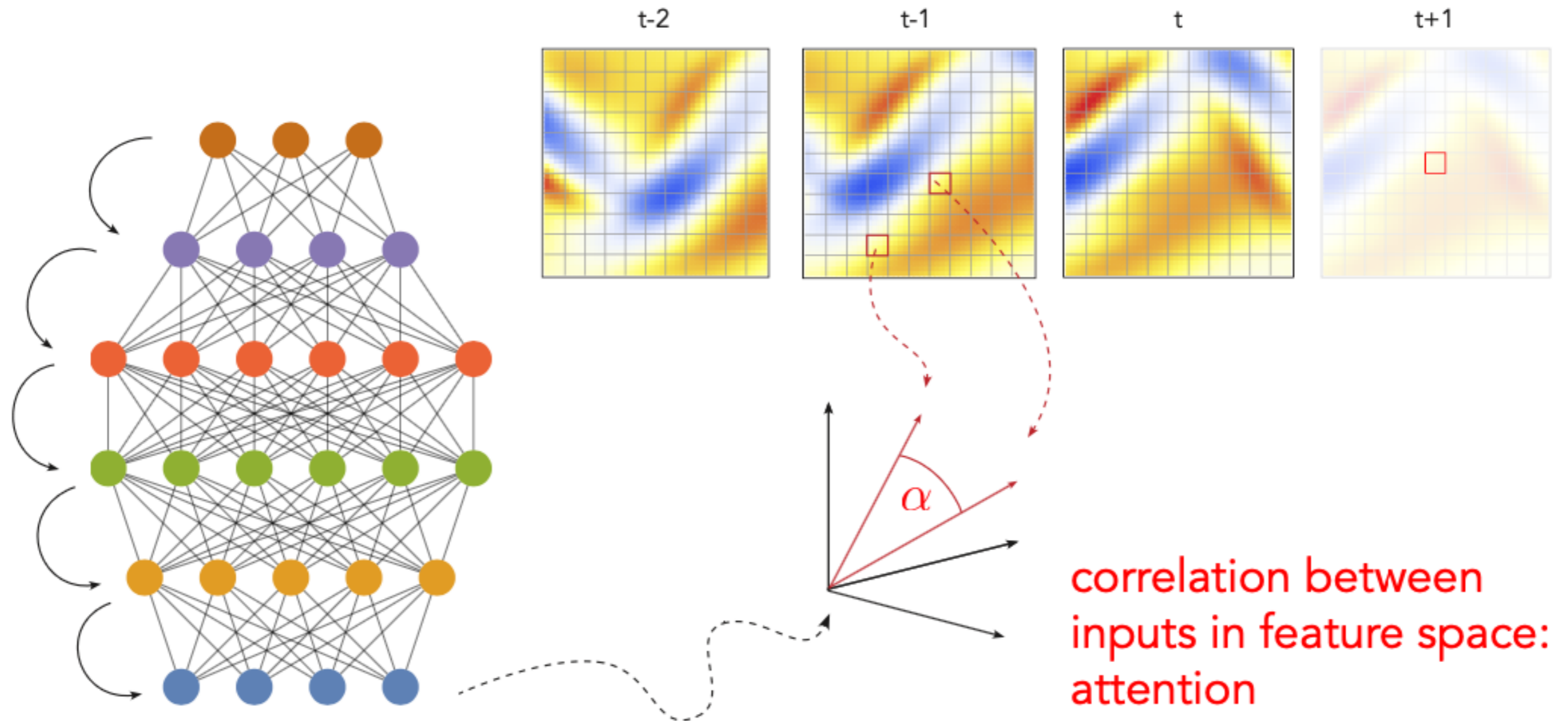
COSMO-REA6



Attention maps and interpretability

Inspect the self-attention mechanism:

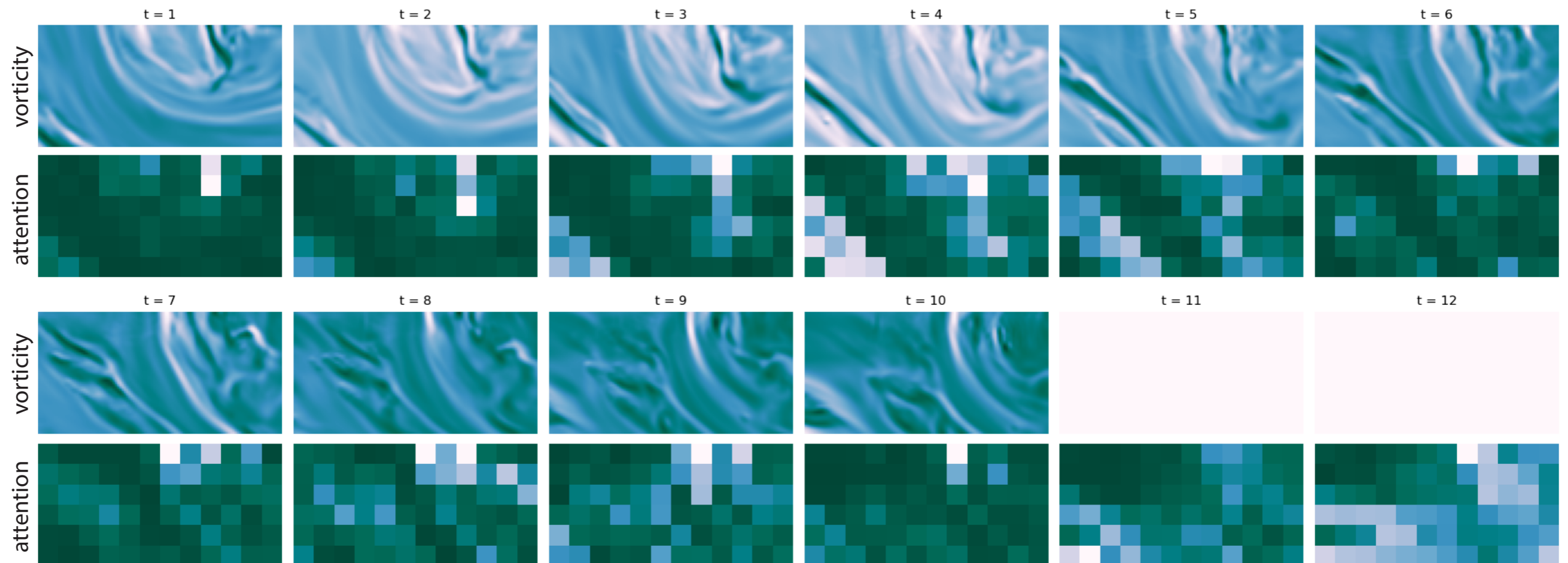
can we identify physics phenomena (e.g. hurricane formation) before they are even created?



Attention maps and interpretability

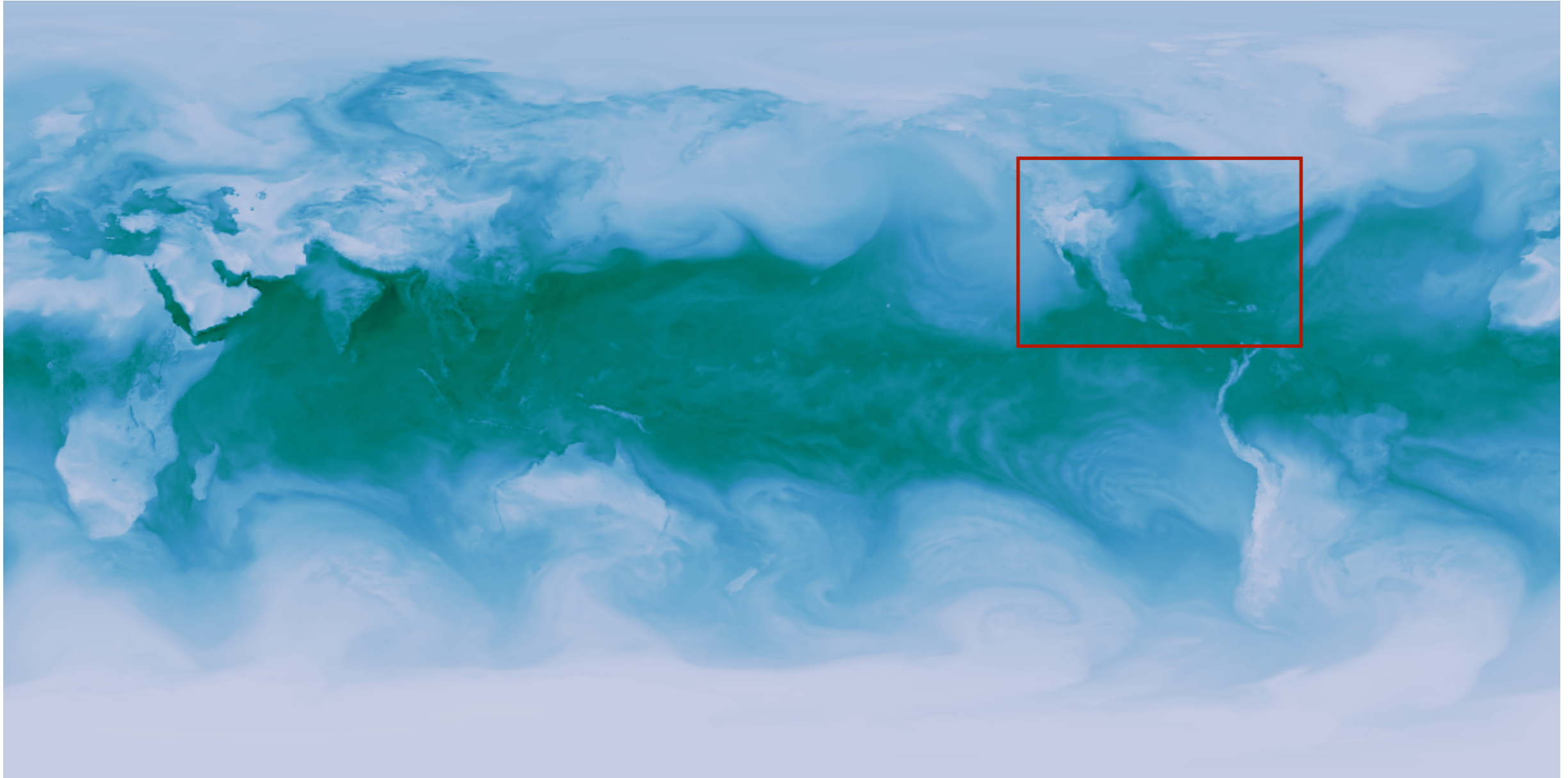
Inspect the self-attention mechanism:

can we identify physics phenomena (e.g. hurricane formation) before they are even created?



Results: Target - ERA5

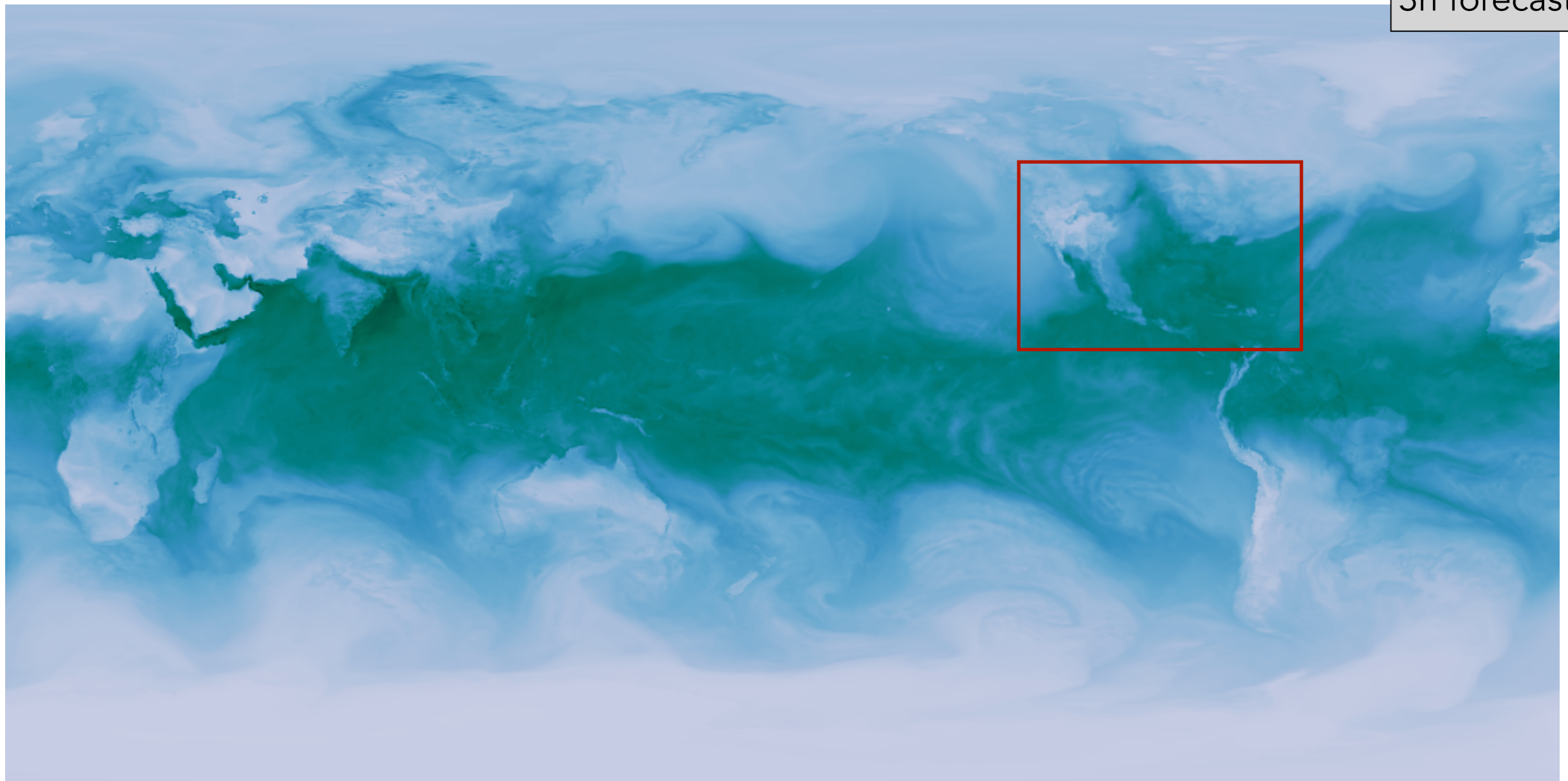
specific humidity, June 15th 2018 13:00 UTC



Results: Prediction - AtmoRep

specific humidity, June 15th 2018 13:00 UTC

3h forecast

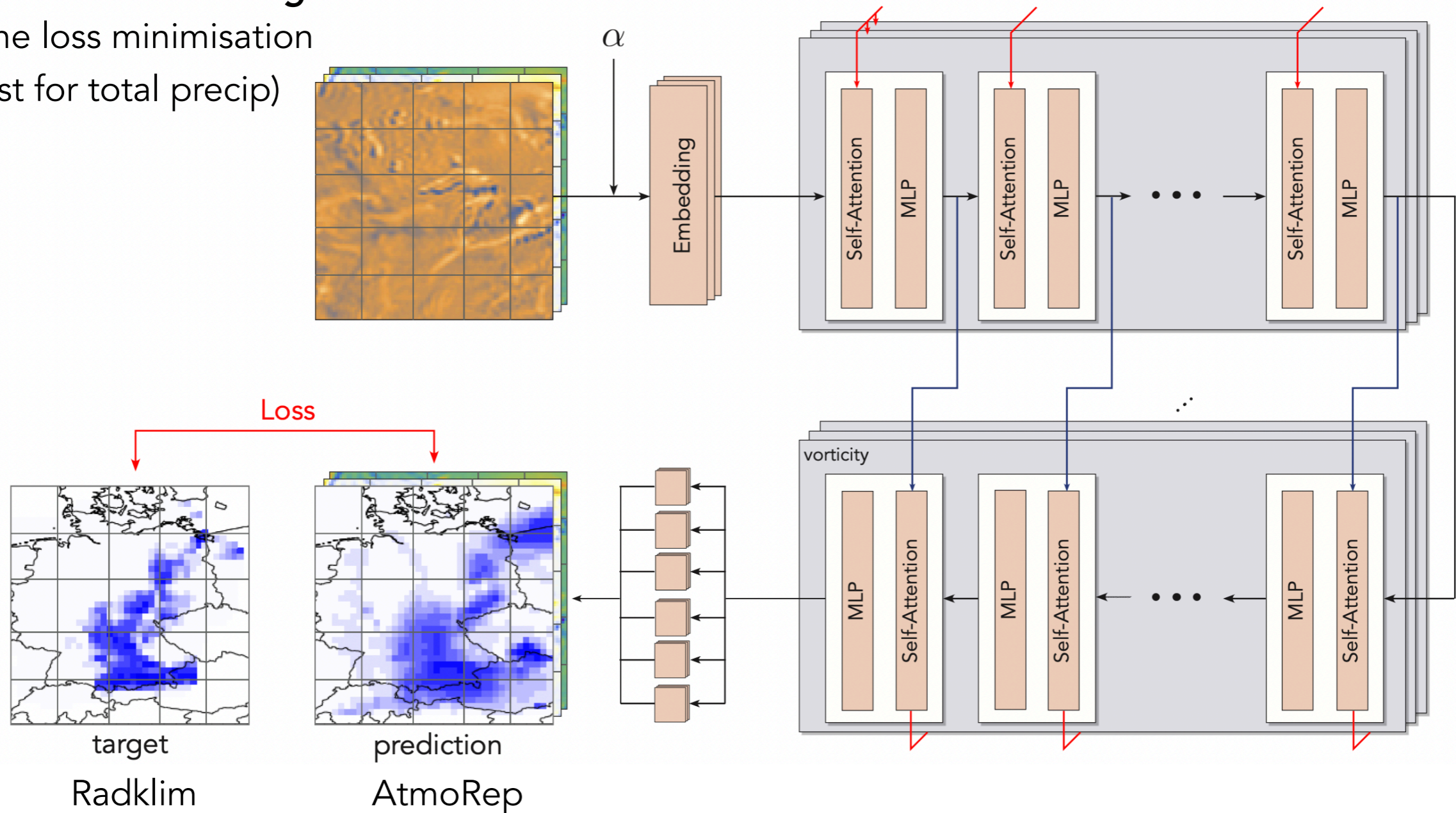


Bias corrections

Precipitation rates are known to be suboptimal in ERA5

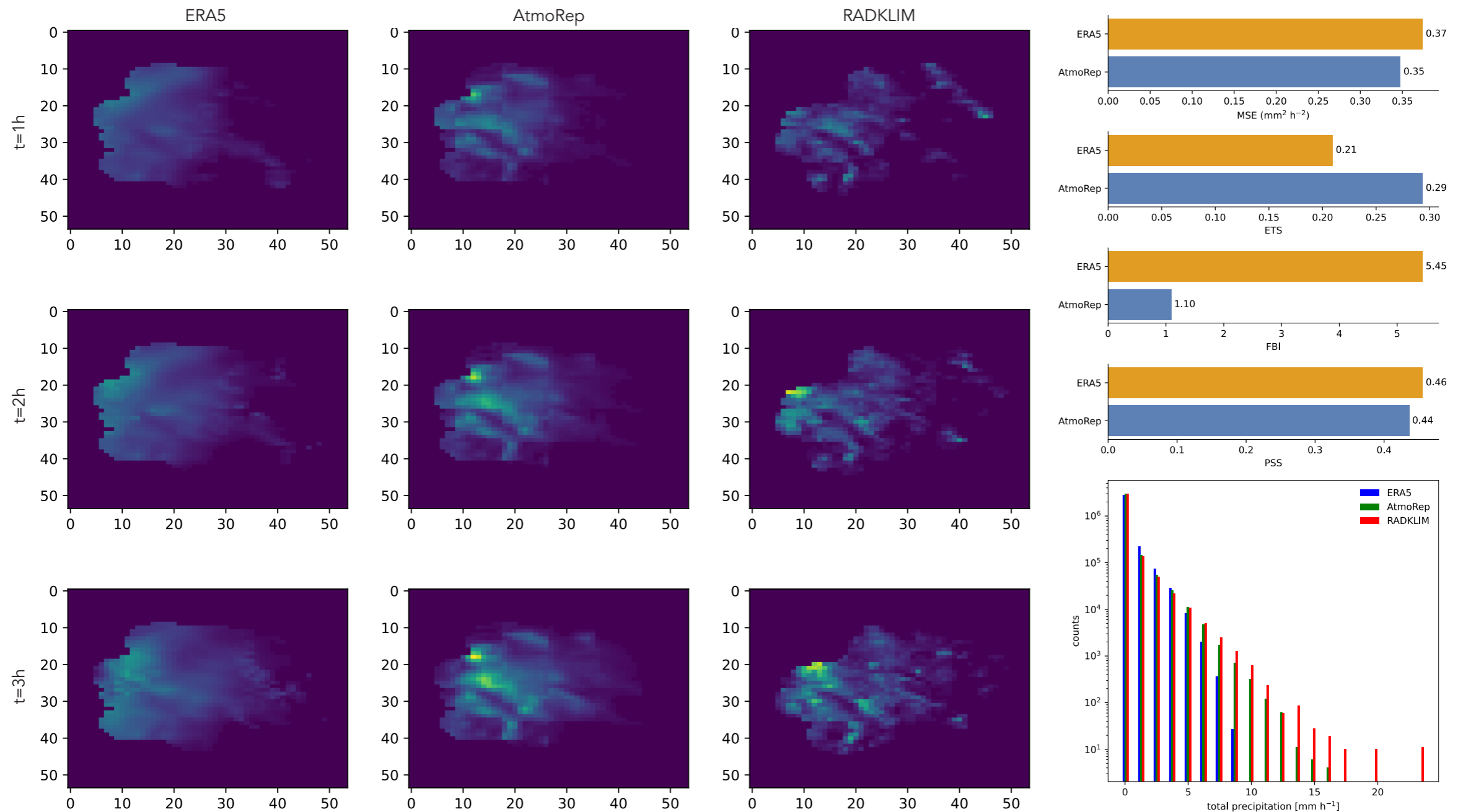
Use RADKLIM radar data to fine-tune the precipitation rates in AtmoRep

Use *Radklim* data as *target*
for the loss minimisation
(just for total precip)



Bias corrections: Results

Precipitation rates are known to be suboptimal in ERA5
Use RADKLIM radar data to fine-tune the precipitation rates in AtmoRep



Quantum Machine Learning

The CERN Quantum Technology Initiative was launched in 2020

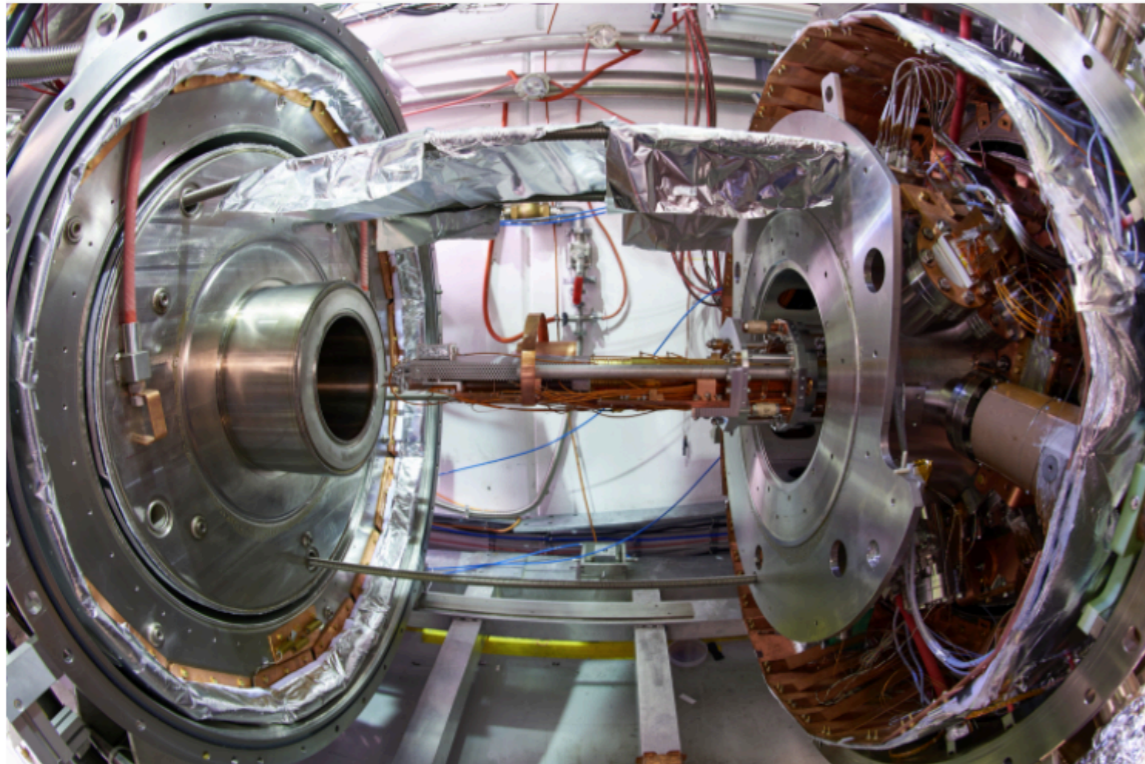
Understand the impact of quantum technologies in HEP

Voir en [français](#)

CERN meets quantum technology

The CERN Quantum Technology Initiative will explore the potential of devices harnessing perplexing quantum phenomena such as entanglement to enrich and expand its challenging research programme

30 SEPTEMBER, 2020 | By [Matthew Chalmers](#)



The AEGIS 1T antimatter trap stack. CERN's AEGIS experiment is able to explore the multi-particle entangled nature of photons from positronium annihilation, and is one of several examples of existing CERN research with relevance to quantum technologies. (Image: CERN)

Quantum simulation and HEP theory applications

Quantum Computing

Quantum Sensing

Quantum Communication

Quantum potential...

Source: McKinsey 2023

<https://www.mckinsey.com/capabilities/mckinsey-digital/our-insights/quantum-technology-sees-record-investments-progress-on-talent-gap>

Principles of quantum mechanics enhance computations

Superposition leads to parallelism

→ **exponential speedup?**

Entanglement

→ **non linear correlation and classical intractability?**

Operations (gates) are unitary transformations

→ **reversible computing?**

Output is the result of a quantum state measurement according to Born rule

→ **stochastic computation ?**

No-cloning theorem

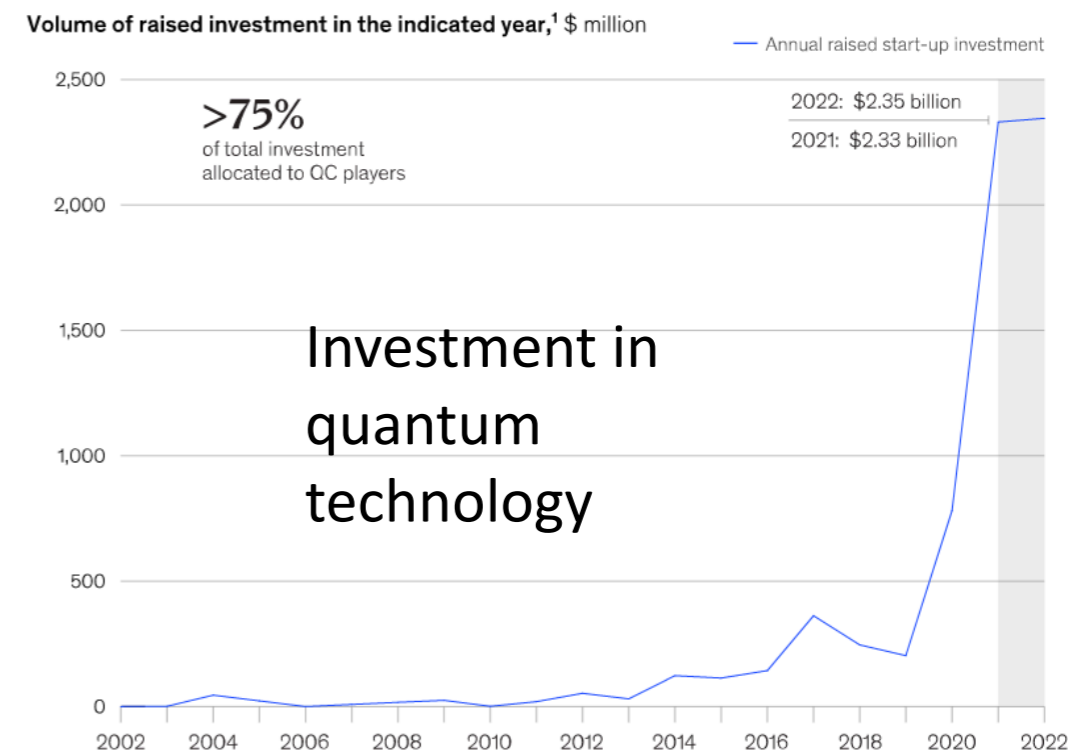
→ **information security**

Quantum state coherence and isolation

→ **computation stability and errors**

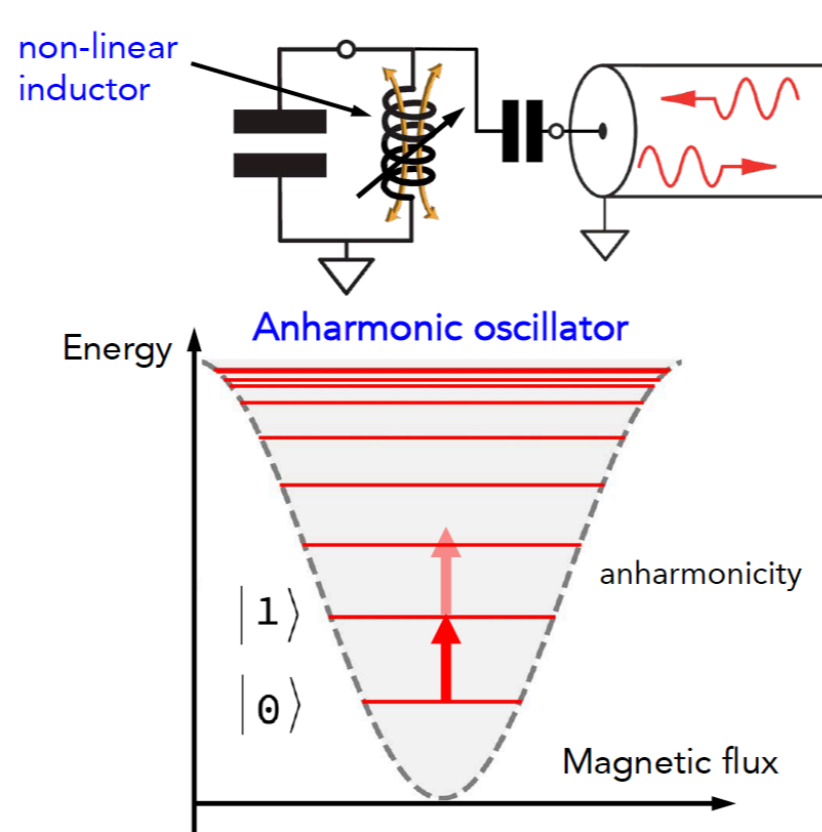
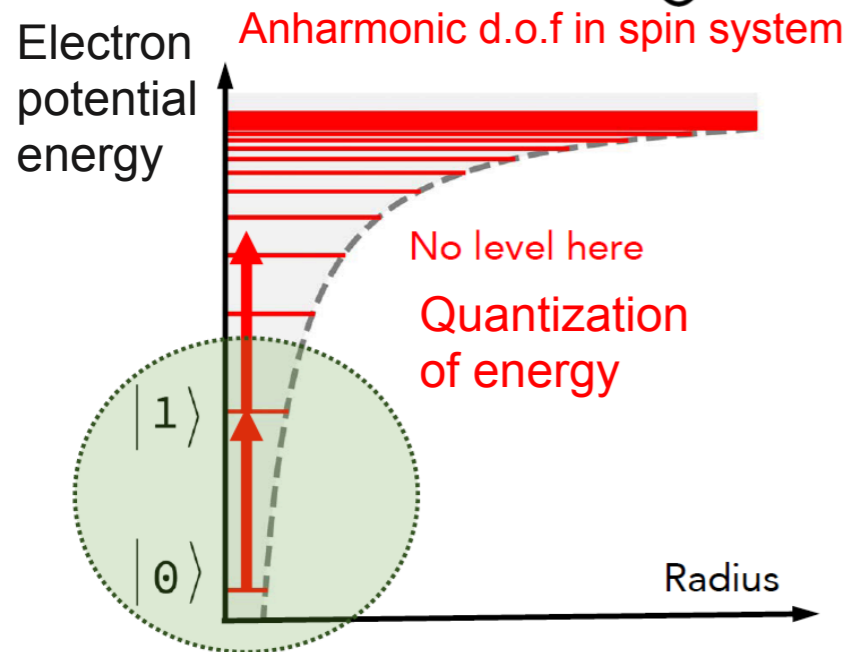
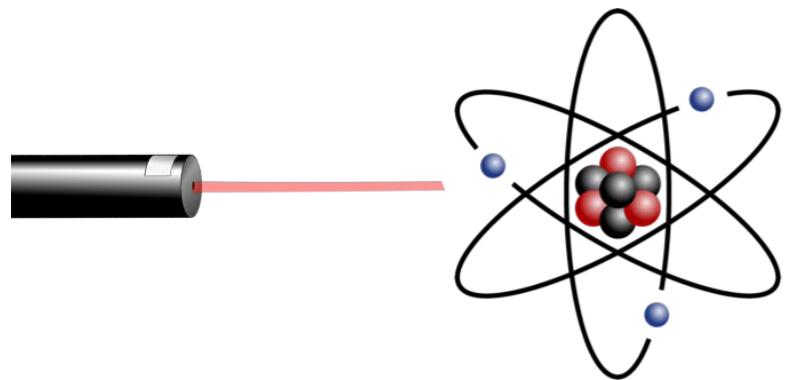
Qubit state collapses

→ **reproducibility?**



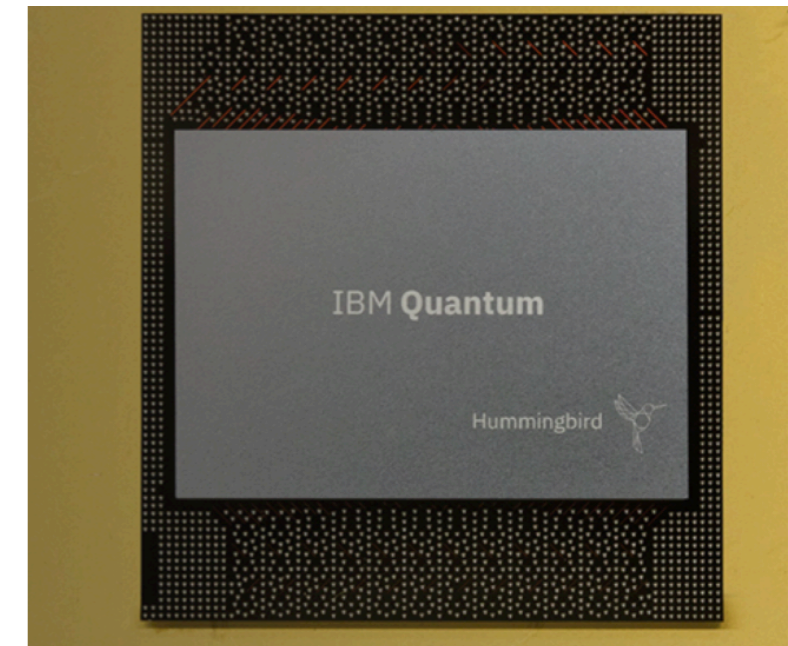
¹Based on public investment data recorded in PitchBook; actual investment is likely higher.
Source: PitchBook

Simple qubits



Z. Mineev, Qiskit Global Summer School 2020

- In zero resistance circuit, current will oscillate
- Microwaves can excite currents in a superposition of states



Ex. Google, IBM, ...

07.10.24

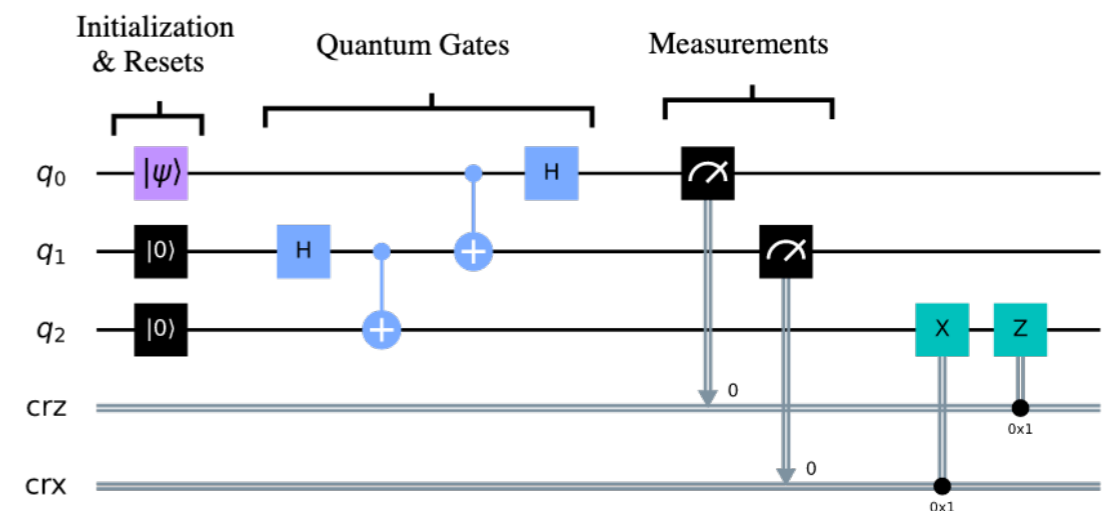
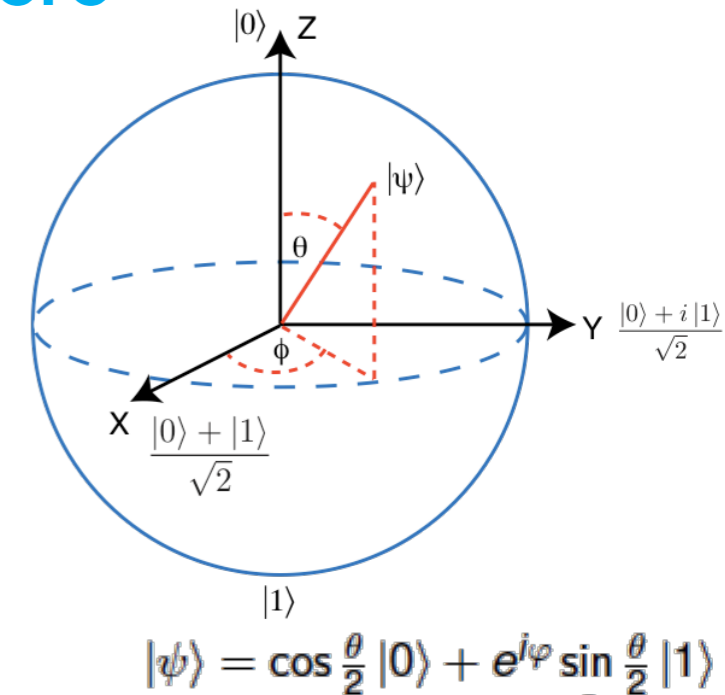
Qubits and algorithms

- Basic Unit of Quantum Computation
 - **Classical bits are binary "0 or 1"**
- Quantum Mechanics predicts **superposition states** (exponential storage information)

- **Dirac notation** $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$

- Operations are **unitary** matrices
 - Input and output states have the **same dimension**
 - Some classical gates (or, and, nand, xor...) **cannot be implemented directly**
 - Can **simulate** any classical computation with small overhead

Bloch Sphere

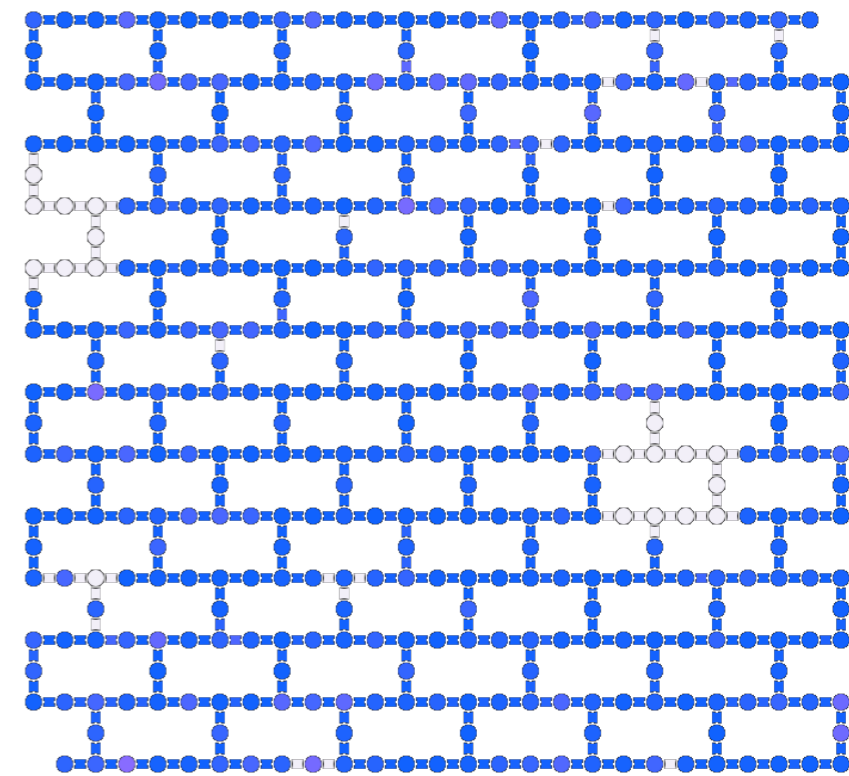
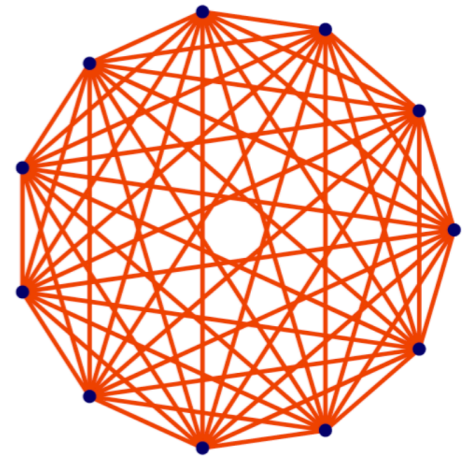


Interest in **multi level** representations: qutrits..

Noisy Intermediate-Scale Quantum devices

- Limitations in terms of **stability** and **connectivity**
 - **Circuit optimisation**
- **De-coherence**, measurement errors or gate level errors (**noise**)
 - Specific **error mitigation techniques**
 - Prefer algorithms **robust against noise**
- **Problem size**
- Initially integrated in **hybrid quantum-classical infrastructure (HPC + QC)**
 - **Quantum Processing Units** as new "hardware accelerators"

Trapped ion technology: *ionQ*
with all-to-all connectivity

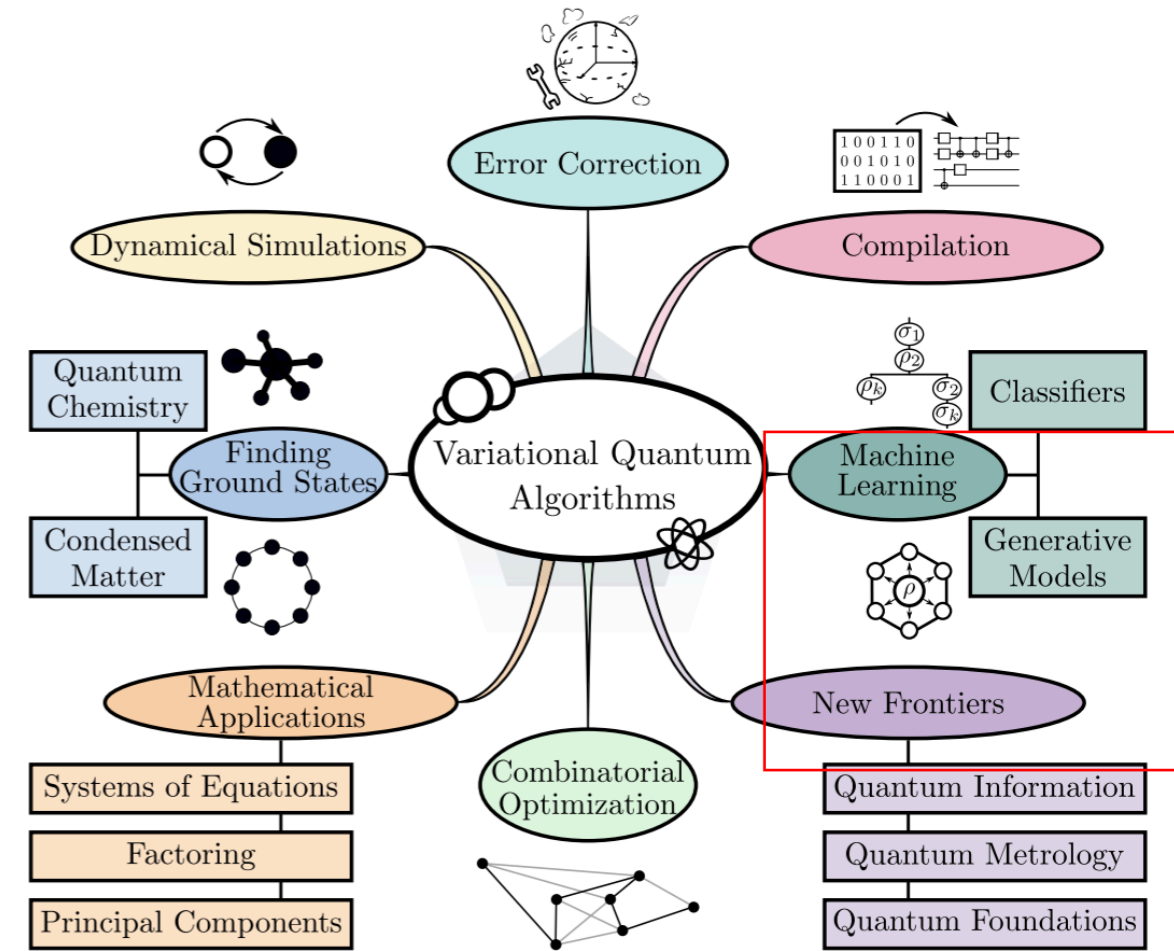


Superconducting qubits:
IBM Seattle

Quantum Machine Learning

Quantum Computing to improve ML

- Speed-up and complexity
- Sample efficiency
- Representational power
- Energy efficiency???
- Evaluate performance on realistic use cases
- QPU as accelerators within classical infrastructure?



Cerezo, Marco, et al. "Variational quantum algorithms." *Nature Reviews Physics* 3.9 (2021)

Study **classical intractability**:

Focus on quantum circuits that are **not efficiently simulable classically?**

IBM Quantum RoadMap

Development Roadmap

IBM Quantum







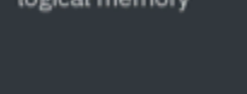


	2016–2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2033+
	Run quantum circuits on the IBM Quantum Platform	Release multi-dimensional roadmap publicly with initial aim focused on scaling	Enhancing quantum execution speed by 100x with Qiskit Runtime	Bring dynamic circuits to unlock more computations	Enhancing quantum execution speed by 5x with quantum serverless and Execution modes	Improving quantum circuit quality and speed to allow 5K gates with parametric circuits	Enhancing quantum execution speed and parallelization with partitioning and quantum modularity	Improving quantum circuit quality to allow 7.5K gates	Improving quantum circuit quality to allow 10K gates	Improving quantum circuit quality to allow 15K gates	Improving quantum circuit quality to allow 100M gates	Beyond 2033, quantum-centric supercomputers will include 1000's of logical qubits unlocking the full power of quantum computing
Data Scientist						Platform						
						Code assistant	Functions	Mapping Collection	Specific Libraries			General purpose QC libraries
Researchers					Middleware							
					Quantum Serverless	Transpiler Service	Resource Management	Circuit Knitting x P	Intelligent Orchestration			Circuit libraries
Quantum Physicist			Qiskit Runtime									
	IBM Quantum Experience	QASM3	Dynamic circuits	Execution Modes	Heron (5K)	Flamingo (5K)	Flamingo (7.5K)	Flamingo (10K)	Flamingo (15K)	Starling (100M)	Blue Jay (1B)	
	Early	Falcon	Eagle		Error Mitigation	Error Mitigation	Error Mitigation	Error Mitigation	Error Mitigation	Error correction	Error correction	
	Canary 5 qubits Albatross 16 qubits Penguin 20 qubits Prototype 53 qubits	Benchmarking 27 qubits	Benchmarking 127 qubits		5k gates 133 qubits Classical modular 133x3 = 399 qubits	5k gates 156 qubits Quantum modular 156x7 = 1092 qubits	7.5k gates 156 qubits Quantum modular 156x7 = 1092 qubits	10k gates 156 qubits Quantum modular 156x7 = 1092 qubits	15k gates 156 qubits Quantum modular 156x7 = 1092 qubits	100M gates 200 qubits Error corrected modularity	1B gates 2000 qubits Error corrected modularity	

Innovation Roadmap

Software Innovation	IBM Quantum Experience	Qiskit	Application modules	Qiskit Runtime	Serverless	AI enhanced quantum	Resource management	Scalable circuit knitting	Error correction decoder			
	Circuit and operator API with compilation to multiple targets	Modules for domain specific application and algorithm workflows	Performance and abstract through Primitives	Demonstrate concepts of quantum centric-supercomputing	Prototype demonstrations of AI enhanced circuit transpilation	System partitioning to enable parallel execution	Circuit partitioning with classical reconstruction at HPC scale	Demonstration of a quantum system with real-time error correction decoder				
Hardware Innovation	Early	Falcon	Hummingbird	Eagle	Osprey	Condor	Flamingo	Kookaburra	Cockatoo	Starling		
	Canary 5 qubits Penguin 20 qubits Albatross 16 qubits Prototype 53 qubits	Demonstrate scaling with I/O routing with Bump bonds	Demonstrate scaling with multiplexing readout	Demonstrate scaling with MLW and TSV	Enabling scaling with high density signal delivery	Single system scaling and fridge capacity	Demonstrate scaling with modular connectors	Demonstrate scaling with nonlocal c-coupler	Demonstrate path to improved quality with logical memory	Demonstrate path to improved quality with logical communication	Demonstrate path to improved quality with logical gates	
						Heron Architecture based on tunable-couplers	Crossbill m-coupler					

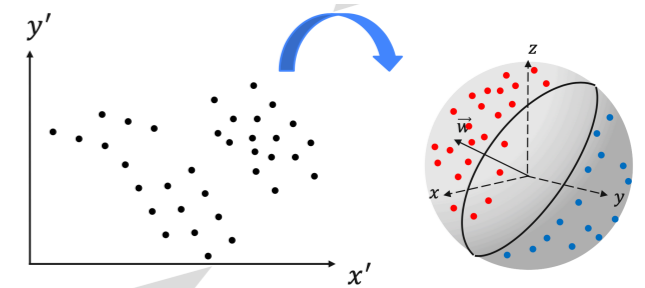
Executed by IBM

On target

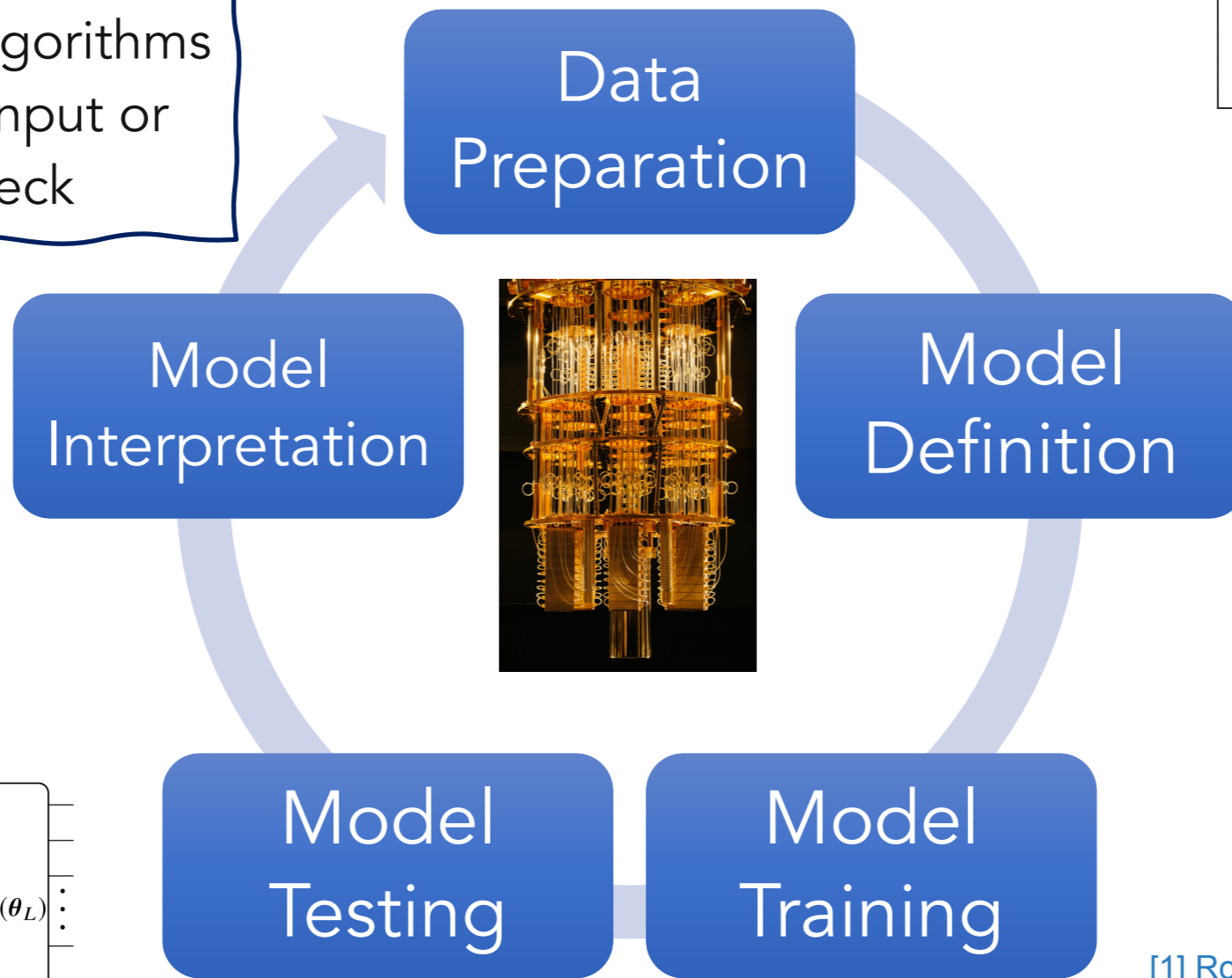
2024	2025	2026	2027	2028
Improving quantum circuit quality and speed to allow 5K gates with parametric circuits	Enhancing quantum execution speed and parallelization with partitioning and quantum modularity	Improving quantum circuit quality to allow 7.5K gates	Improving quantum circuit quality to allow 10K gates	Improving quantum circuit quality to allow 15K gates
Platform				
Code assistant 	Functions	Mapping Collection	Specific Libraries	
Transpiler Service 				
Resource Management	Circuit Knitting x P	Intelligent Orchestration		
Heron (5K)  Error Mitigation 5k gates 133 qubits Classical modular 133x3 = 399 qubits	Flamingo (5K) Error Mitigation 5k gates 156 qubits Quantum modular 156x7 = 1092 qubits	Flamingo (7.5K) Error Mitigation 7.5k gates 156 qubits Quantum modular 156x7 = 1092 qubits	Flamingo (10K) Error Mitigation 10k gates 156 qubits Quantum modular 156x7 = 1092 qubits	Flamingo (15K) Error Mitigation 15k gates 156 qubits Quantum modular 156x7 = 1092 qubits
Resource management  System partitioning to enable parallel execution	Scalable circuit knitting Circuit partitioning with classical reconstruction at HPC scale	Error correction decoder Demonstration of a quantum system with real-time error correction decoder		
Flamingo  Demonstrate scaling with modular connectors 	Kookaburra Demonstrate scaling with nonlocal c-coupler 	Demonstrate path to improved quality with logical memory 	Cockatoo Demonstrate path to improved quality with logical communication 	Starling Demonstrate path to improved quality with logical gates 

Quantum Machine Learning Lifecycle

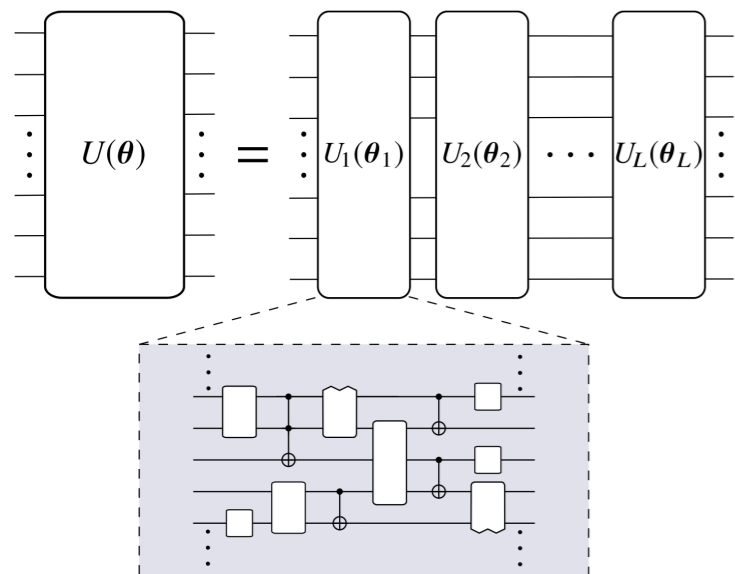
The quantum advantage of many known QML algorithms is impeded by an input or output bottleneck



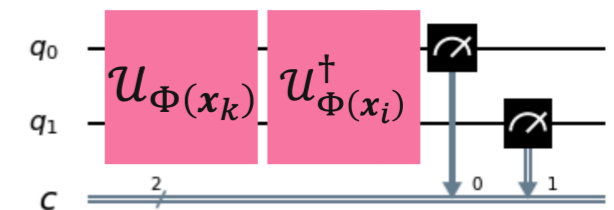
*Data Reduction
Data Encoding
[1,2,3]*



Trainability (BP...)



Read Out



[1] Robust data encodings for quantum classifiers, Ryan LaRose and Brian Coyle, Phys. Rev. A 102, 032420

[2] Quantum convolutional neural network for classical data classification, <https://arxiv.org/pdf/2108.00661.pdf>

[3] Quantum Support Vector Machines for Continuum Suppression in B Meson Decays, <https://arxiv.org/abs/2103.12257>

Models

Variational algorithms (ex. QNN)

Gradient-free or gradient-based optimization

Data Embedding can be learned

Ansatz design can leverage data symmetries¹

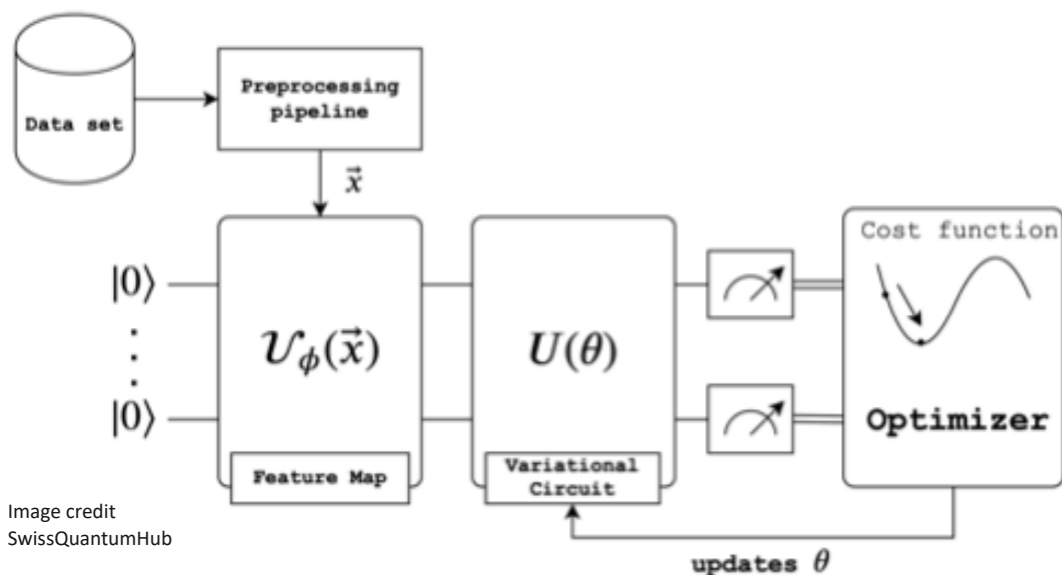


Image credit
SwissQuantumHub

Kernel methods (ex. QSVM)

Feature maps as quantum kernels

Classical kernel-based training
(convex losses)

Identify classes of kernels that relate to
specific data structures²

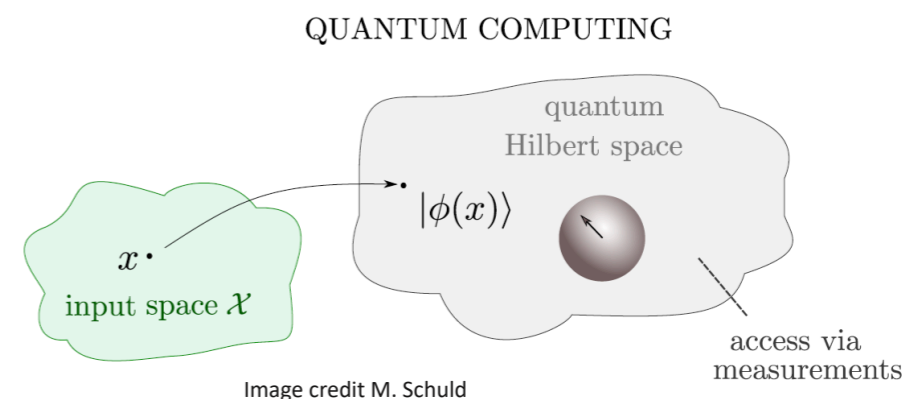


Image credit M. Schuld

Energy-based ML (ex. QBM)

Build networks of **stochastic binary units**
and optimise their energy.

Quantum Boltzmann Machines has
quadratic energy function that follows the
Boltzmann distribution (Ising Hamiltonian)

¹ Bogatskiy, Alexander, et al. "Lorentz group equivariant neural network for particle physics." PMLR, 2020.

³ Jerbi, Sofiene, et al. "Quantum machine learning beyond kernel methods." arXiv:2110.13162 (2021).

Parameter optimization

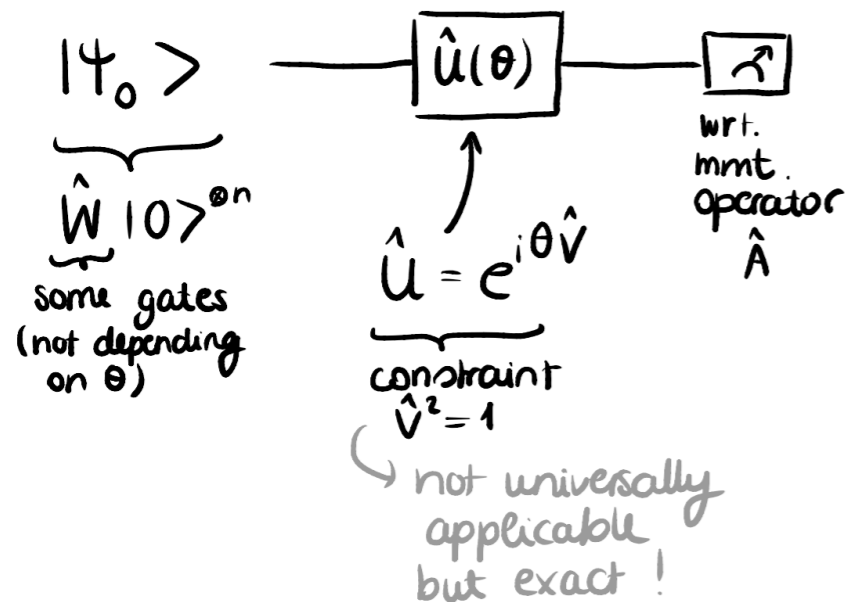
See C. Rieger's [summer students lecture](#)

The parameter-shift rule (gradient-based)

$$\theta \rightarrow \theta - \eta \nabla_{\theta} f$$

$\uparrow \langle \hat{A}(\theta) \rangle$

Compute **partial derivative** of variational circuit parameter θ , alternative to analytical gradient computation and classical finite difference rule (numerical errors and resource cost considerations)



$$\Rightarrow \nabla_{\theta} \langle \hat{A} \rangle = u \left[\langle \hat{A}(\theta + \frac{\pi}{4u}) \rangle - \langle \hat{A}(\theta - \frac{\pi}{4u}) \rangle \right]$$

Evaluate Quantum Circuit twice at shifted parameters to compute gradient

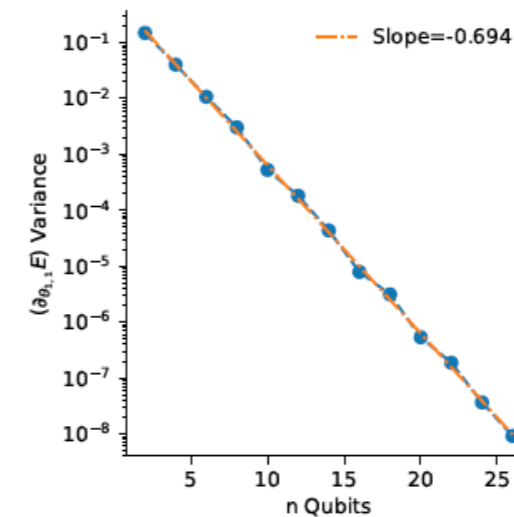
Gradients decay and Model Convergence

Classical gradients **vanish exponentially** with the number of layers (J.McClean *et al.*, arXiv:1803.11173)

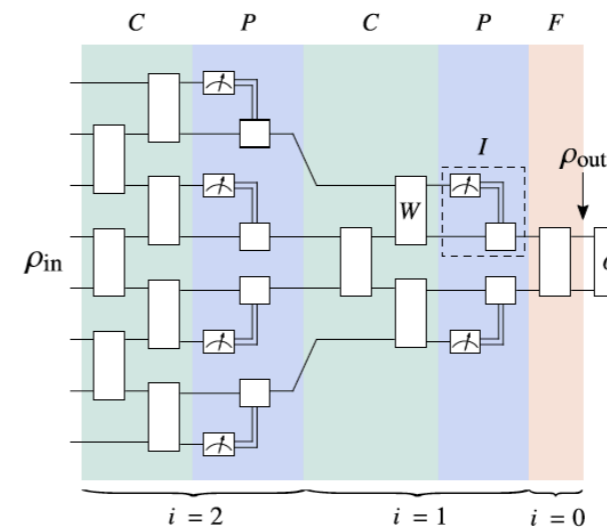
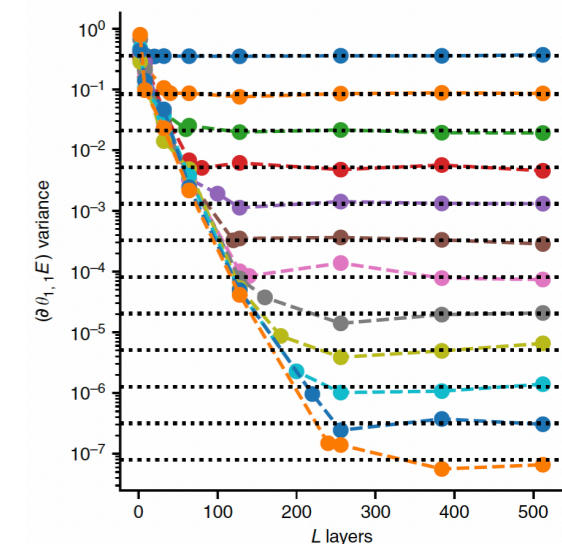
- Convergence still possible if gradients consistent between batches.

Quantum gradient **decay exponentially** in the number of qubits (number of graph paths is exponential in the number of gates)

- Random circuit initialization
- Loss function locality in shallow circuits (M. Cerezo *et al.*, arXiv:2001.00550)
- Ansatz choice: TTN, CNN (Zhang *et al.*, arXiv:2011.06258, A Pesah, *et al.*, *Physical Review X* 11.4 (2021): 041011.)
- Noise induced barren plateau (Wang, S *et al.*, *Nat Commun* 12, 6961 (2021))



J. McClean *et al.*, arXiv:1803.11173



QCNN: A Pesah, *et al.*, *Physical Review X* 11.4 (2021): 041011

Quantum Convolutional NN:
Convolution: general SU(4)
Pooling: reduces number of qubits

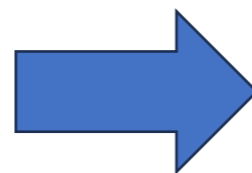
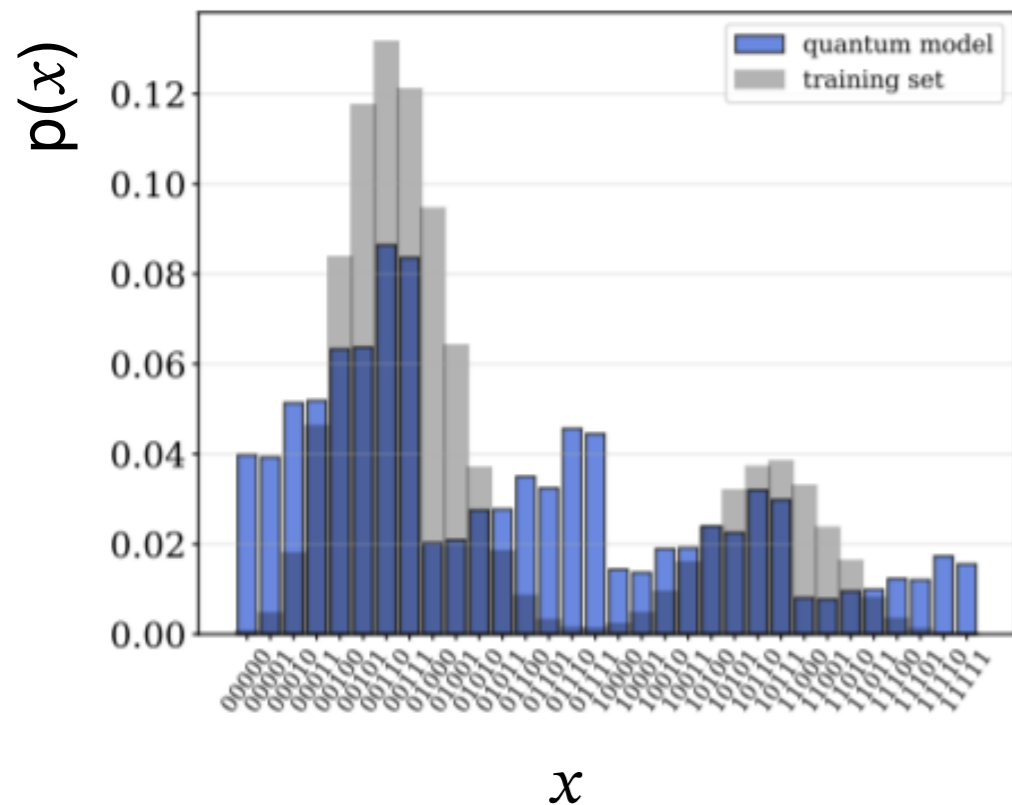
Large number of measurements: $1/\epsilon^2$ measurements to estimate a cost to precision ϵ

Quantum Generative Models

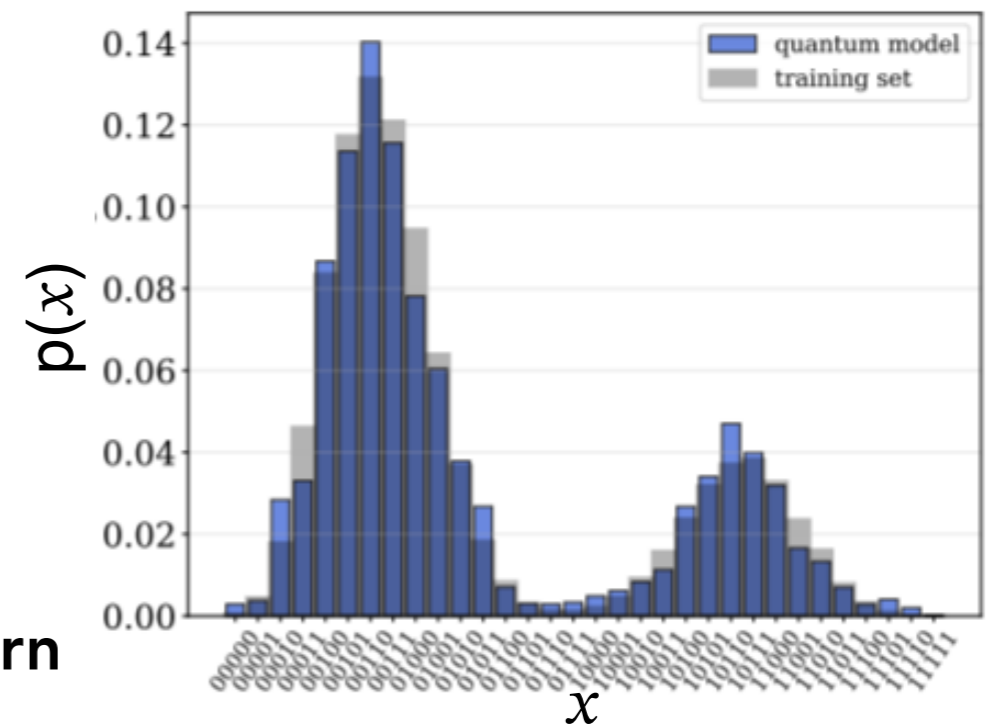
Learn probability distribution that best describes a data set

Quantum Circuit Born Machine

Sample variational pure state $|\psi(\theta)\rangle$ by projective measurement through **Born rule**: $p_{\theta}(\mathbf{x}) = |\langle \mathbf{x} | \psi(\theta) \rangle|^2$.



Deeper circuits learn better representations..
Or don't they ??



Implicit and Explicit Models

Classified according to whether or not they **have access to the probability distribution function**

Explicit Models have access to PDF in polynomial time

- Use explicit losses that are defined by probabilities
- Ex. TN or autoregressive models

$$\text{Explicit} \\ \sum_{\mathbf{x}} f(\tilde{p}(\mathbf{x}), \tilde{q}_{\theta}(\mathbf{x}))$$

Ex. KL Divergence

$$D_{\text{KL}}(P||Q) = \sum_i P(i) \log\left(\frac{P(i)}{Q(i)}\right)$$

Implicit models do not have access to PDF. Can sample from it

- Use implicit losses built on samples
- Ex. GAN, QBM, VAE... QCBM...

$$\text{Implicit} \\ \mathbb{E}_{\mathbf{x}, \mathbf{y}} [g(\mathbf{x}, \mathbf{y})]$$

Ex. MMD

$$\text{MMD}(\mathbb{P}_r, \mathbb{P}_g) = \left(\mathbb{E}_{\substack{\mathbf{x}_r, \mathbf{x}'_r \sim \mathbb{P}_r, \\ \mathbf{x}_g, \mathbf{x}'_g \sim \mathbb{P}_g}} \left[k(\mathbf{x}_r, \mathbf{x}'_r) - 2k(\mathbf{x}_r, \mathbf{x}_g) + k(\mathbf{x}_g, \mathbf{x}'_g) \right] \right)^{\frac{1}{2}}$$

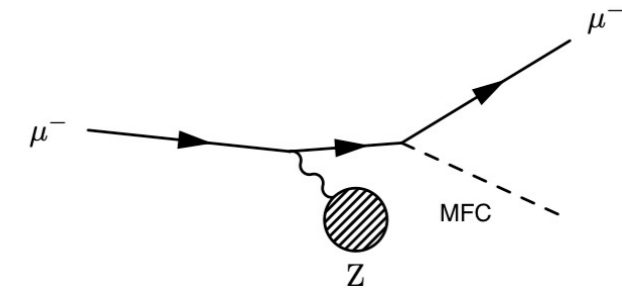
Strong impact on trainability!

Quantum Circuit Born Machine for Event Generation

Born machine:

Produces statistics according to Born's measurement rule using parametrized quantum circuit $|\psi(\theta)\rangle$

$$p_{\theta}(x) = \left| \langle x | \psi(\theta) \rangle \right|^2, x \in \{0,1\}^{3n}$$



Muon fixed target scattering experiment

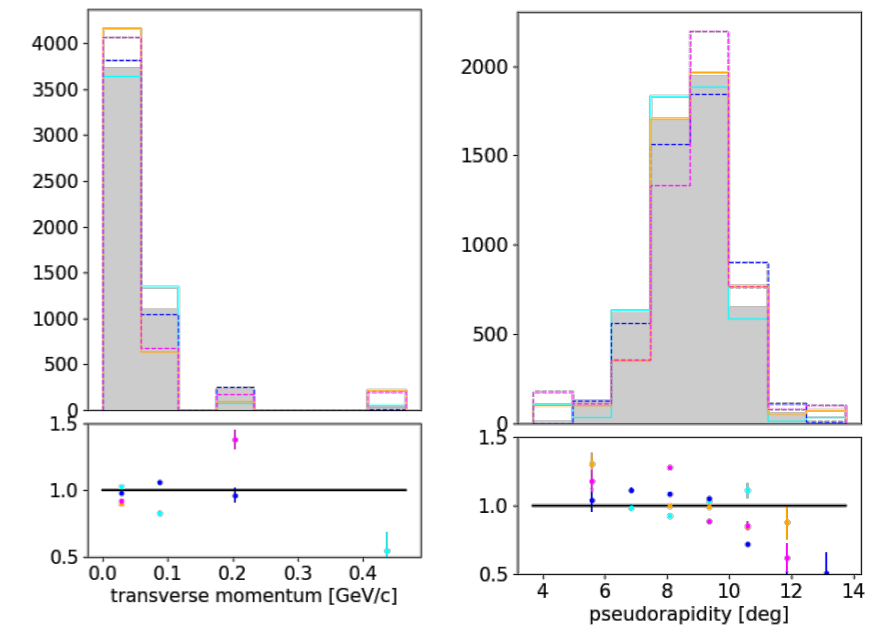
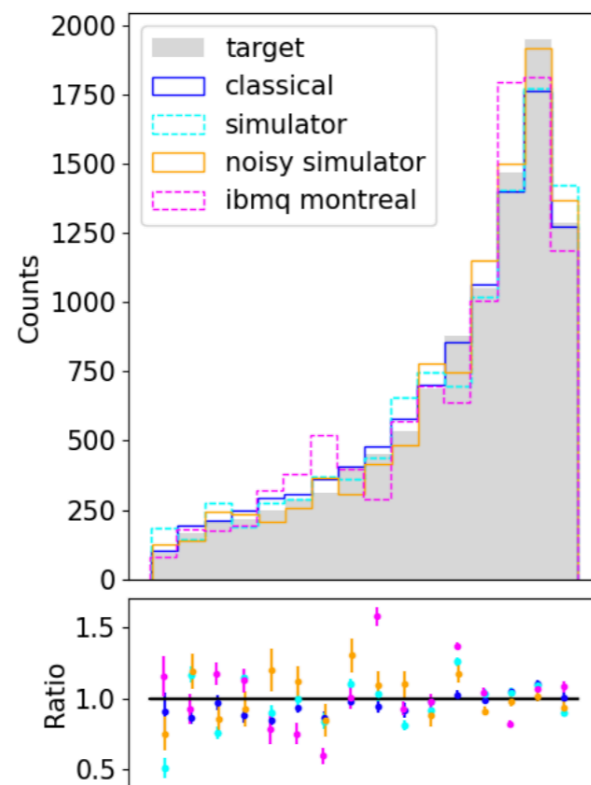
Train using Maximum Mean Discrepancy loss function:

$$\text{MMD}(P,Q) = \mathbb{E}_{\substack{X \sim P \\ Y \sim P}} [K(X, Y)] + \mathbb{E}_{\substack{X \sim Q \\ Y \sim Q}} [K(X, Y)] - 2\mathbb{E}_{\substack{X \sim P \\ Y \sim Q}} [K(X, Y)]$$

Gaussian kernel

$$K(x, y) = \exp\left(-\frac{(x-y)^2}{2\sigma}\right)$$

Generate discrete PDFs (continuous in the limit increasing no. of qubits)



A classification task

Analysis setup

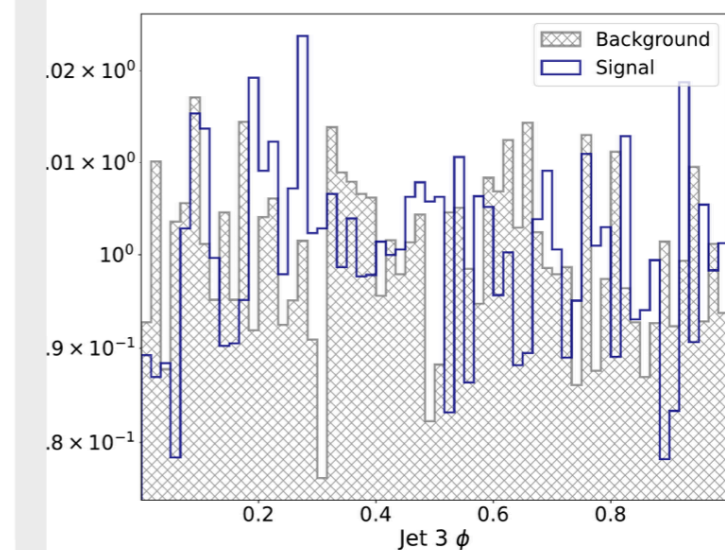
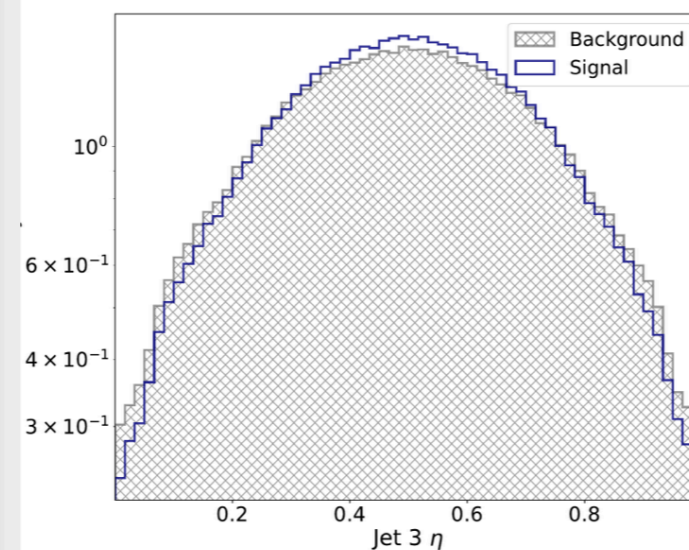
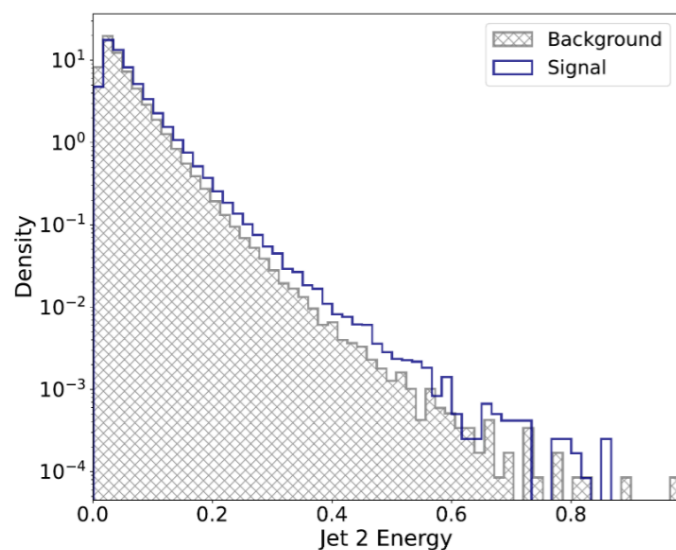
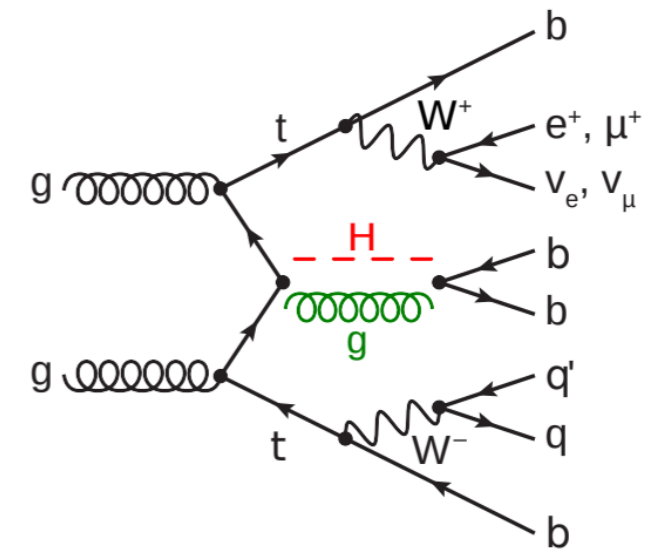
Analysis

Discrimination of the signal over the overwhelming background

Features

- For the each jet we have 8 features: $(p_T, \eta, \phi, E, b \text{ tag}, p_x, p_y, p_z)$
- For MET we have 4 features: (p_T, p_x, p_y, ϕ)
- For the lepton (electron or muon) we have 7 features: $(p_T, \eta, \phi, E, p_x, p_y, p_z)$

$$\#features = 8 \times 7(\text{jets}) + 7(1\text{lepton}) + 4(\text{MET}) = 67$$

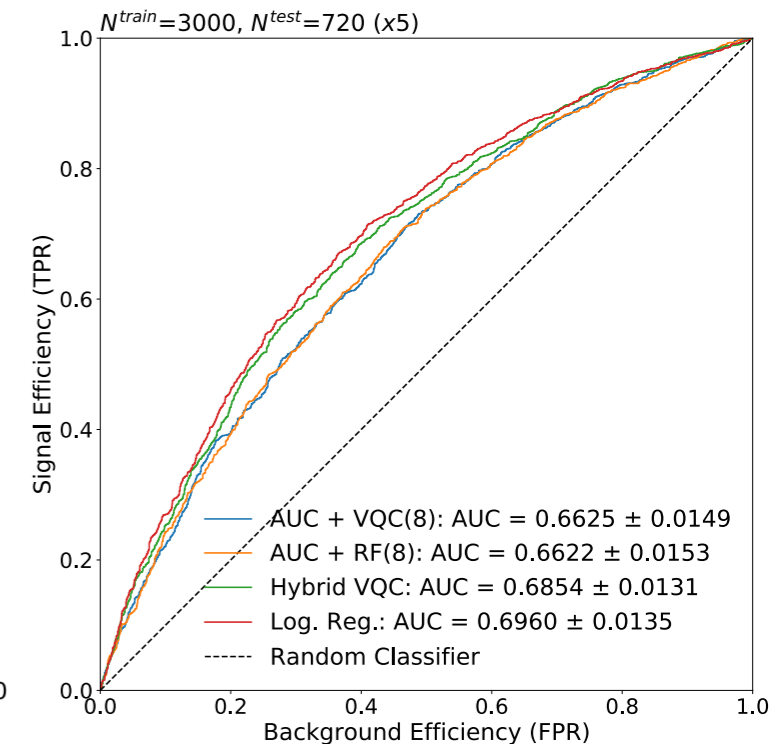
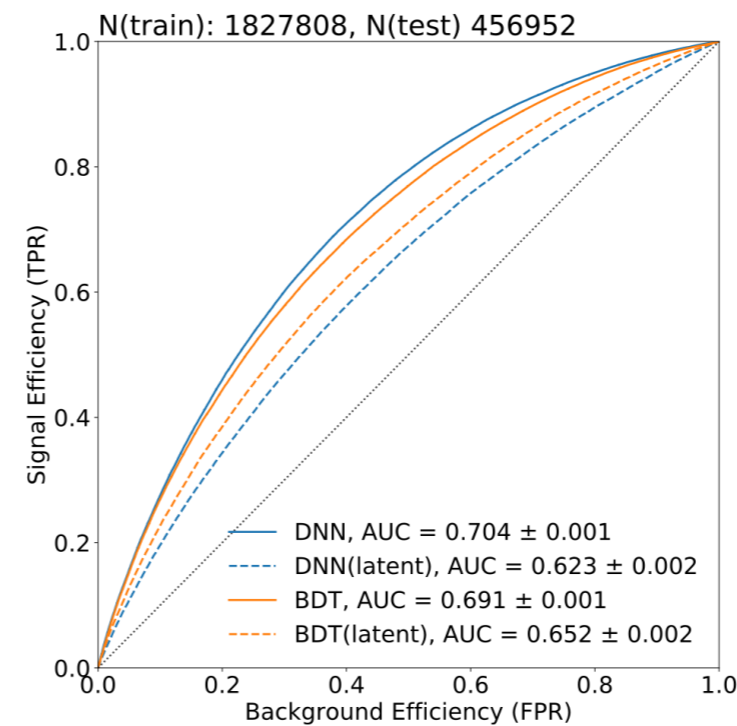
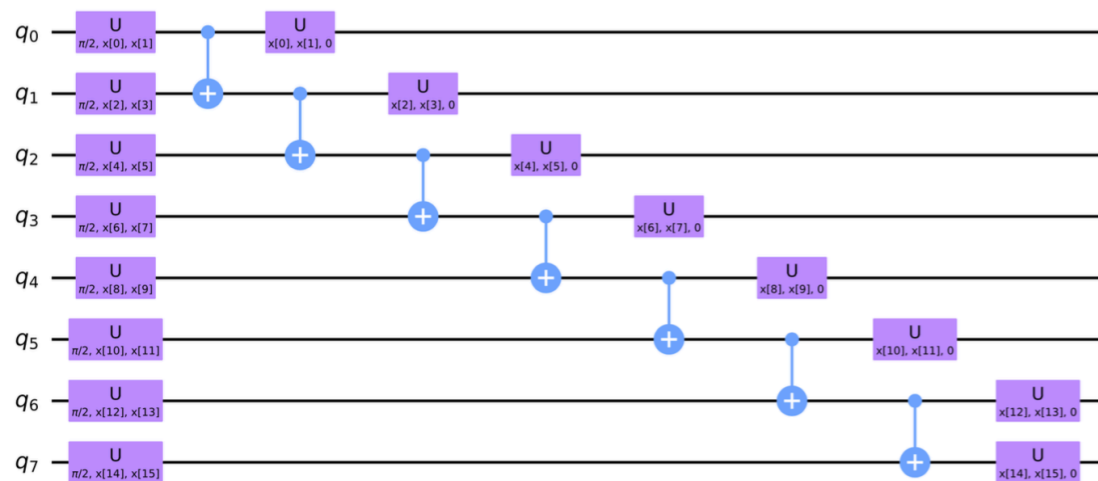


Quantum SVM for Higgs Classification

Input dimensionality reduction through an Auto-Encoder projects to a lower dimension latent space (8,16)

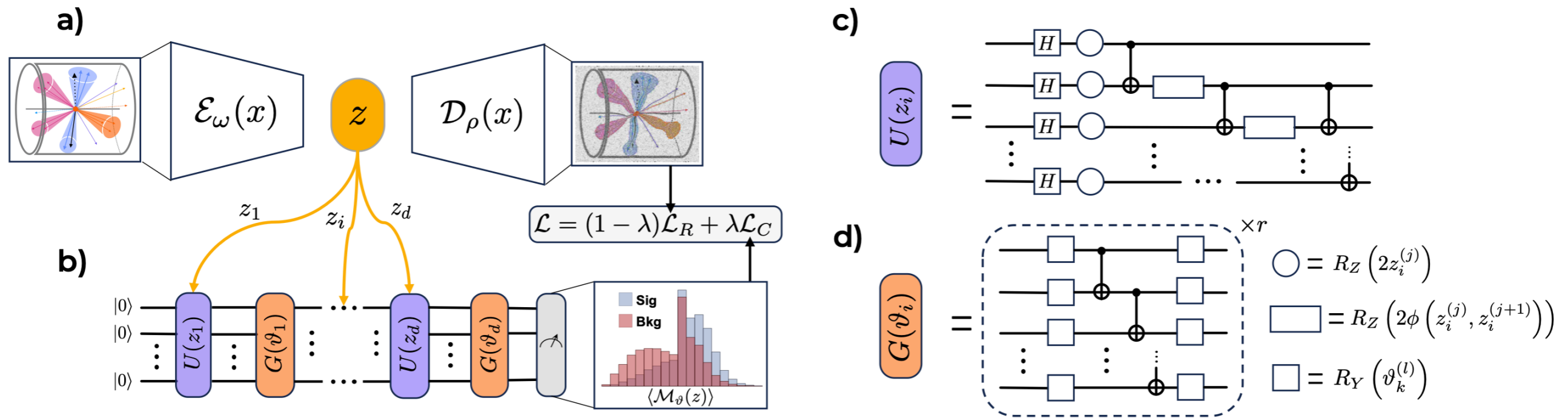
Feature selection + Model	AUC
AUC + QSVM	0.66 ± 0.01
PyTorch AE + QSVM	0.62 ± 0.03
AUC + SVM rbf	0.65 ± 0.01
PyTorch AE + SVM rbf	0.62 ± 0.02
KMeans + SVM rbf	0.61 ± 0.02

Feature selection + Model	AUC
AUC + QSVM	0.68 ± 0.02
AUC + Linear SVM	0.67 ± 0.02
Logistic Regression	0.68 ± 0.02



Data encoding circuit serving as feature map for the 8-qubit QSVM implementation.

Guided Quantum Compression



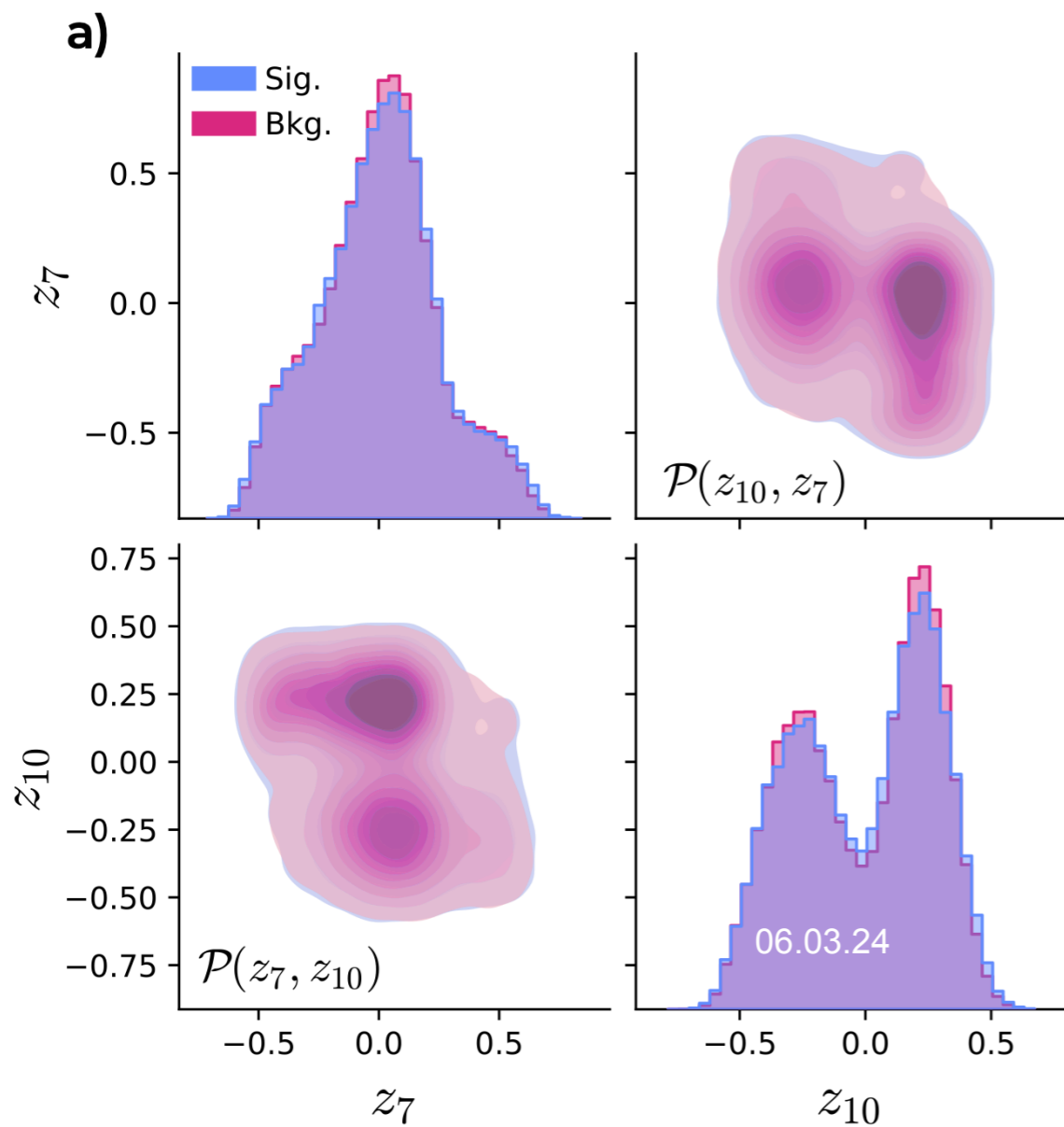
Two hybrid quantum-classical strategies:

GQC: Joint training

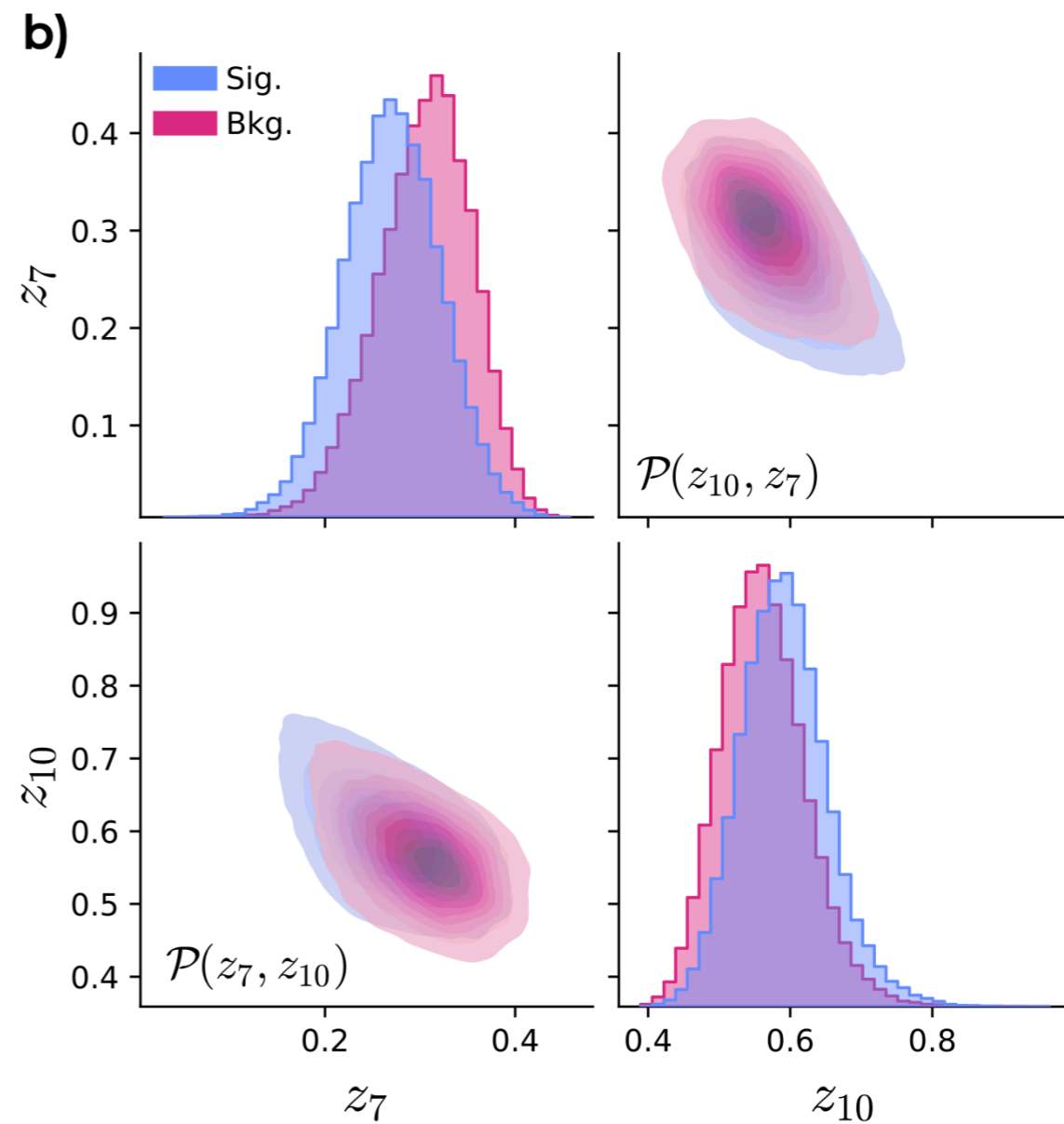
2Steps: The data compression step is independently trained

Latent Space Representation

2 Steps

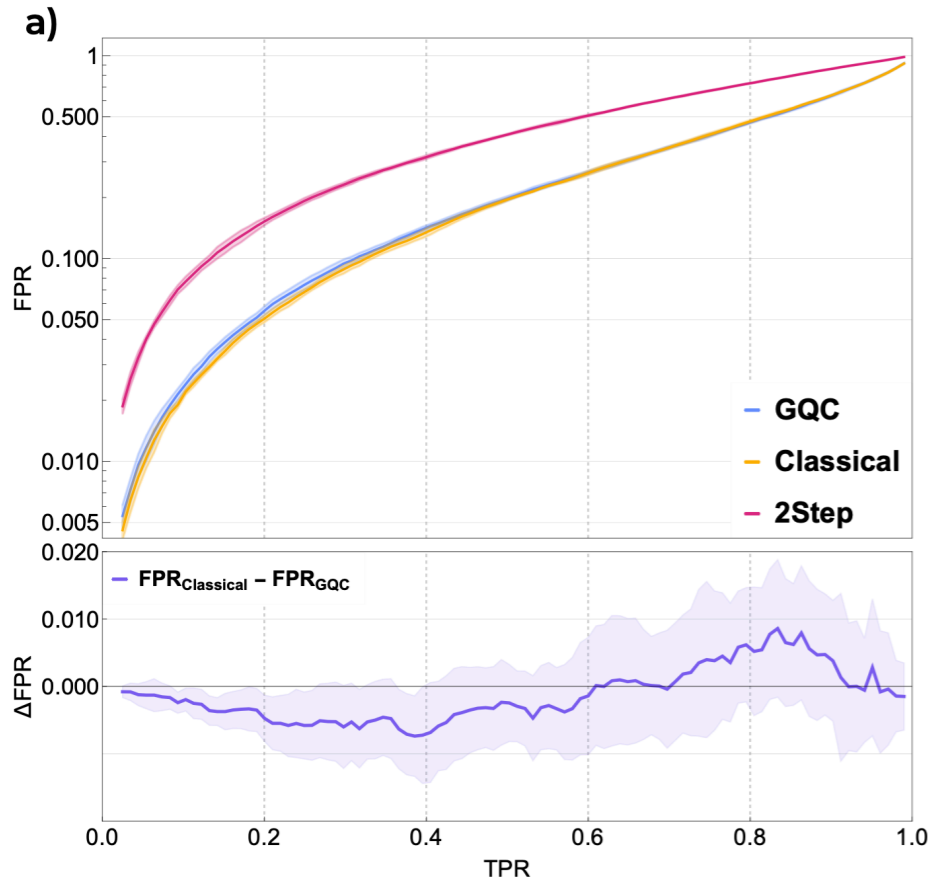


GQC

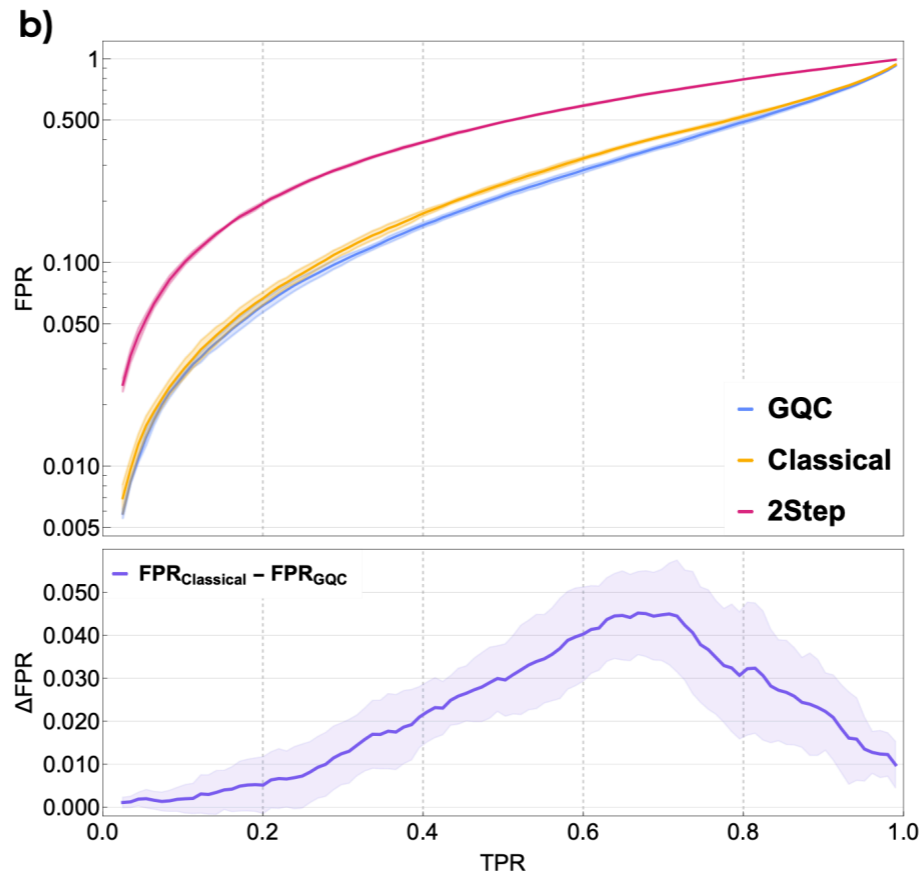


Results

Including b-tagging

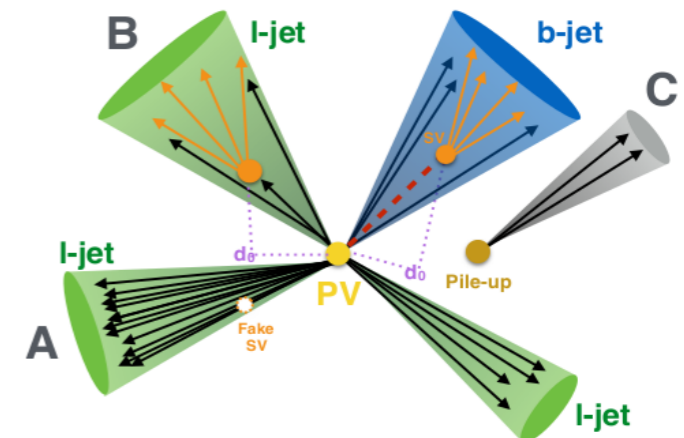


No b-tagging



compression method has significant impact on the classifier performance.

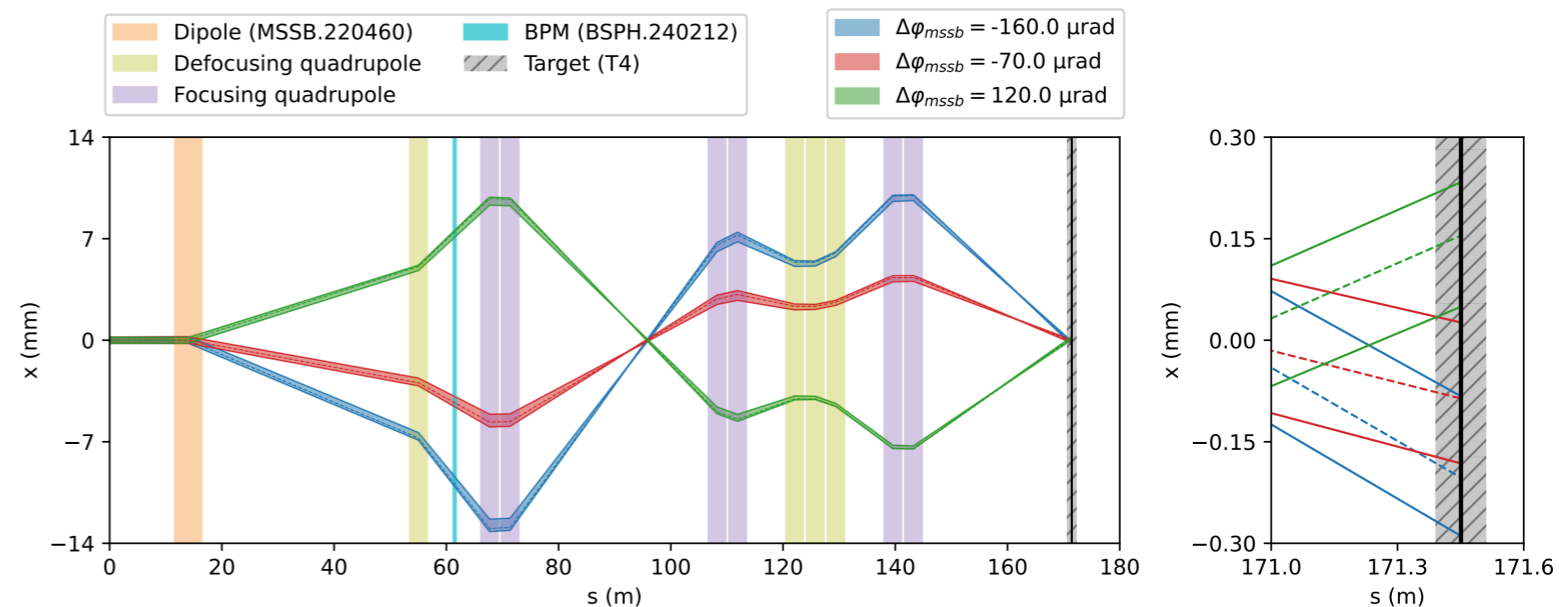
NB: b-tag features are high level features containing information about the quark content



Reinforcement Learning for steering CERN beams

1D beam steering inspired by the CERN North Area transfer line

- **Action:** (discrete) deflection angle
- **State:** (continuous) BPM position
- **Reward:** integrated beam intensity on target
- **Optimality:** fraction of states in which the agent takes the right decision



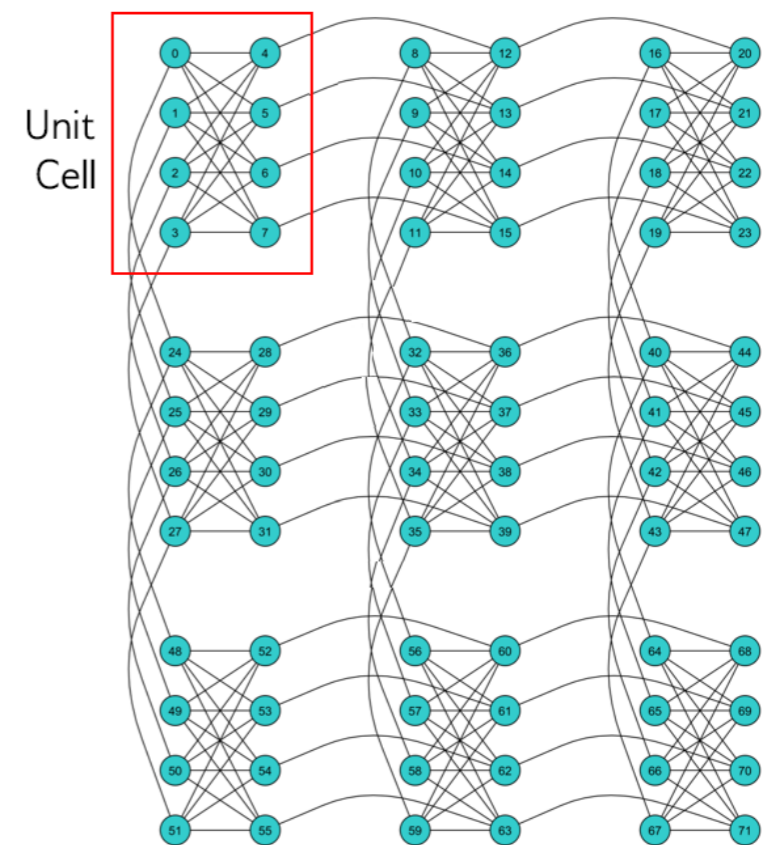
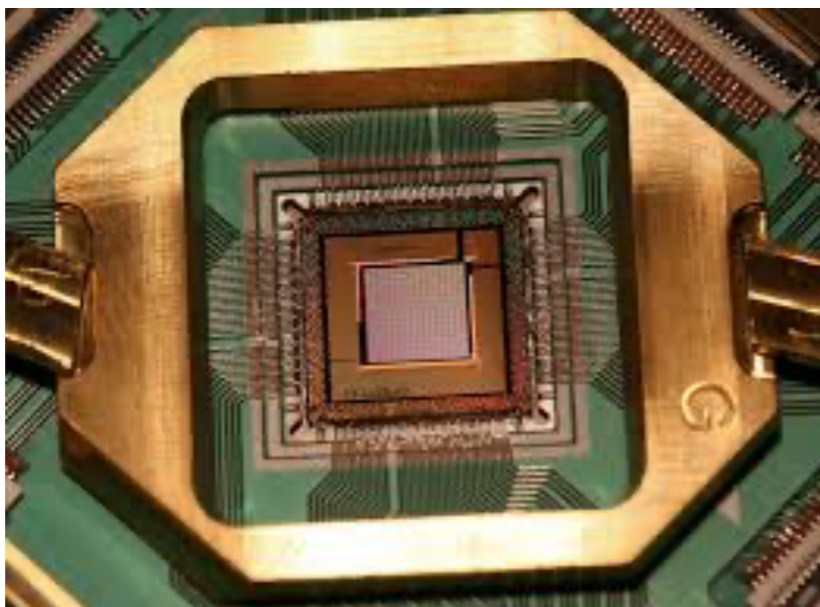
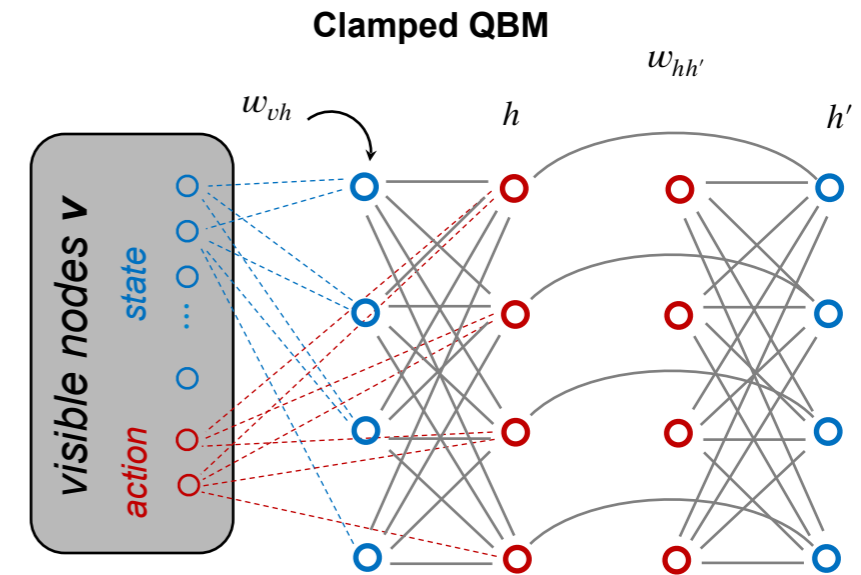
Approach based on Q-learning : the reward is estimated using a Q-function

Quality of the Q-function drives performance

- **Classical Deep Q-learning (DQN)**
Feed-forward neural net
- **Free-energy based RL (FERL)**
Quantum Boltzmann machine (QBM)

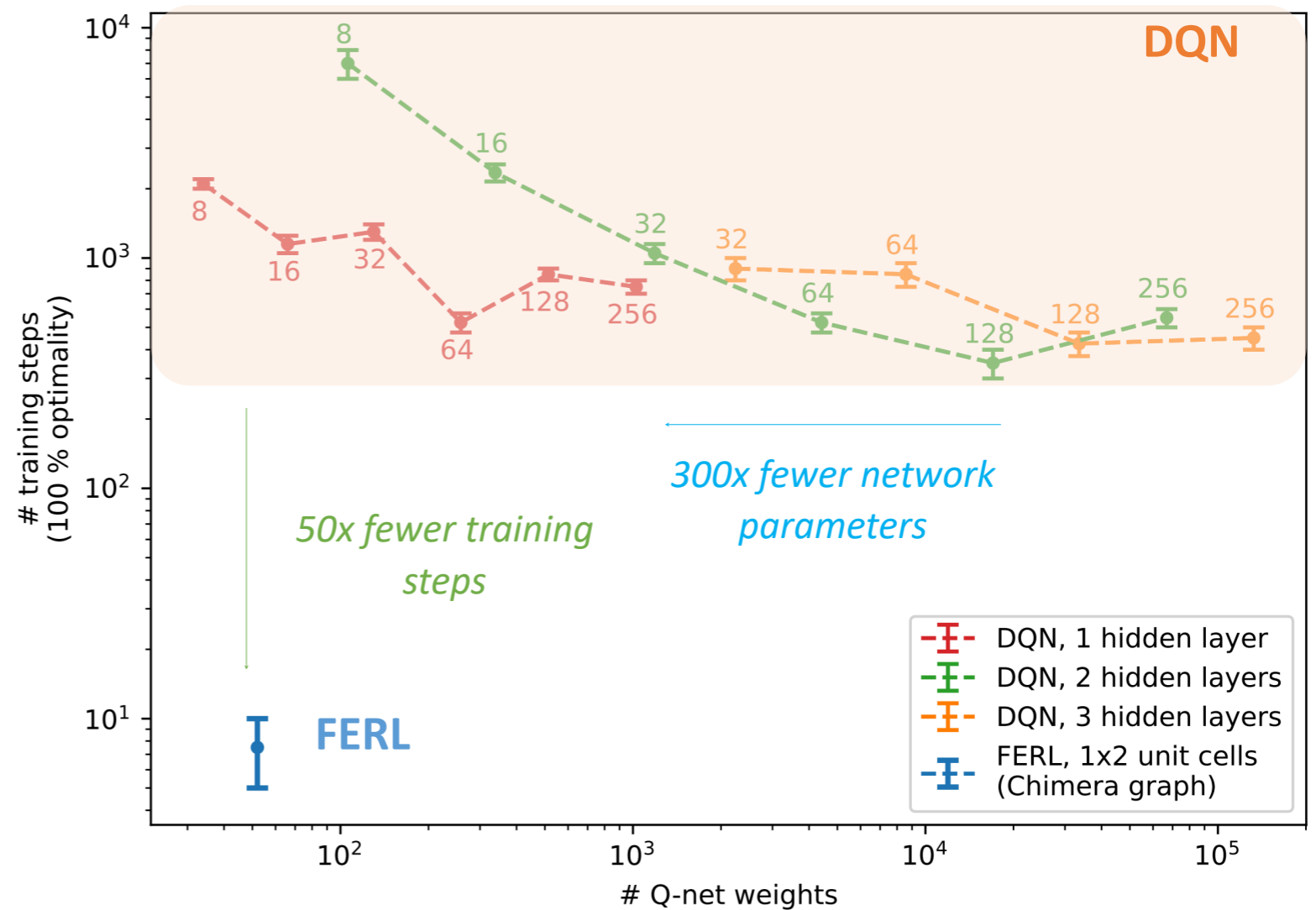
Quantum Boltzmann Machines

- Create a network of qubits similar to the binary units in a classical Boltzmann machine
- Map network to the quantum computer graph
- Train by minimising the qubits system energy



Free-energy based RL (FERL)

Sample-efficiency is really important given cost of training (beam time)



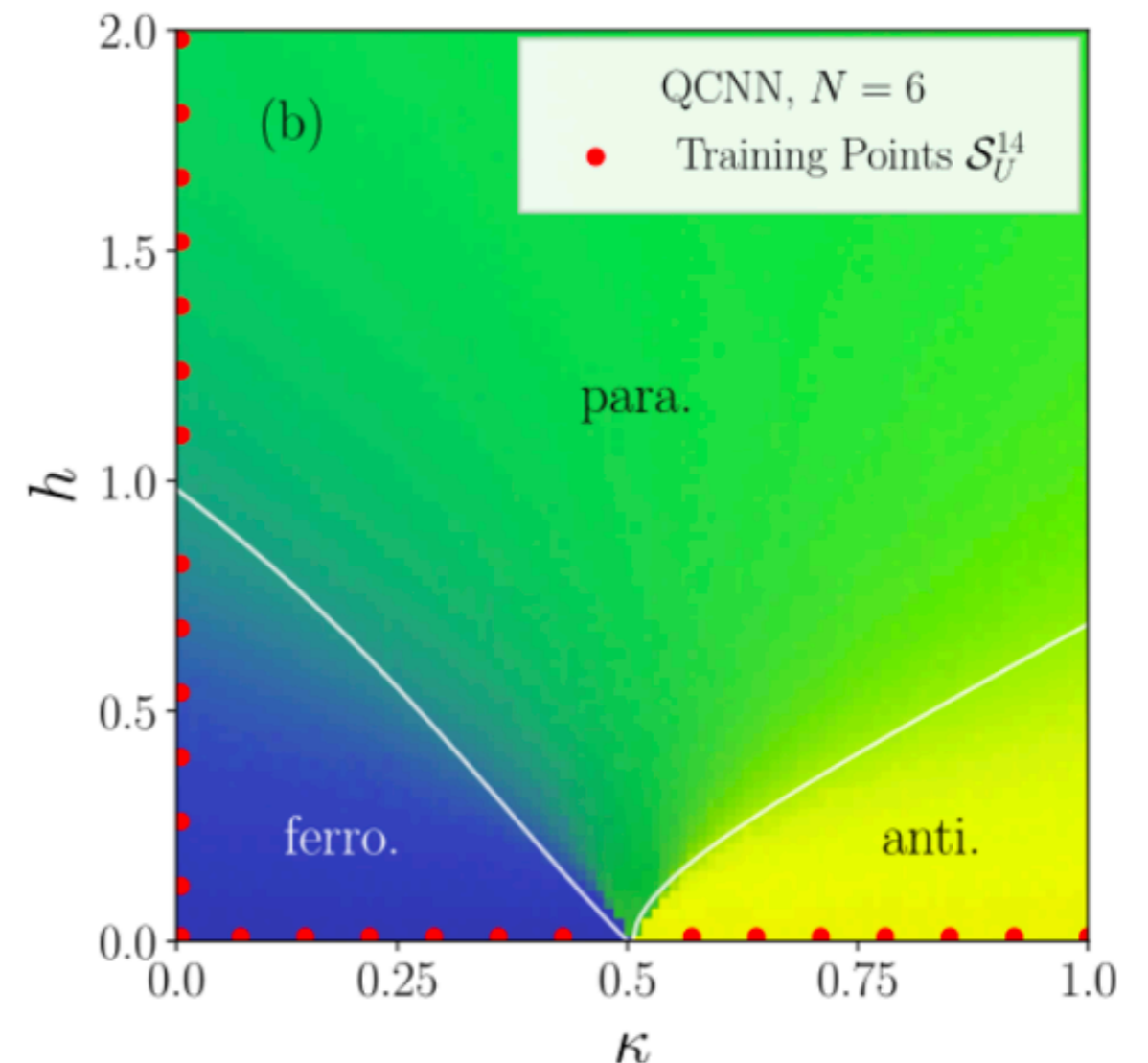
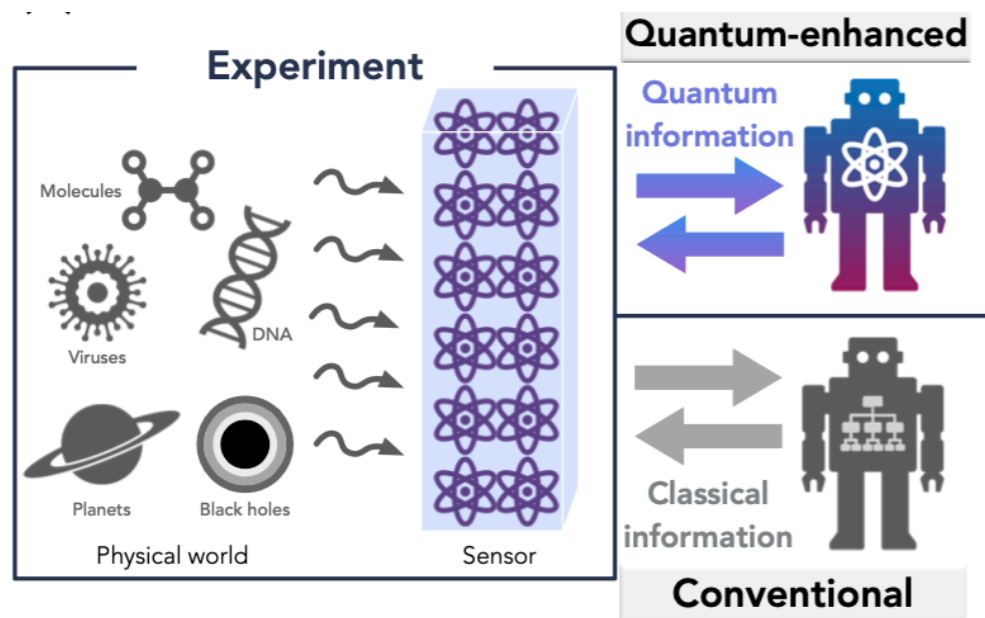
Classifying quantum data

Saverio Monaco et al., **Quantum phase detection generalisation from marginal quantum neural network models**, arXiv:2208.08748v1.

Generate **quantum states** directly on the device

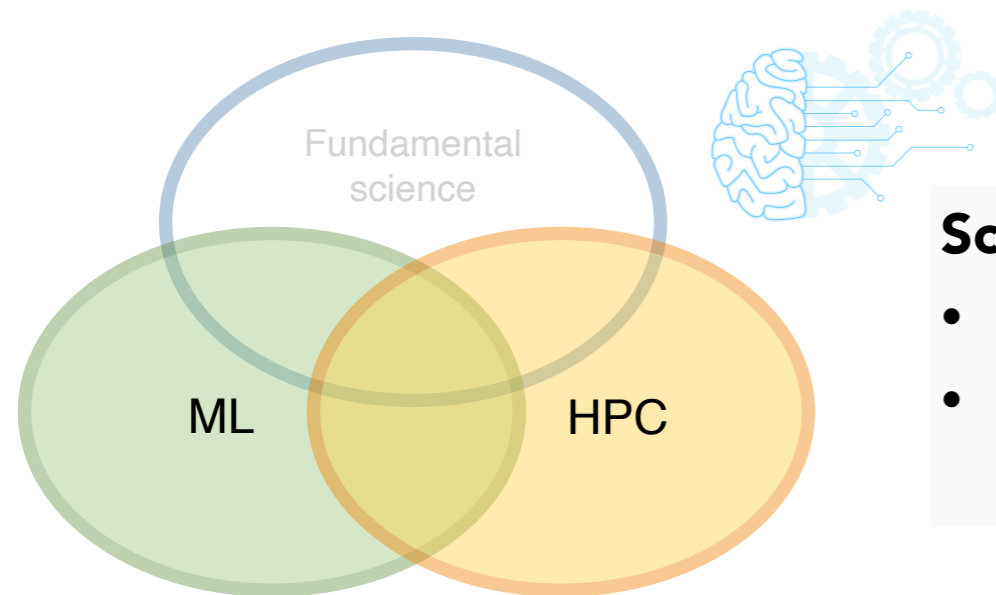
Train QCNN to **classify quantum states**

Use marginal datasets \rightarrow **OOD generalization !**



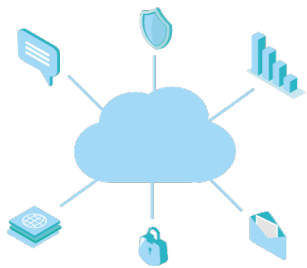
Backup

Future challenges



Scaling:

- **Efficiently scaling distributed training to larger models**
- Develop the software infrastructure and model architecture suitable for such big models



Accessibility:

- **Deployment of the models on the cloud**
- we need an integration of the HPC centers to provide **seamless access** and data movement in the background (example: Google Cloud)

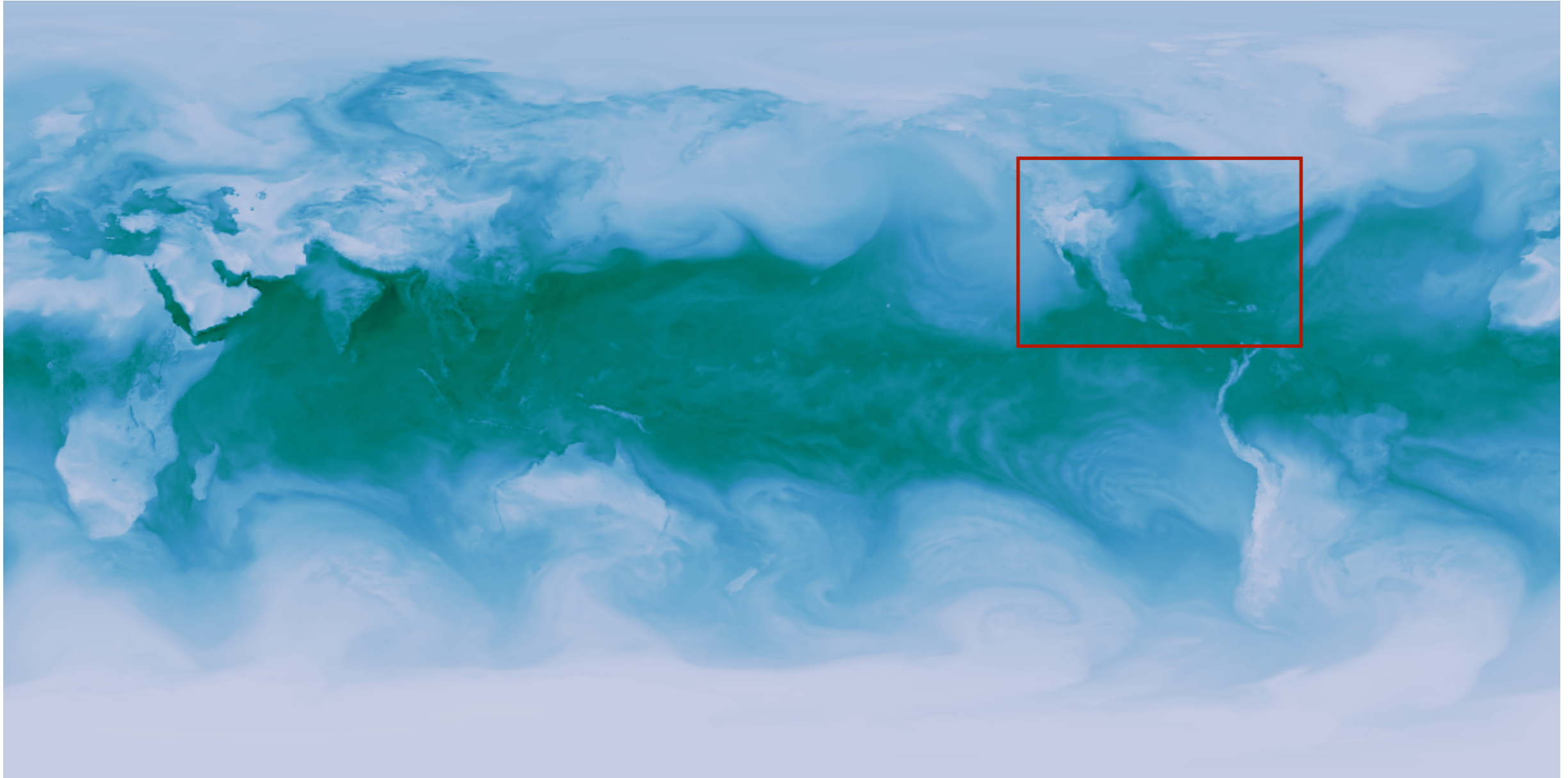


Maintenance:

- **How to integrate new incoming data**
- How to **expand** to new fields/variables without fully retraining the model each time?

Results: Target - ERA5

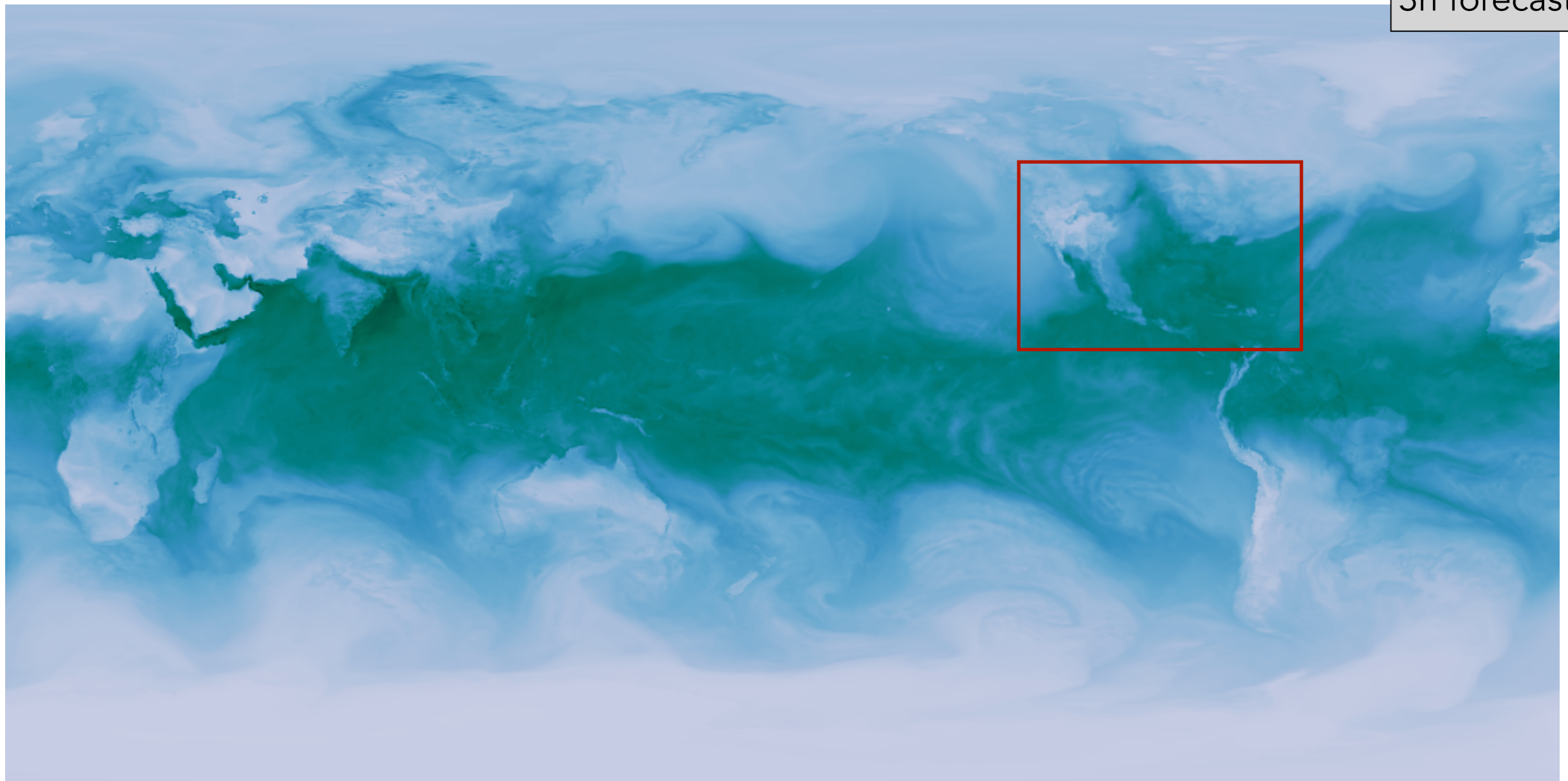
specific humidity, June 15th 2018 13:00 UTC



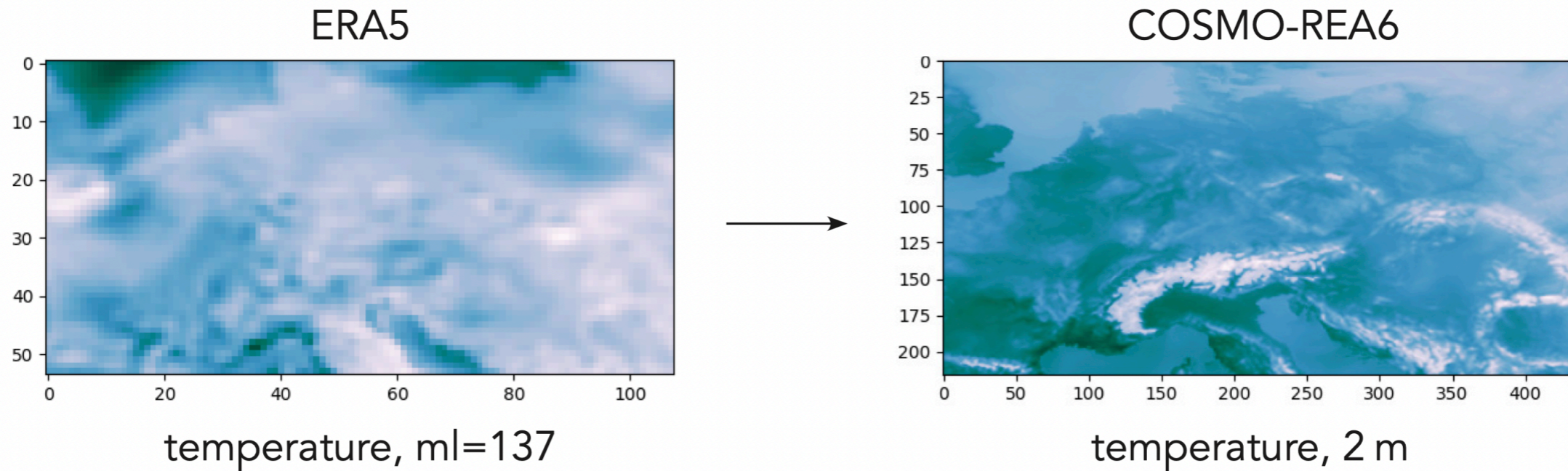
Results: Prediction - AtmoRep

specific humidity, June 15th 2018 13:00 UTC

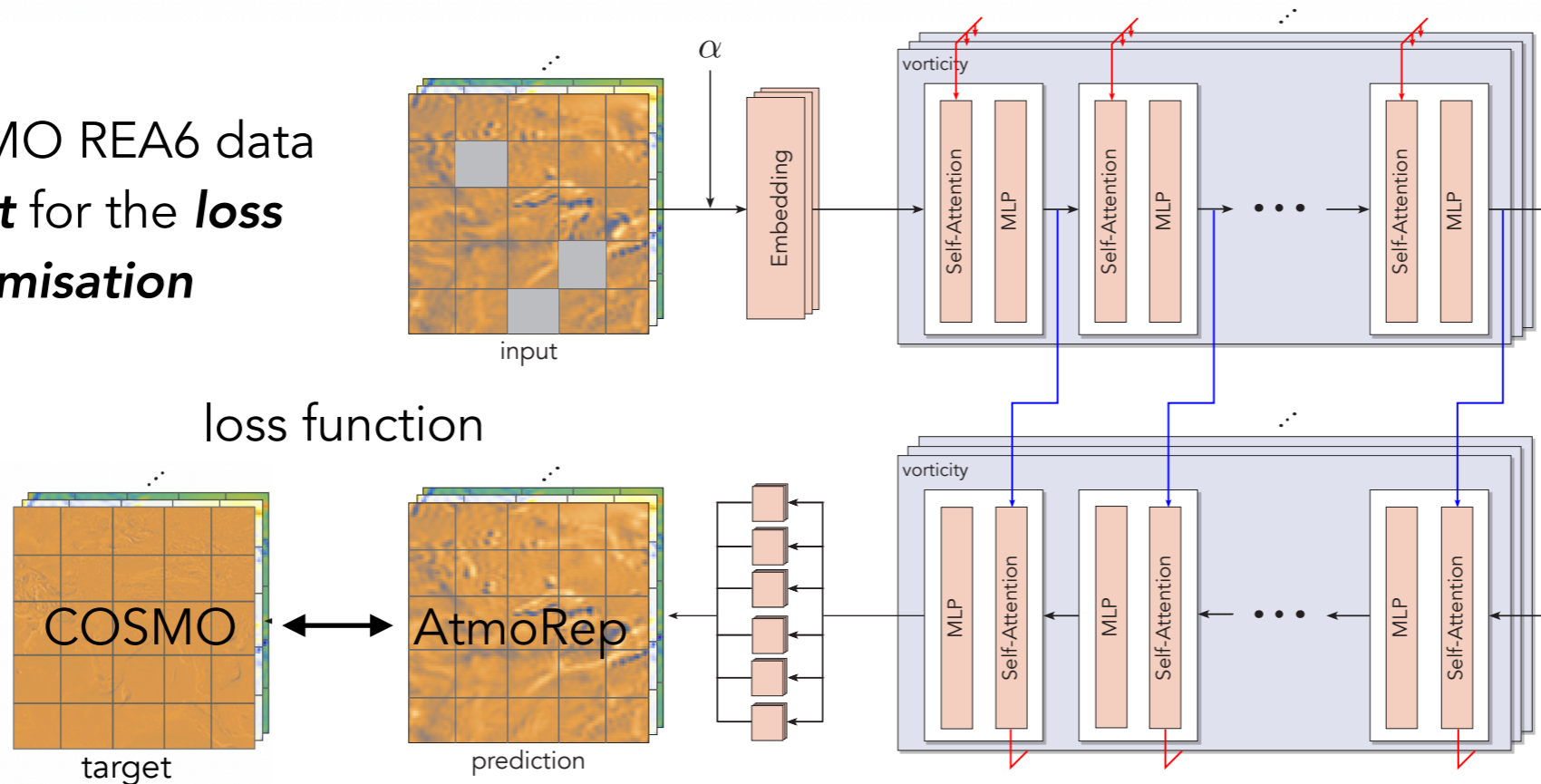
3h forecast



Downscaling



Use COSMO REA6 data as **target** for the **loss minimisation**

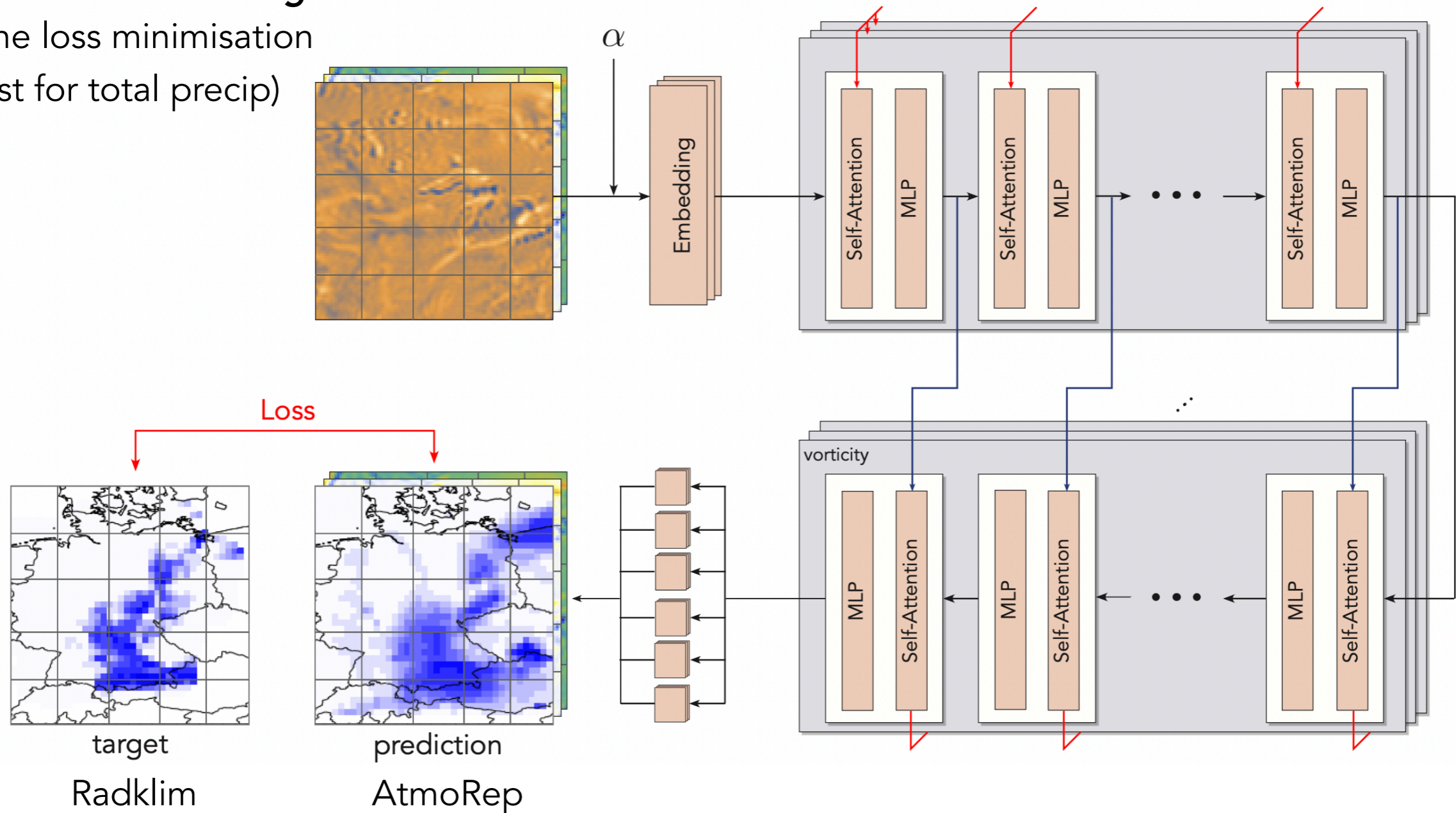


Bias corrections

Precipitation rates are known to be suboptimal in ERA5

Use RADKLIM radar data to fine-tune the precipitation rates in AtmoRep

Use *Radklim* data as *target*
for the loss minimisation
(just for total precip)



Bias corrections: Results

Precipitation rates are known to be suboptimal in ERA5
Use RADKLIM radar data to fine-tune the precipitation rates in AtmoRep

