DLR Quantencomputing Initiative

Quantum Computing for Earth System Modelling

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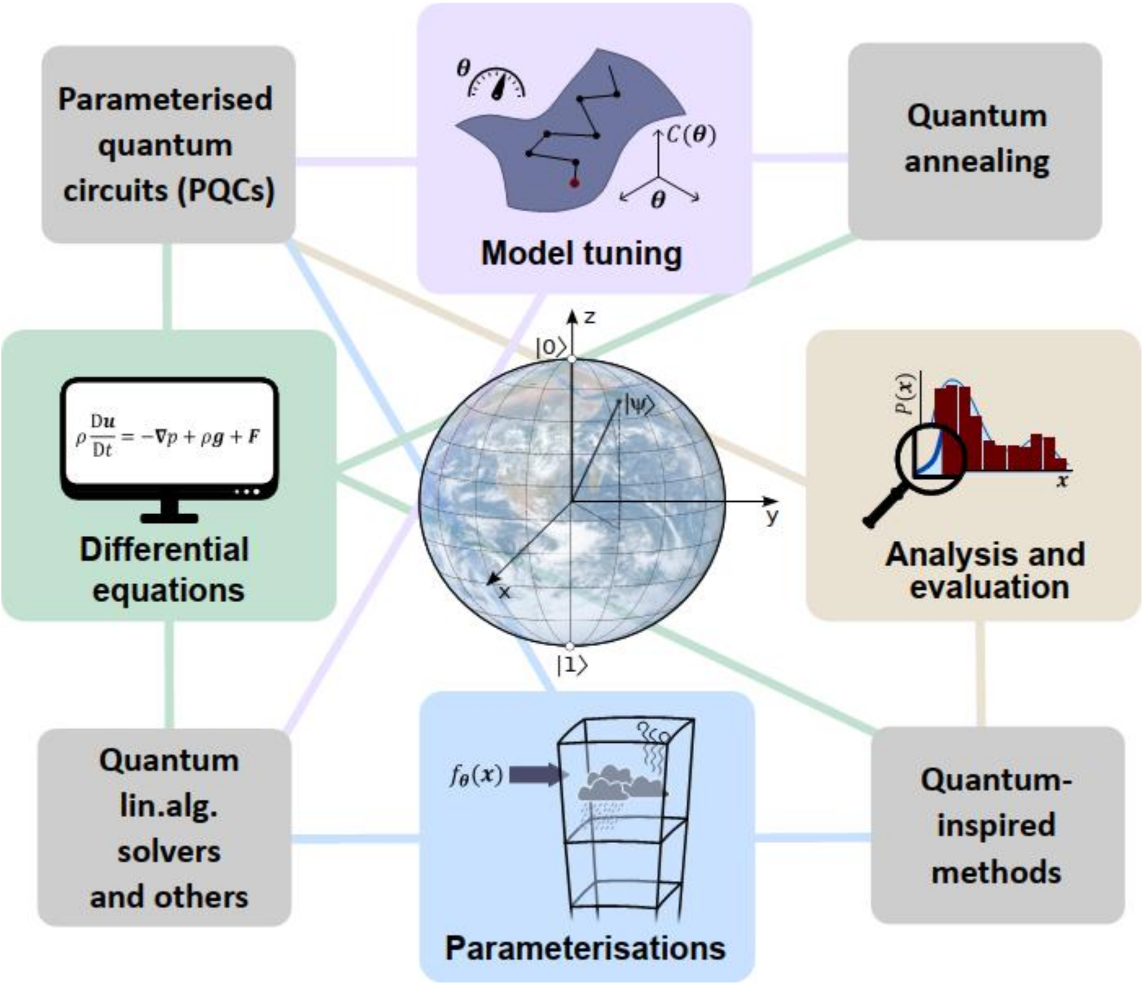
Contributions by V. Eyring, F. Herbort, H. Keller, J. Klamt, N. Klement, J.d.D. Rodriguez Garrido, E. Sarauer

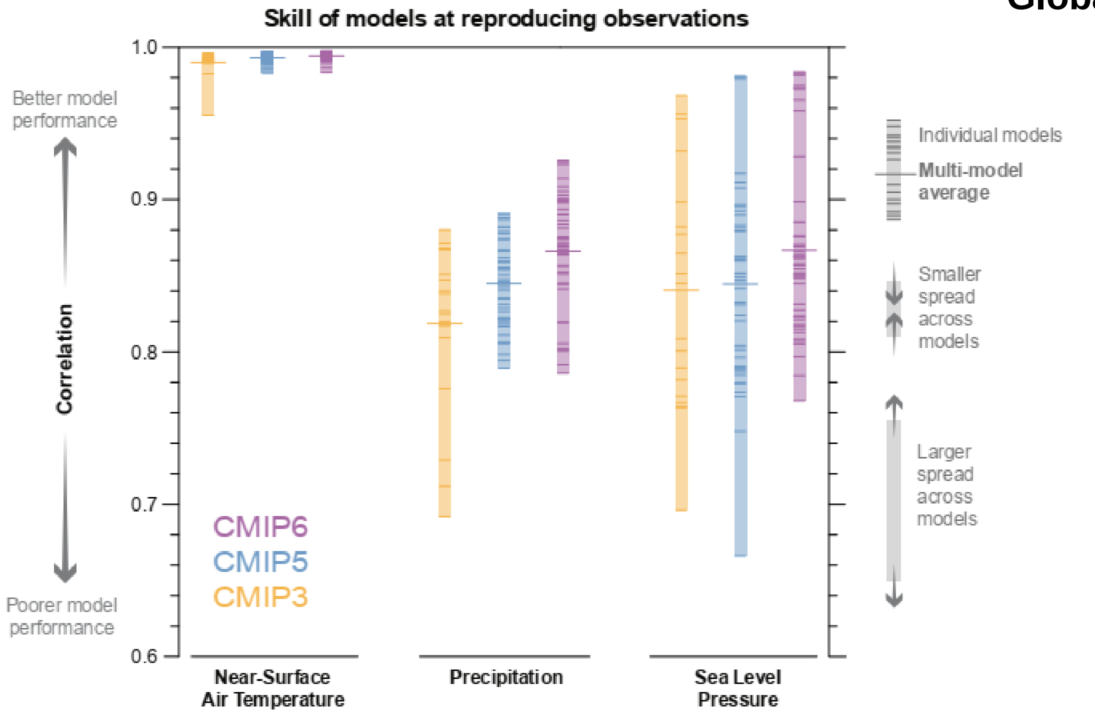
Outline

+ Introduction
+ Improving subgrid-scale parameterizations
+ Quantum computing for PDEs
+ Quantum-assisted model tuning
+ Conclusion

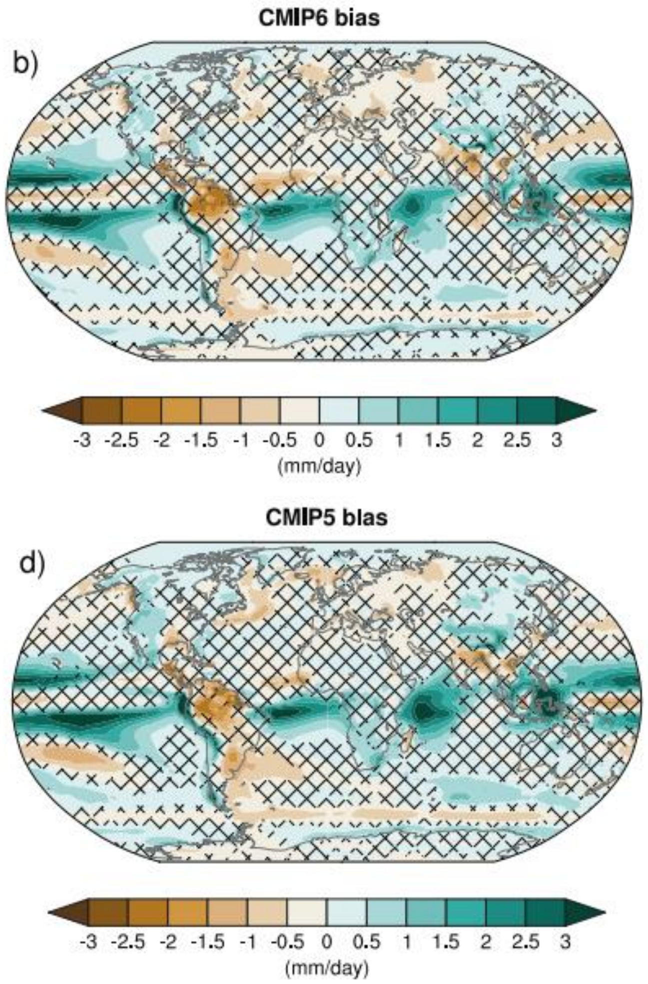


Schwabe et al: Env. Data Sci. 4, e35 (2025)

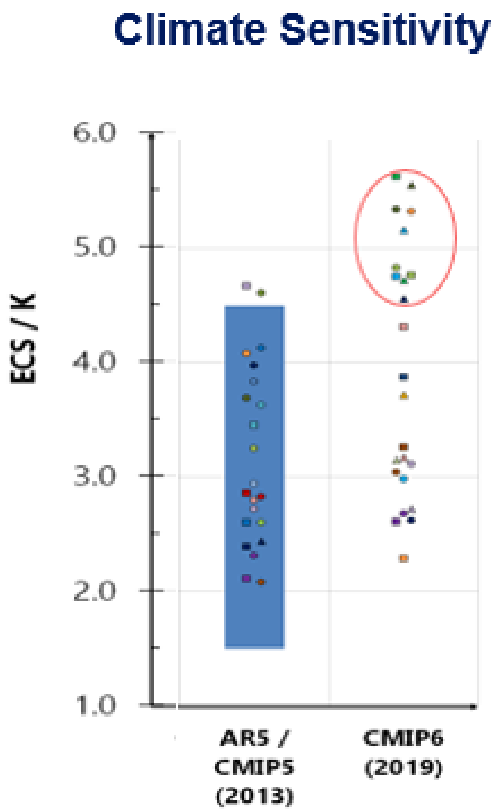
Climate models are improving, yet systematic biases remain.



Precipitation bias (1995–2014) to Global Precipitation Climatology Project (GPCP)



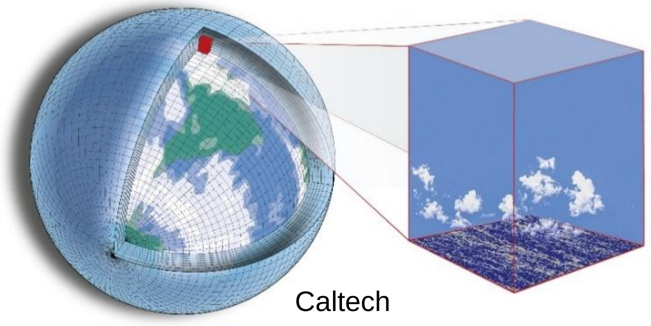
Colour Robust bias Conflicting signals



Eyring et al., IPCC AR6 WGI, Chapter 3: "Human influence on the climate system", 2021

Subgrid-scale parameterizations are problematic.

Not all motions (e.g., convective plumes) **and processes** (e.g., cloud droplet formation) **can be explicitly represented by the model** ("resolved" at grid-scale). Yet, these can impact the resolved "grid-scale" state.



Caltech

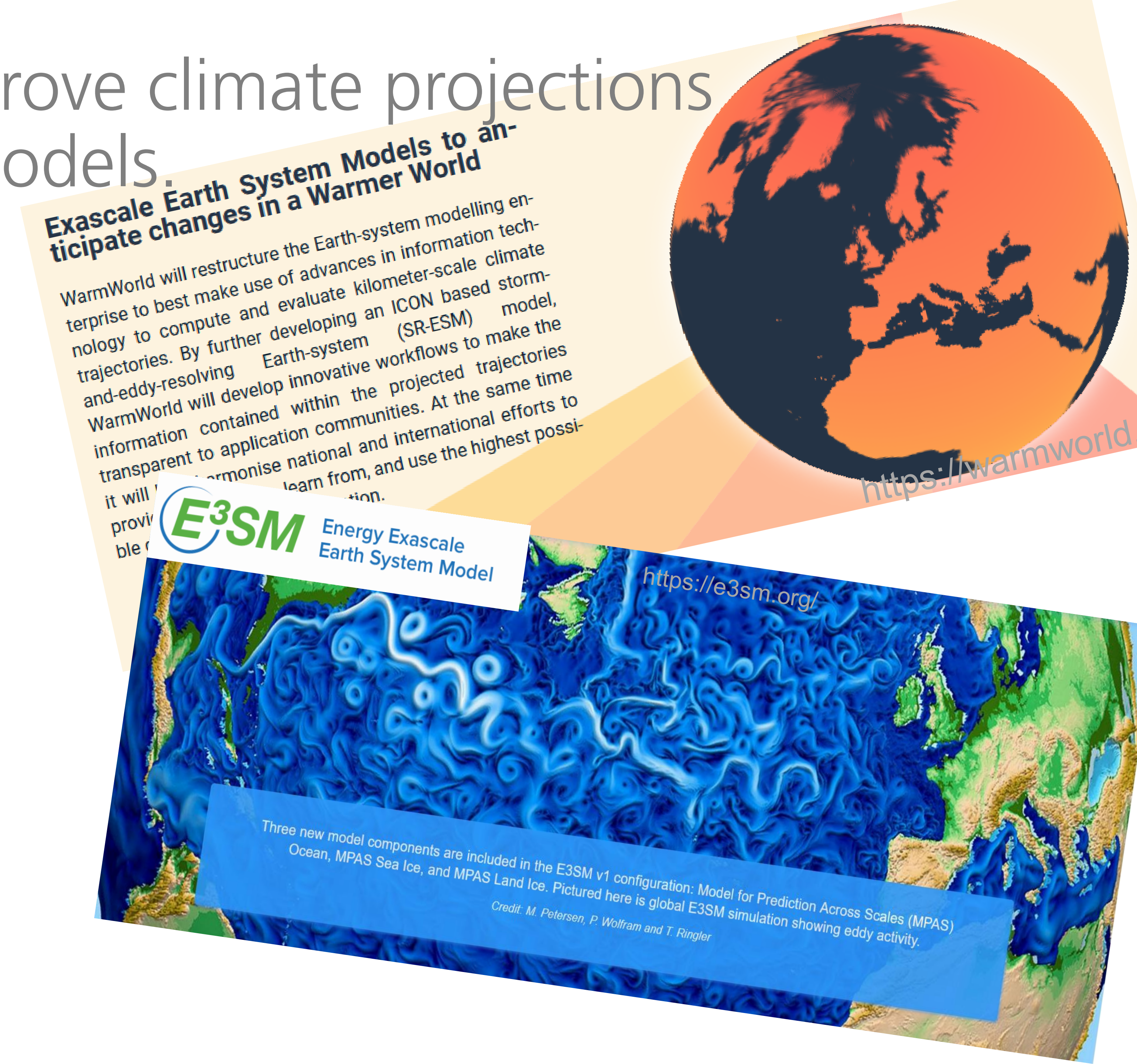
~50-150 km

<u>Solution</u>: **Describe the impact of subgrid-scale processes on the mean state of the system in a statistical manner** using information of the grid-scale state with **Parameterizations**

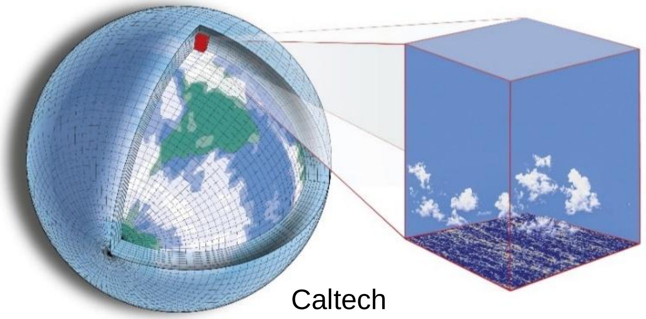
- Parametrizations **do not represent processes exactly -** rather the statistical effect of a given process (or combination of processes) at grid scale of the GCM
- Often rely on factors that are uncertain or non-observable → have to be **tuned (e.g., trial and error) to lie within estimated observed bounds**

One approach to improve climate projections are high-resolution models.

+ High-resolution ($O(km)$) models resolve various dynamical processes, e.g. deep convection and eliminate many biases
+ However, only part of spectrum resolved (e.g., not shallow convection)
+ Need for parameterizations still remains (e.g., turbulence and microphysics)



Data-driven methods can improve the subgrid-scale parametrizations.



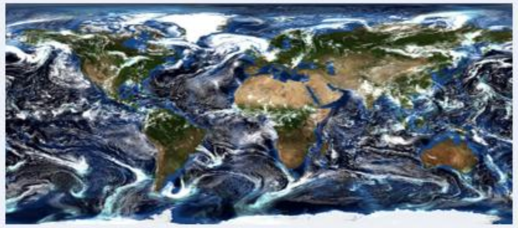
~50-150 km

Improved Climate Projections and Understanding

… our approach

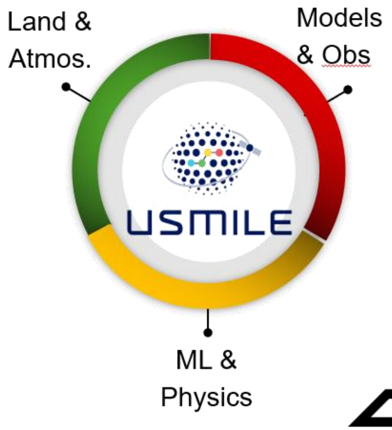
1. Massive data from Earth observation

2. High-resolution cloud resolving models



3. Progress in machine learning

Coupled hybrid model
(ICON-ML-ESM)

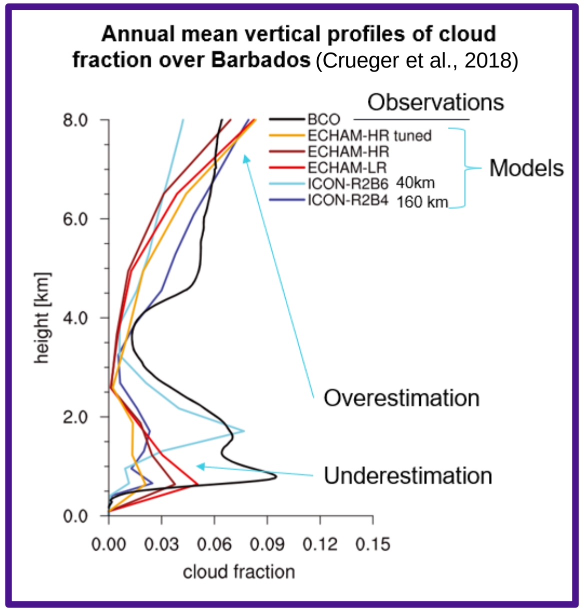


DLR

Feedforward NN for Cloud cover parametrization in ICON

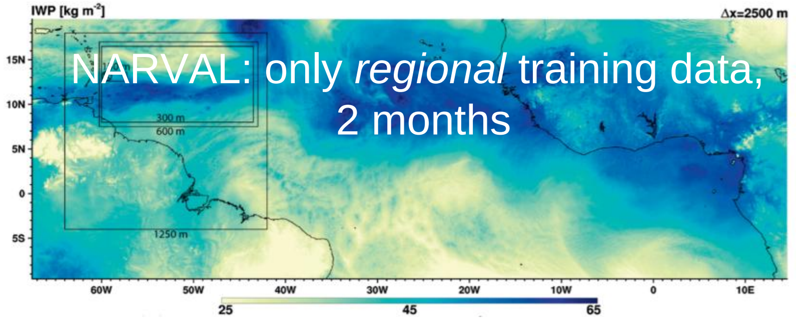
Estimated as a diagnostic (Sundqvist et al., 1989)

- Based on relative humidity (RH)
- And a semi-empirical parameterization with tuning parameters
- Cloud cover exists whenever RH exceeds a critical RH level (T,p)



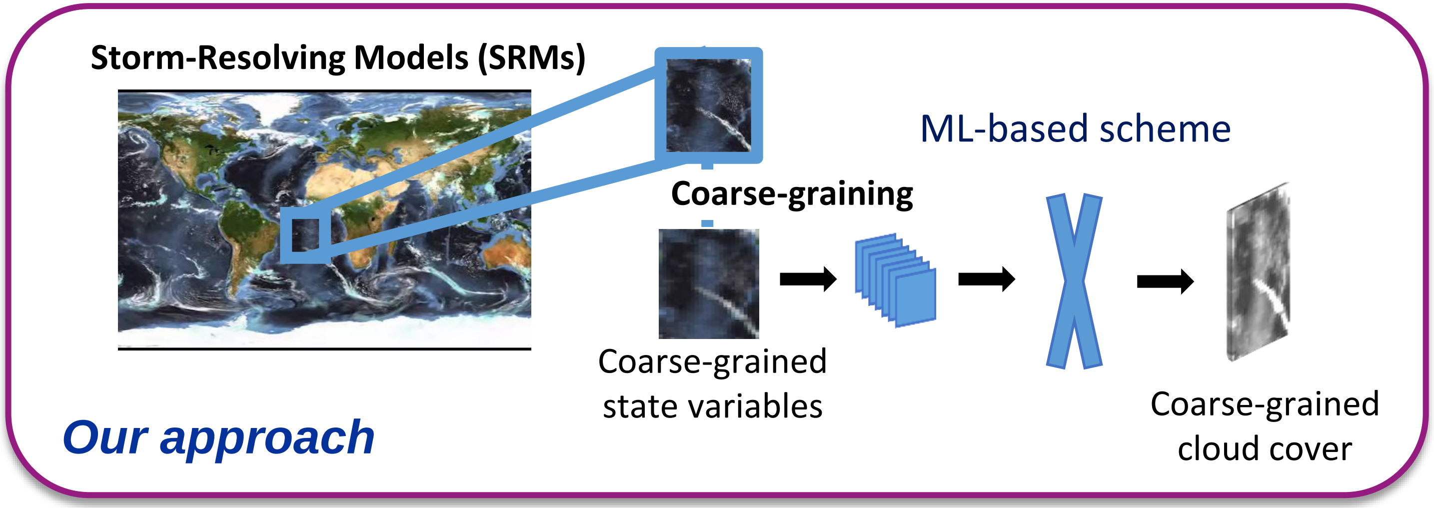
ICON Storm Resolving Model Simulations NARVAL, QUBICC, DYAMOND (~2-5 km)

- Explicit treatment of (deep) convection
- Improved representation of clouds & convection (Stevens et al. 2020, Hohenegger et al. 2020)

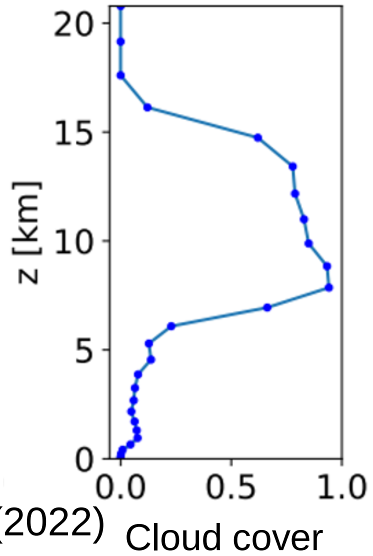


Potential features

- Temperature
- Humidity
- Pressure
- Water vapor
- Cloud water
- Cloud ice

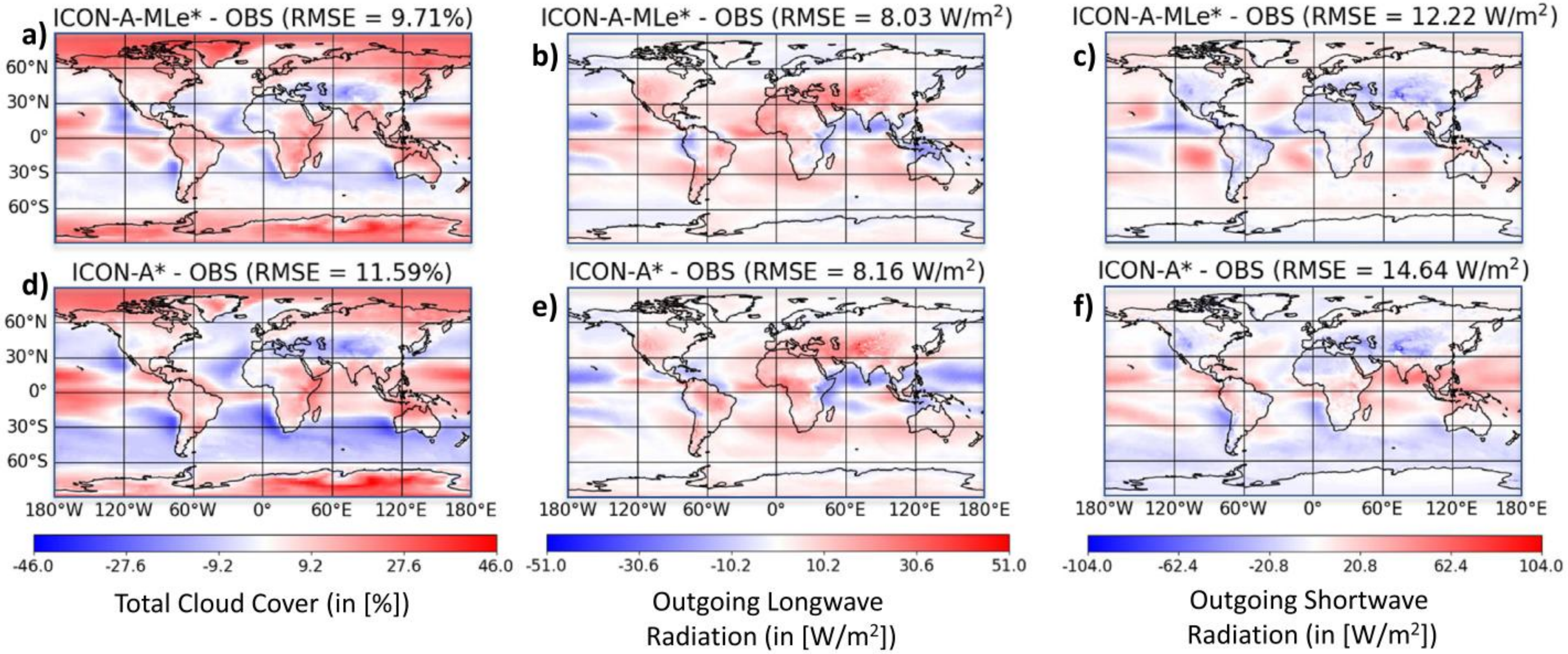


Target



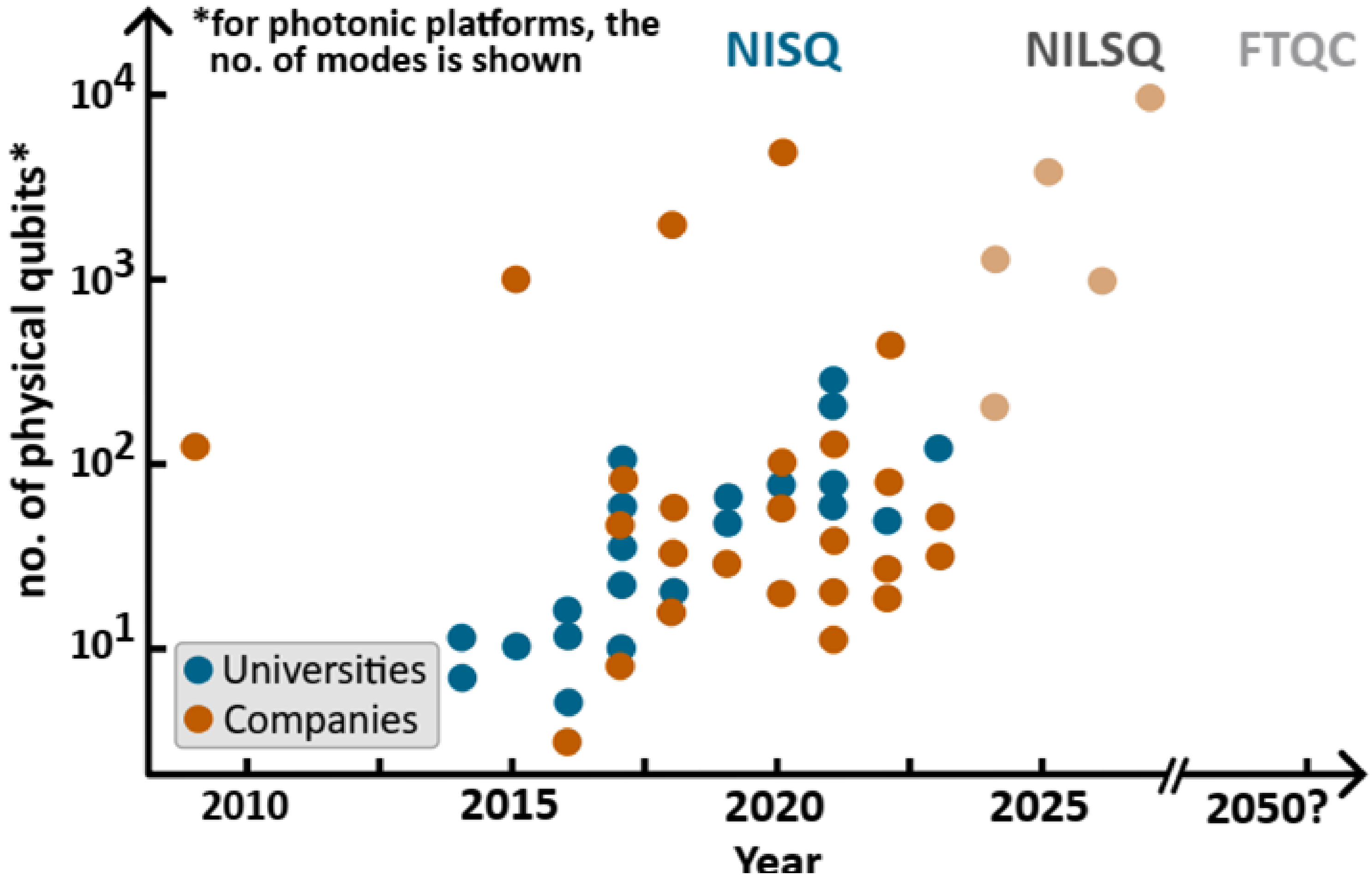
Grundner et al., DL Based Cloud Cover Parameterization for ICON, https://doi.org/10.1029/2021MS002959 (2022)

ML for cloud cover reduces the climate model error.



Grundner et al., Scientific Reports 15:43836 (2025)

Explore potential of quantum computing for climate modelling



Hope from literature for, e.g.

- Better generalization properties (Cong et al., 2019; Abbas et al., 2021; Caro et al., 2022, 2023)
- Faster training (Abbas et al., 2021) (but: barren plateaus)
- Application for generative modelling (Amin et al., 2018; Dallaire-Demers and Killoran, 2018; Coyle et al., 2020)

Schwabe et al: Env. Data Sci. 4, e35 (2025)

Quantum computing for parameterizations

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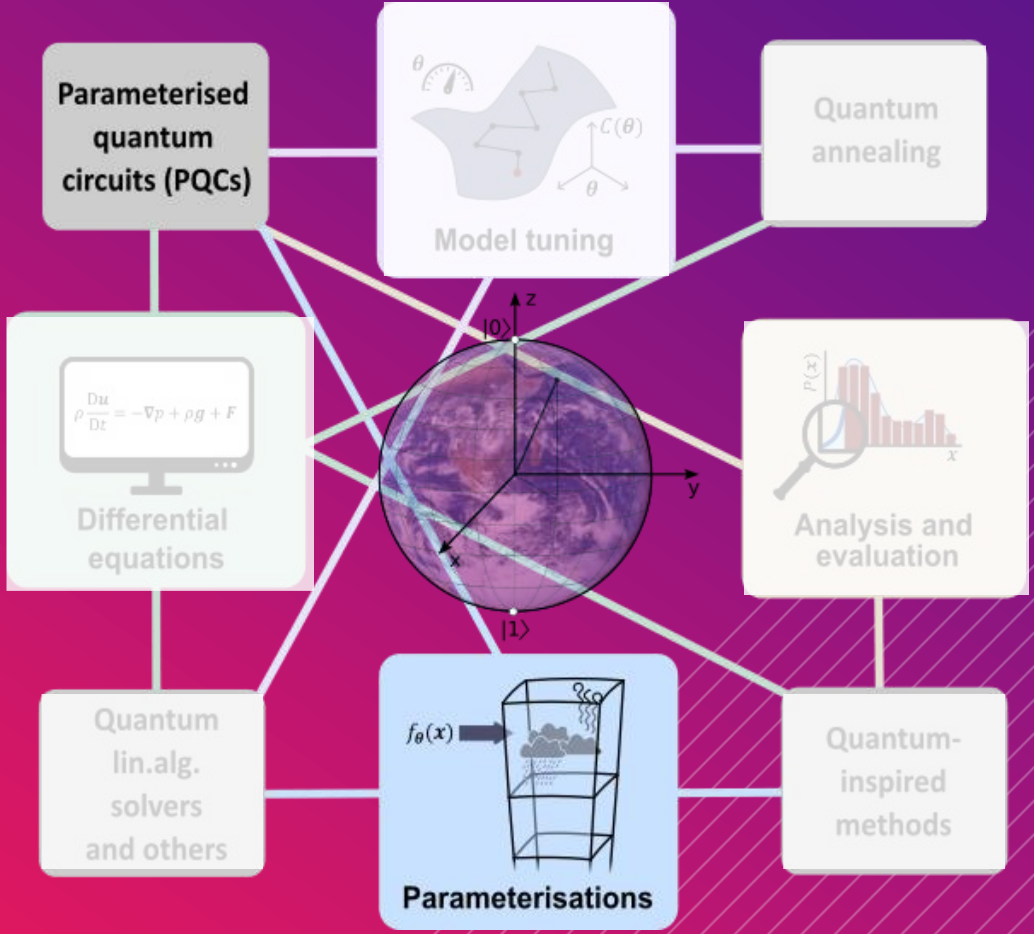
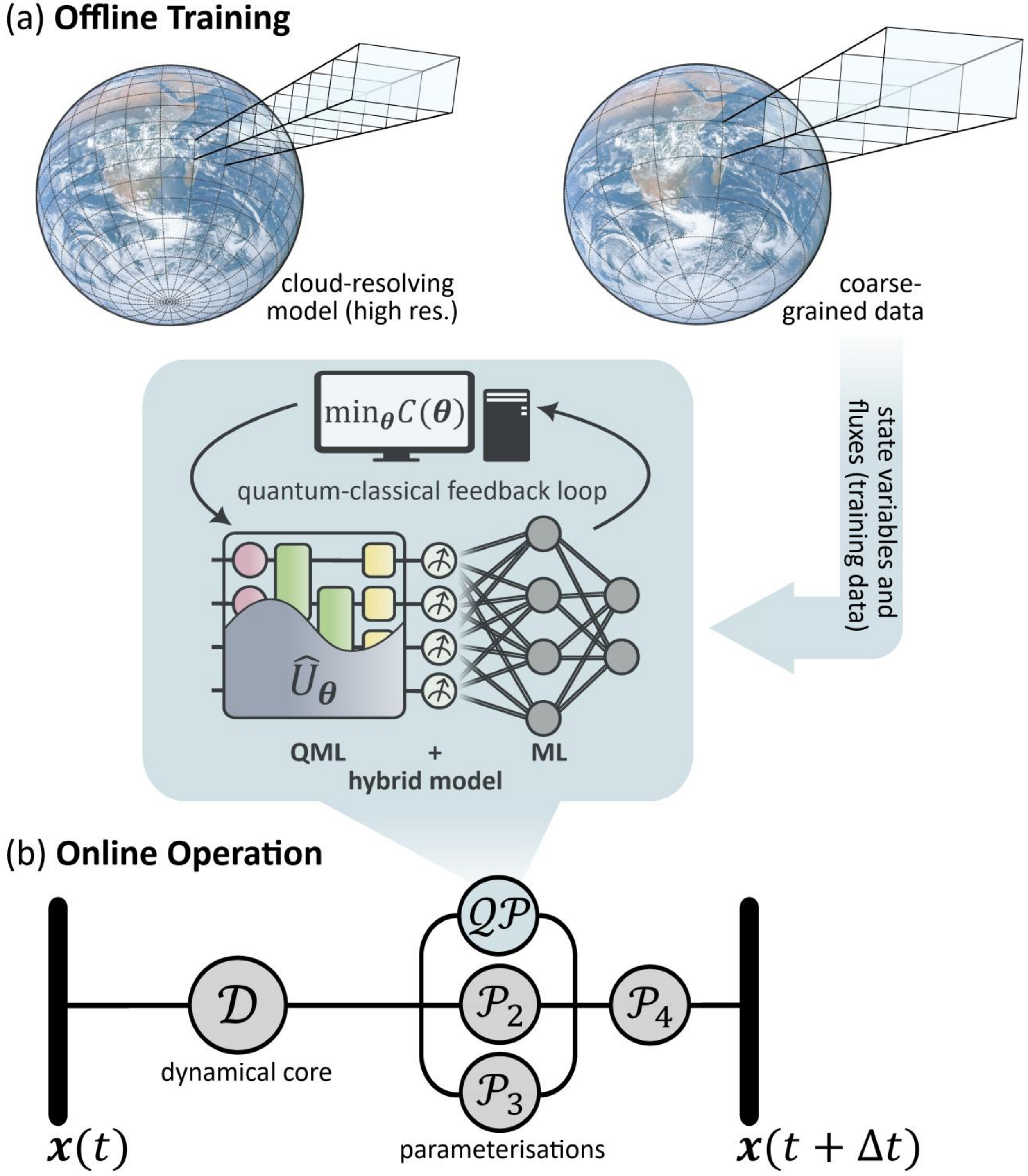


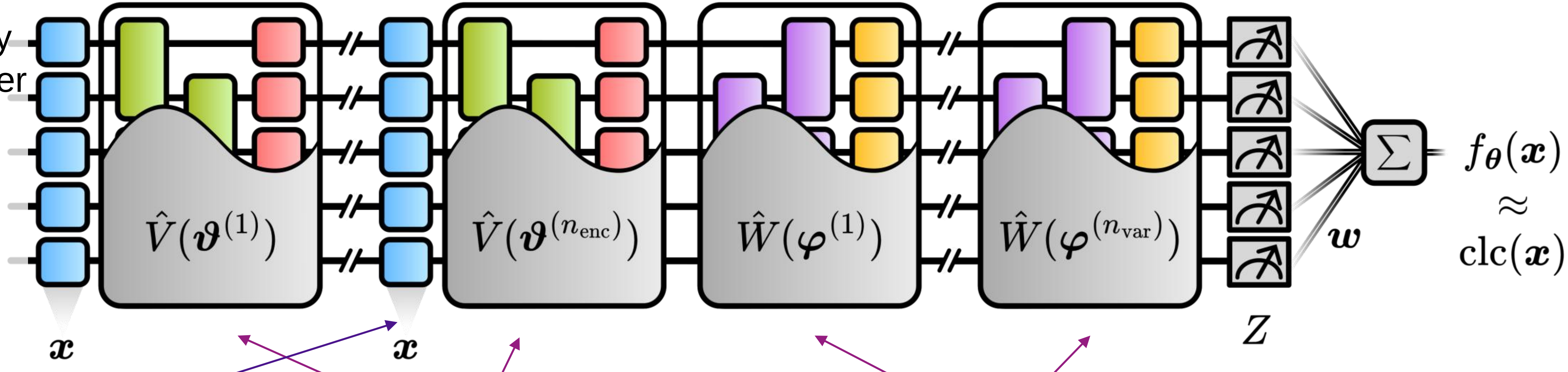
The workflow for developing data-driven quantum computing-based parameterizations is similar as for classical para-meterizations.



Schwabe et al: Env. Data Sci. 4, e35 (2025)

QNN architectures for cloud cover

Inputs:
Specific humidity
Cloud liquid water
Cloud ice water
Air temperature
Pressure
Horizontal wind



Input features **x** encoded as angles of single-qubit rotations in encoding layer $\hat{S}(\boldsymbol{x}) = \hat{\boldsymbol{R}}_{\boldsymbol{x}}(x)$

Variational blocks $\hat{V}(\theta)$ with entangling gates and trainable parameters θ

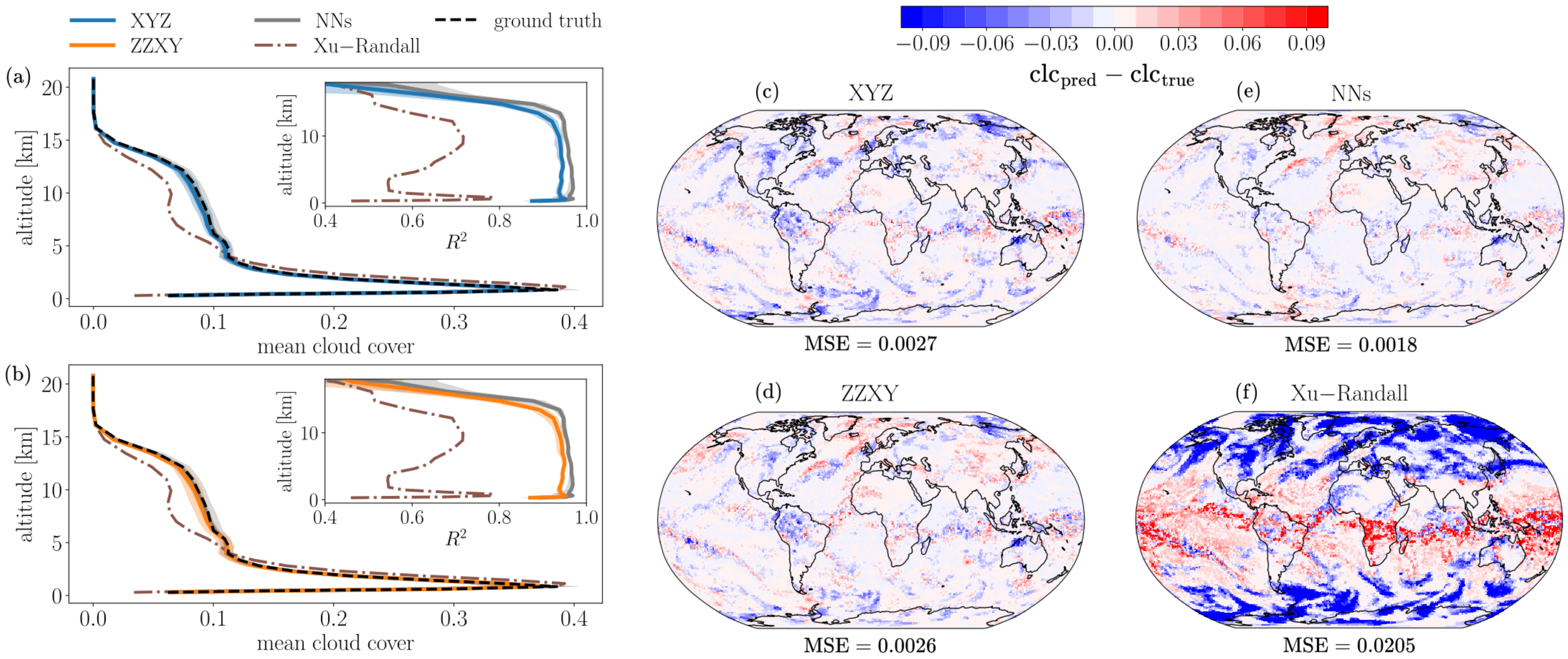
Additional variational blocks $\widehat{W}(\varphi)$ with entangling gates and trainable parameters φ

Repeated n_{enc} times

Repeated n_{var} times

Pastori et al: Machine Learning: Earth 2 (1), 015008 (2026)

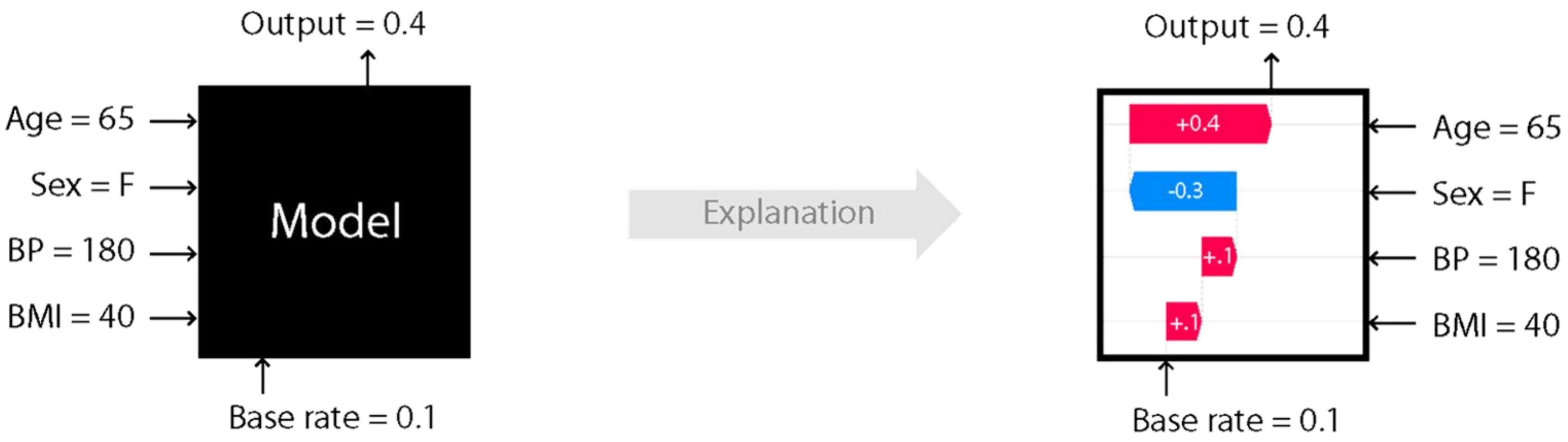
Quantum neural networks for cloud cover



- For a fair comparison, classical NN has 200 trainable parameters, comparable to quantum NNs
- Quantum (XYZ and ZZXY) and classical NNs have comparable performances and biases
- Can XAI pinpoint more differences? Test on more complex parametrizations?

Pastori et al: Machine Learning: Earth 2 (1), 015008 (2026)

Shapley values quantify the influence of input features



https://shap.readthedocs.io/en/latest/index.h

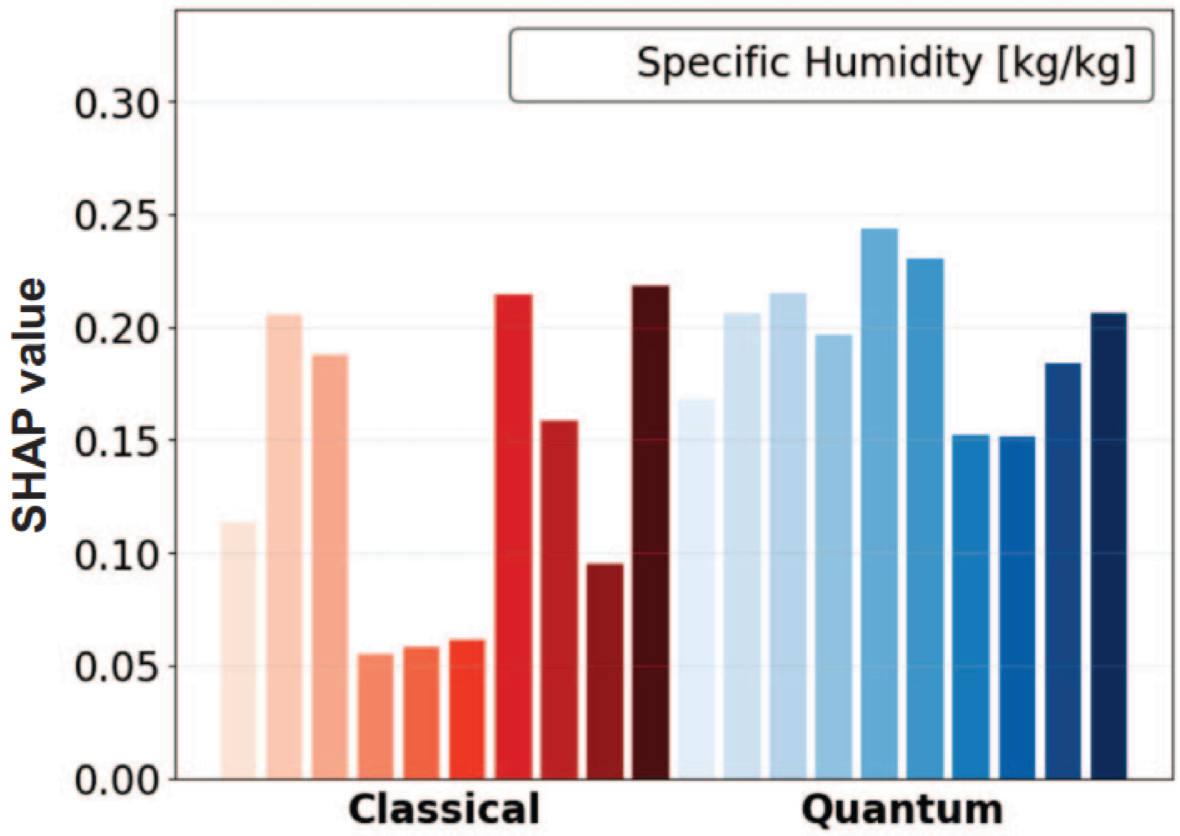
SHAP package: Shapley Additive exPlanations (Lundberg & Lee, 2017): efficiently compute approximations of Shapley values for deep NNs

According to analyzing SHAP values: The QML parameterizations for cloud cover learn more robustly than the classical ones.

Network (Classical)	MSE	R^2	Network (Quantum)	MSE	R^2
NN(θ_1)	0.007	0.93	QNN(θ_1)	0.010	0.90
NN(θ_2)	0.006	0.94	QNN(θ_2)	0.009	0.91
NN(θ_3)	0.006	0.94	QNN(θ_3)	0.009	0.90
NN(θ_4)	0.006	0.94	QNN(θ_4)	0.009	0.91
NN(θ_5)	0.006	0.94	QNN(θ_5)	0.011	0.89
NN(θ_6)	0.006	0.94	QNN(θ_6)	0.011	0.89
NN(θ_7)	0.006	0.94	QNN(θ_7)	0.010	0.90
NN(θ_8)	0.006	0.94	QNN(θ_8)	0.010	0.90
NN(θ_9)	0.008	0.92	QNN(θ_9)	0.009	0.91
NN(θ_{10})	0.006	0.94	QNN(θ_{10})	0.010	0.90

Table 9: Summary of MSE and R^2 values for different parameter sets in classical and quantum architectures. The architecture remains consistent across all experiments, while the parameter set θ (labeled with subscripts from 1 to 10) represents the selected set of parameters. All values are computed using a dataset of 100,000 points, as in previous cases.

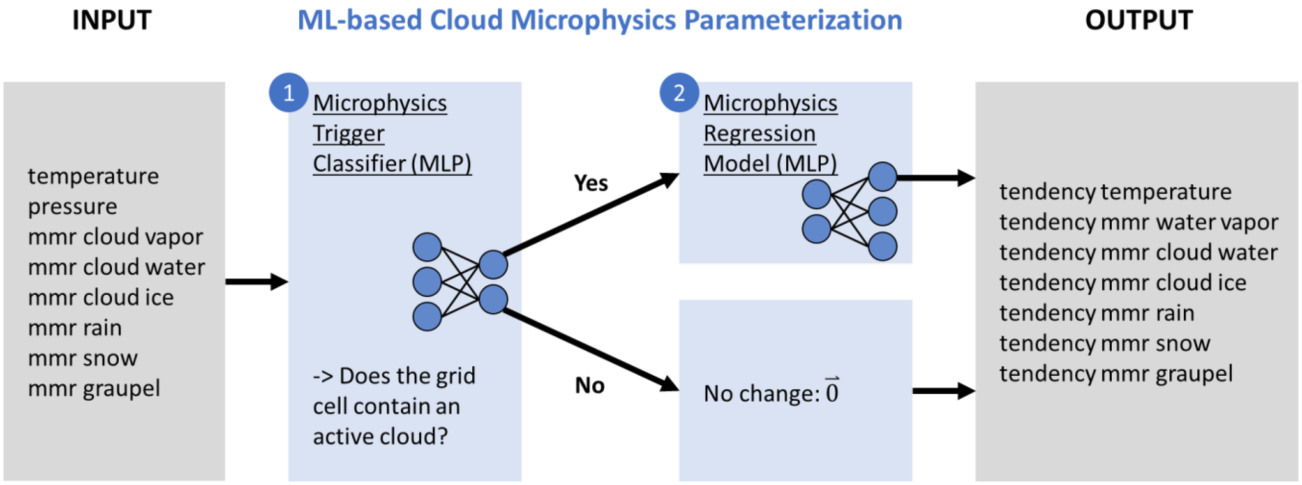
- Train ten classical and ten quantum neural networks with varying random seeds
- Analyse feature importance with SHAP values (XAI)
- Quantum networks show more stable feature importances

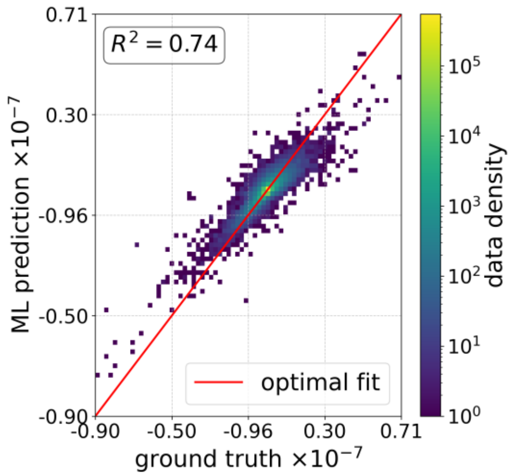


Sarandrea, Master‘s Thesis, LMU Munich (2025)
Schwabe, Proc. IEEE QAI 73-78 (2025)

QML learns cloud microphysics, but less well than a classical NN

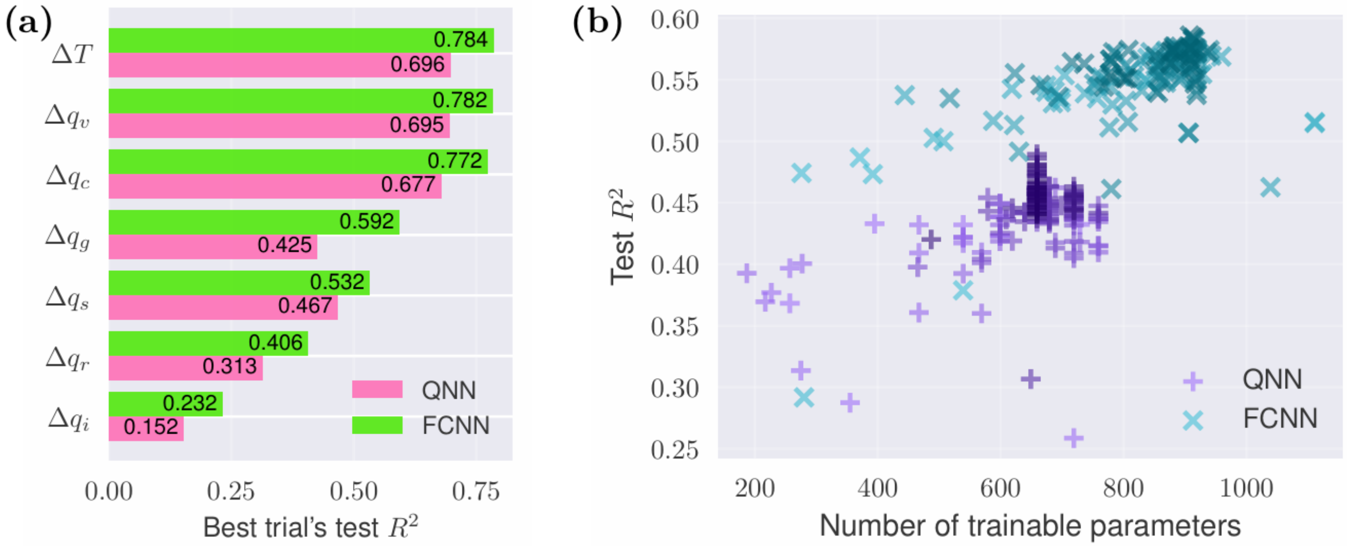
Baseline ML-based para-meterization of cloud microphysics





Sarauer et al., Env. Data Sci. 4, e40 (2025)

Comparison classical Fully Connected Neural Network with Quantum Neural Network



Herbort et al., arXiv:2607.04915 (2026)

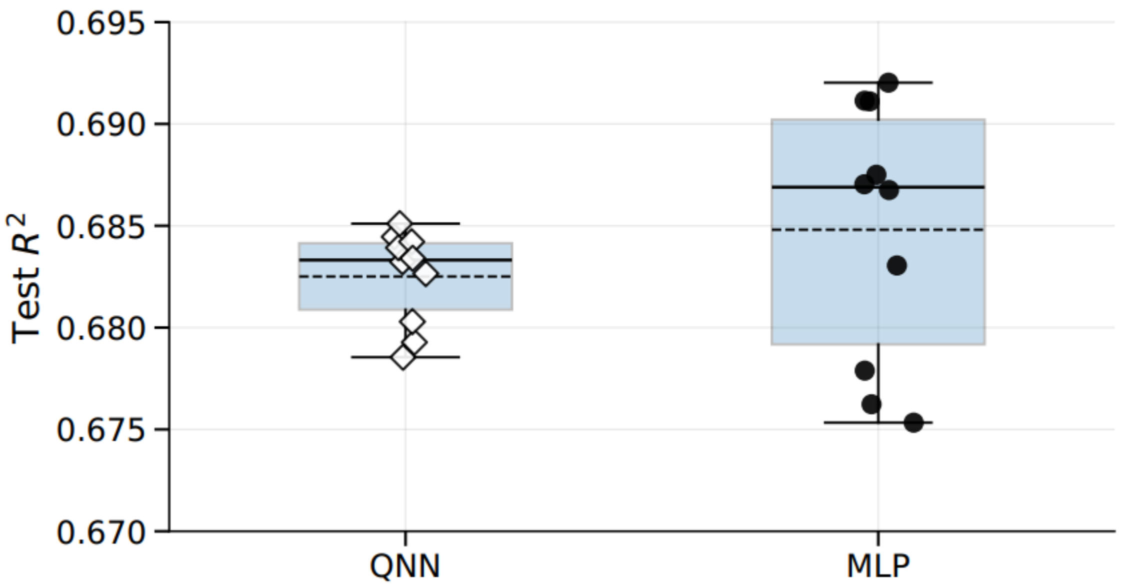
Further work on QML-based parameterizations

+ Parameterizations under development: Microphysics, turbulent fluxes, boundary layer height, convection (stochastic parameterization)

Repeatedly observed:

more stable training results

Rodríguez Garrido, University of Murcia, Master's Thesis (2026)



+ Ongoing work on coupling QML-based parameterizations with ESM ICON-XPP

See Virtual Poster by H. Keller on Tuesday at 2 PM

Quantum computing for differential equations

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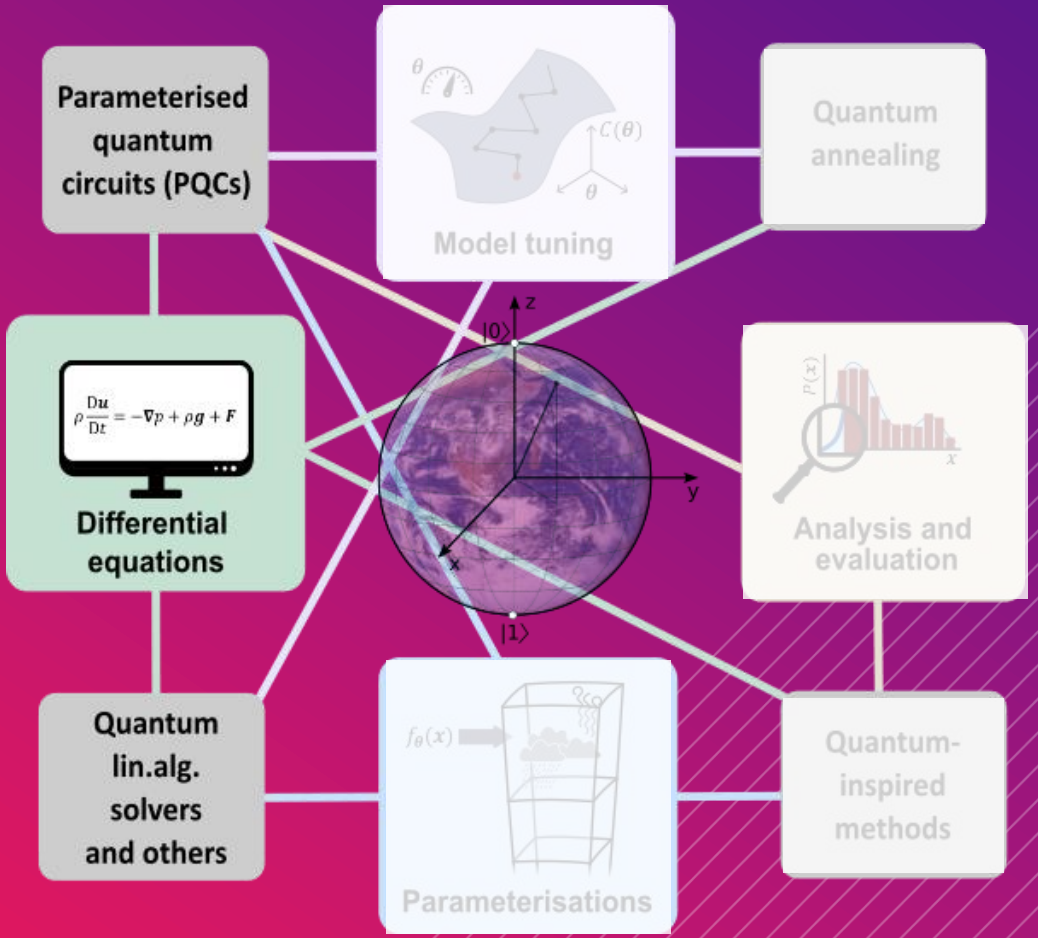
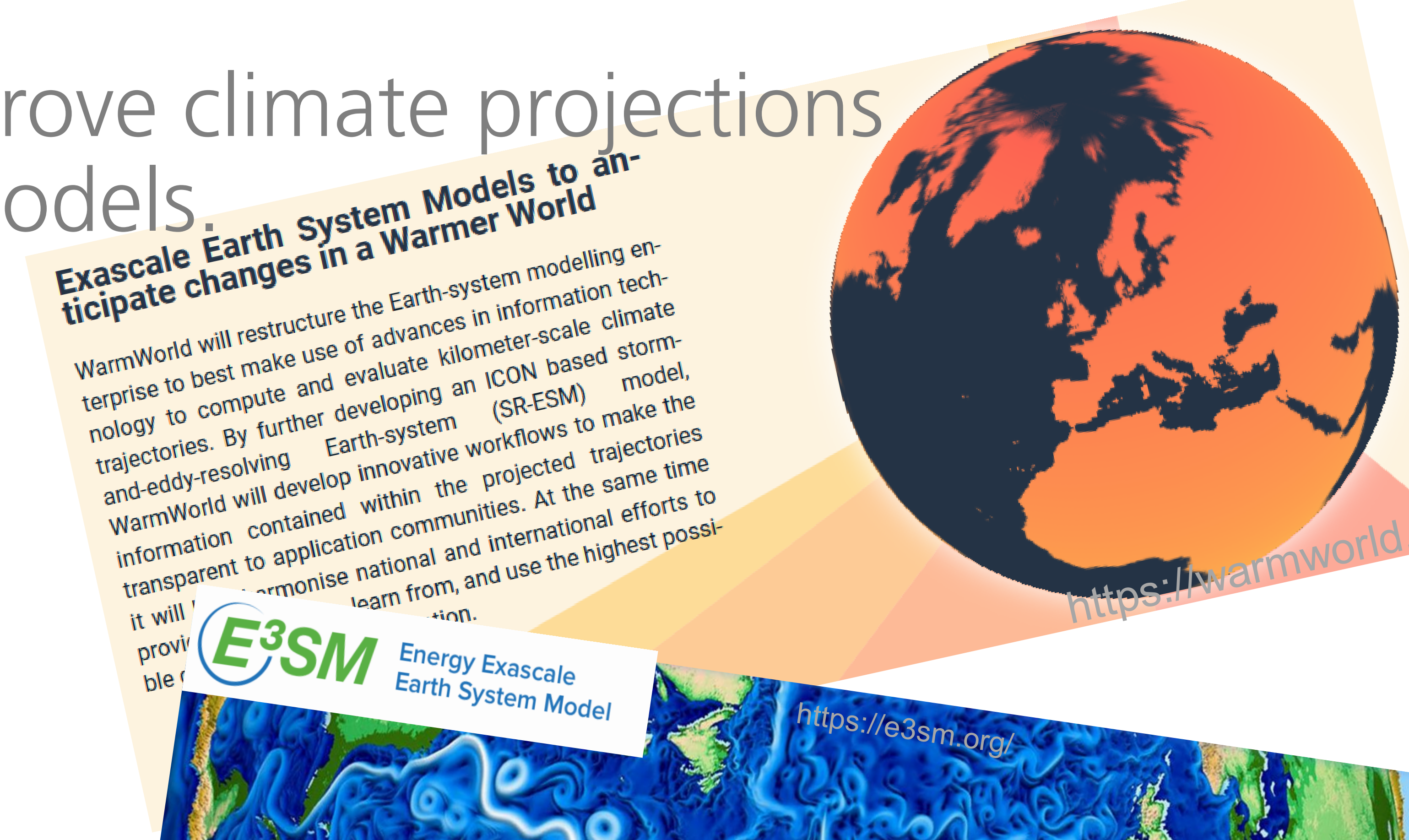


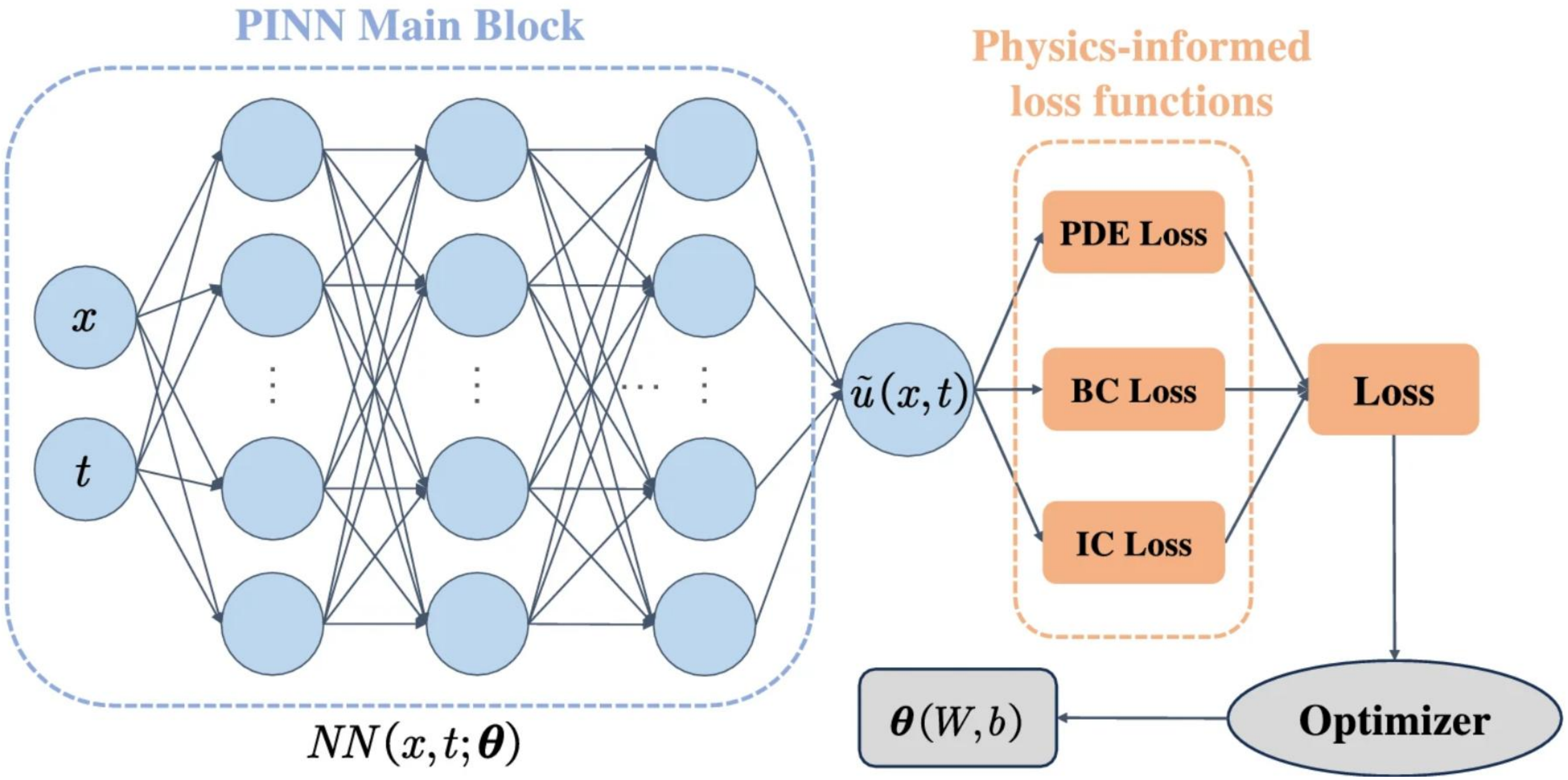
One approach to improve climate projections are high-resolution models.

+ High-resolution ($O(km)$) models resolve various dynamical processes, e.g. deep convection and eliminate many biases
+ However, only part of spectrum resolved (e.g., not shallow convection)
+ Need for parameterizations still remains (e.g., turbulence and microphysics)

→ **Quantum computing for fluid dynamics**

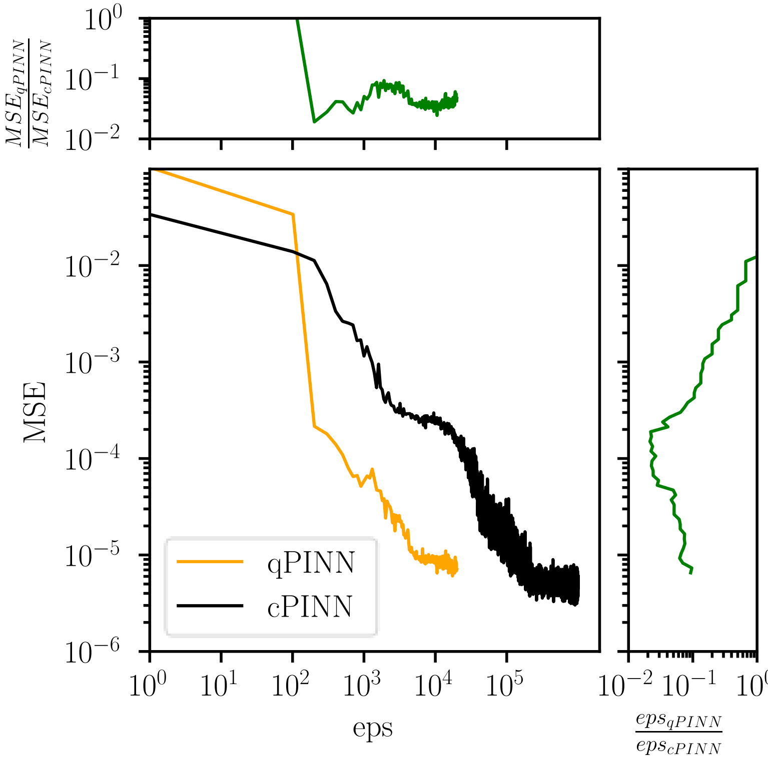


PINNs can be used to approximate the solution of PDEs, but can be slow.



Luo et al., AI Rev. 58, 323 (2025)

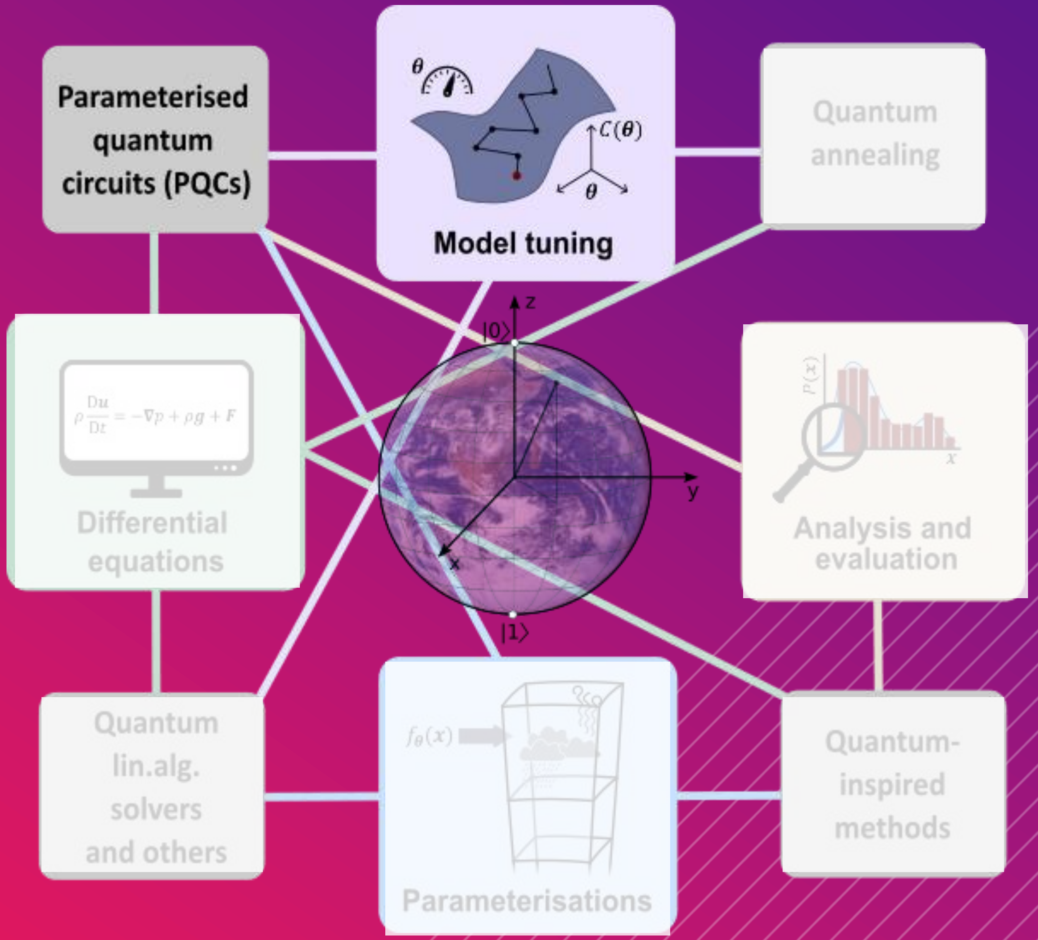
PINNs with quantum components converge faster in terms of epochs than vanilla PINNs.



- qPINNs and cPINNs (same number of trainable parameters) reach similar performance
- qPINNs are trained significantly faster in terms of epochs in the complex loss landscape of PINNs
- Mean squared error (MSE) of qPINN goes up when more parameters in classical part rather than quantum part

Klement et al., arXiv:2601.15046 (2026) – see his talk on Tuesday at 10 AM!

Quantum computing for climate model tuning



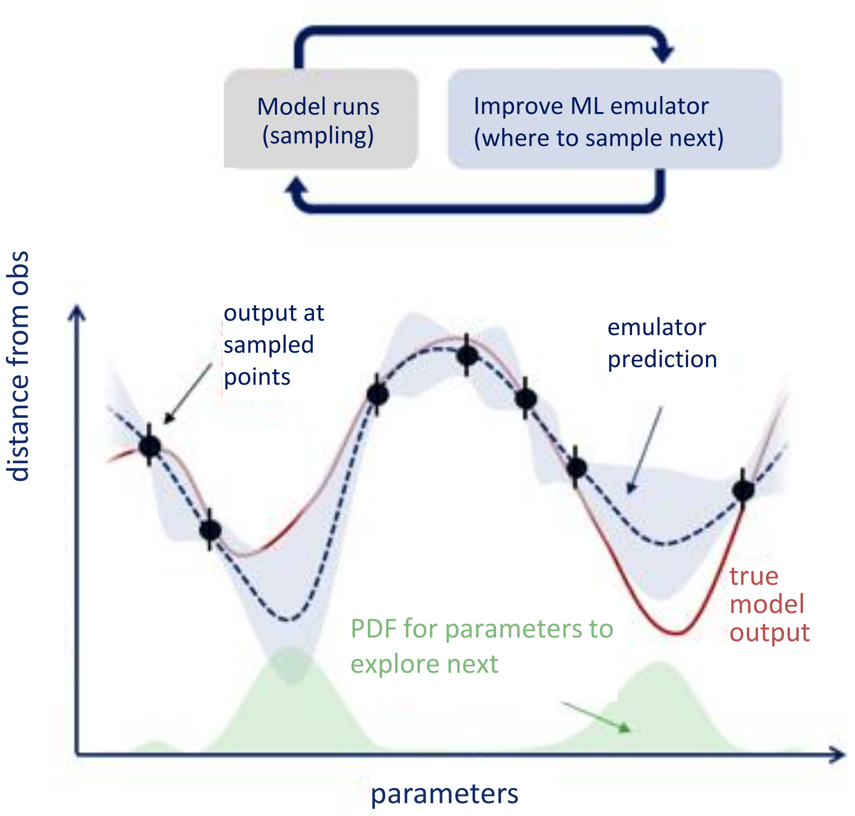
ML-assisted Automatic Tuning Framework

- Preliminary step: choose metrics to tune for and identify parameters to tune (e.g. sensitivity analysis)
- Iterative optimization: Bayesian scher applicable to costly 'black-box' funct

1. Perturbed parameters ensemble (PPE): N model runs for randomly sampled parameters
2. Fit ML model (emulator) to PPE
3. Generate very large PPE with emulator
4. Shrink parameter space (history matching)

$$\mathrm{IM}(\boldsymbol{\theta}) = \sqrt{\frac{(y_{\mathrm{emul}}(\boldsymbol{\theta}) - y_{\mathrm{obs}})^2}{\sigma^2_{\mathrm{emul}}(\boldsymbol{\theta}) + \sigma^2_{\mathrm{obs}}}} < \rho$$

5. Reiterate from PPE generation



History Matching (HM)

- Balance between **exploration of the parameter** space **and exploitation of the already explored, and potentially promising, parameter regions**.

Exploration-exploitation tradeoff achieved by shrinking parameter space according to an implausibility criterion:

- Only parameters which the emulator finds promising (i.e, $(y_{\mathrm{emul}}(\boldsymbol{\theta}) - y_{\mathrm{obs}})^2$ is small), or where the emulator is very uncertain (i.e., $\sigma^2_{\mathrm{emul}}(\boldsymbol{\theta})$ is large), will be kept in the next iteration of the protocol.

Bonnet & Pastori et al., Geosci. Model Dev., https://doi.org/10.5194/gmd-18-3681-2025, 2025

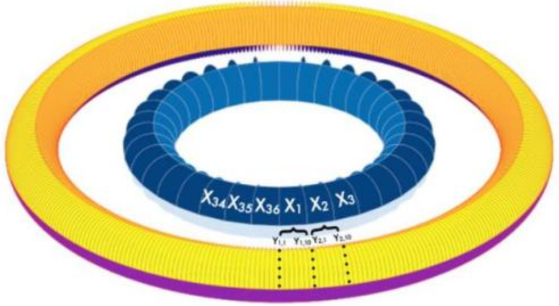
Quantum Gaussian process emulators applied to Lorenz-96 toy model

Quantum GPs: replace classical with quantum kernel, i.e., kernel evaluated from quantum circuit

→ Start with Lorenz-96 as toy model

$$\frac{dX_k}{dt} = \underbrace{-X_{k-1}(X_{k-2} - X_{k+1})}_{\text{Advection}} \underbrace{-X_k}_{\text{Diffusion}} \underbrace{+F}_{\textit{Forcing}} \underbrace{-\frac{hc}{b}\sum_{j=1}^{J} Y_{j,k}}_{\textit{Coupling}}$$

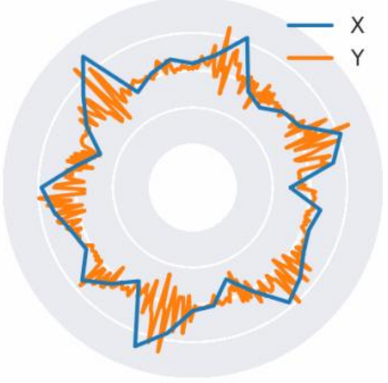
$$\frac{dY_{j,k}}{dt} = \underbrace{-cbY_{j+1,k}(Y_{j+2,k} - Y_{j-1,k})}_{\text{Advection}} \underbrace{-cY_{j,k}}_{\text{Diffusion}} \underbrace{+\frac{hc}{b}X_k}_{\text{Coupling}}$$



- Simplified substitute model
- *X* variables correspond to slow processes (e.g., ocean system)
- *Y* correspond to fast processes (e.g. atmosphere)

Metrics to consider for tuning:

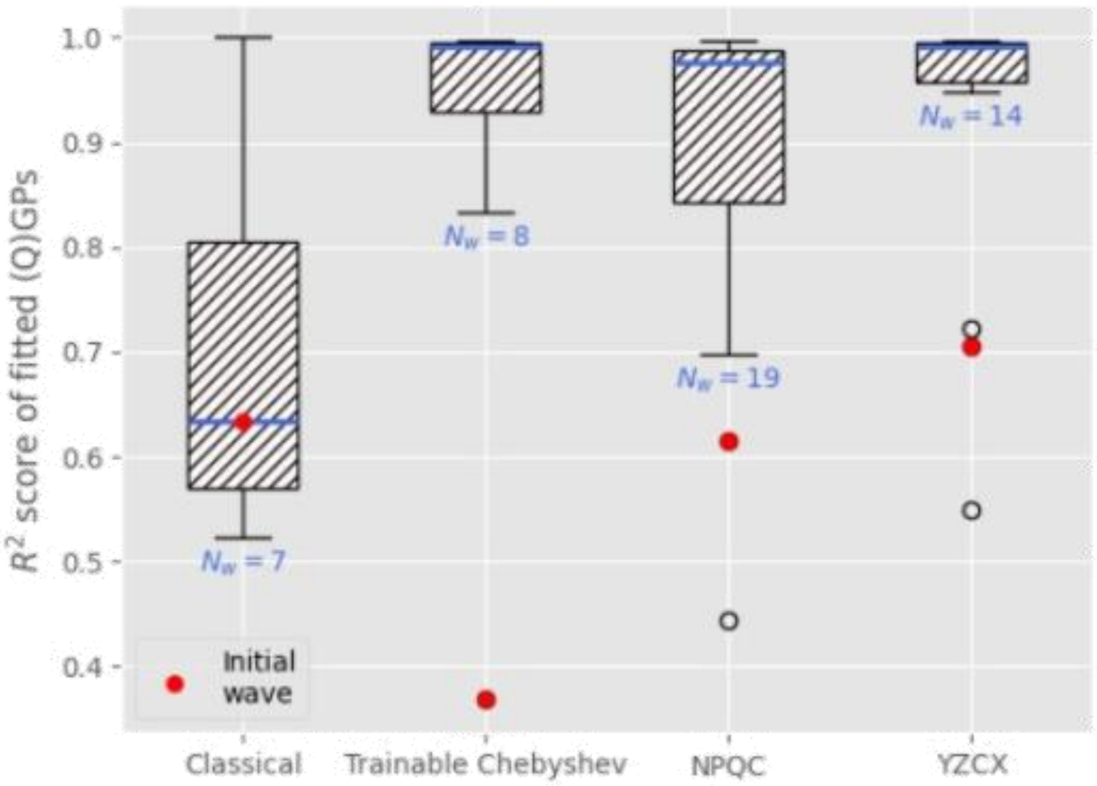
$$\boldsymbol{f}(\boldsymbol{p}) = \begin{pmatrix} \langle \boldsymbol{X} \rangle_\tau \\ \langle \overline{\boldsymbol{Y}} \rangle_\tau \\ \langle \boldsymbol{X}^2 \rangle_\tau \\ \langle \boldsymbol{X}\overline{\boldsymbol{Y}} \rangle_\tau \\ \langle \overline{\boldsymbol{Y}}^2 \rangle_\tau \end{pmatrix}$$

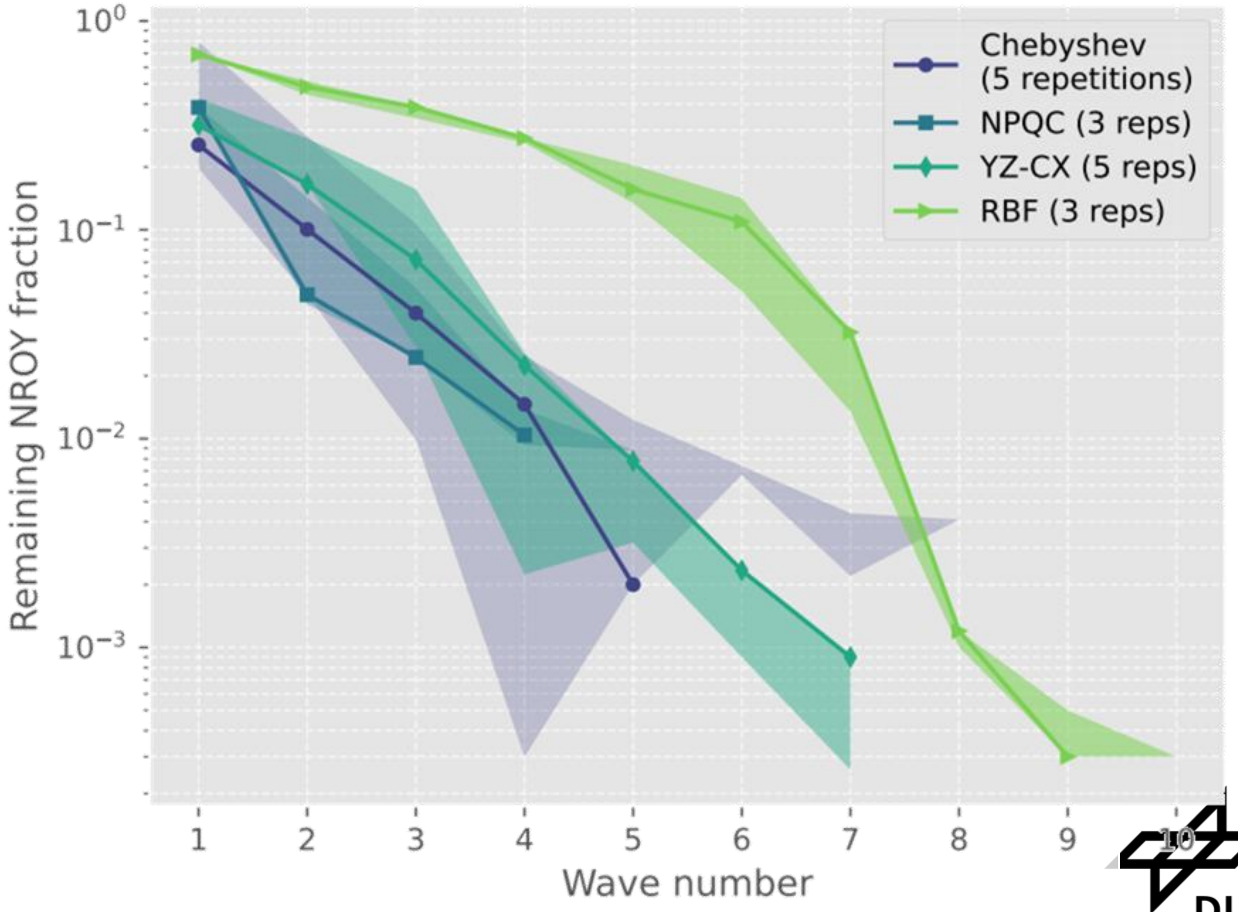


Christiansen & Ohl de Mello et al., arXiv:2512.20437 (2025)

Quantum kernels show good performance

Quantum GPs: replace classical with quantum kernel, i.e., kernel evaluated from quantum circuit

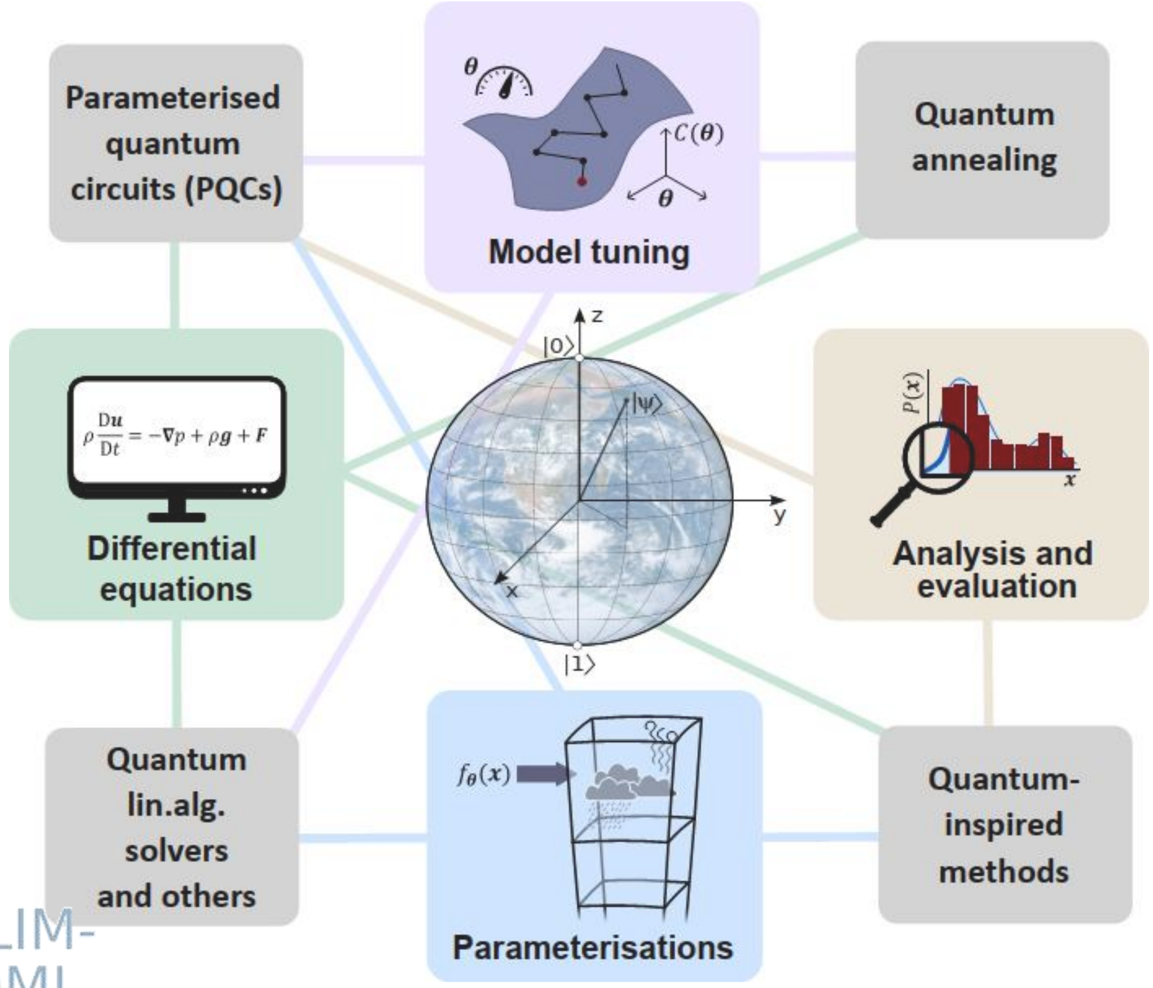




Christiansen & Ohl de Mello et al., arXiv:2512.20437 (2025)

Summary

+ Climate models can be improved with classical machine learning
+ Potential of quantum computing to boost climate modelling
+ Important for community to position itself to take advantage of rapid QC progress, advocate for QC developments with applications in mind, advance hardware-software/application co-design



Bundesministerium für Wirtschaft und Klimaschutz
DLR Quantencomputing Initiative

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KLIM-QML

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Schwabe et al: Env. Data Sci. 4, e35 (2025)

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