Understanding and Modelling the Earth System with Machine Learning

Veronika Eyring [1,2]

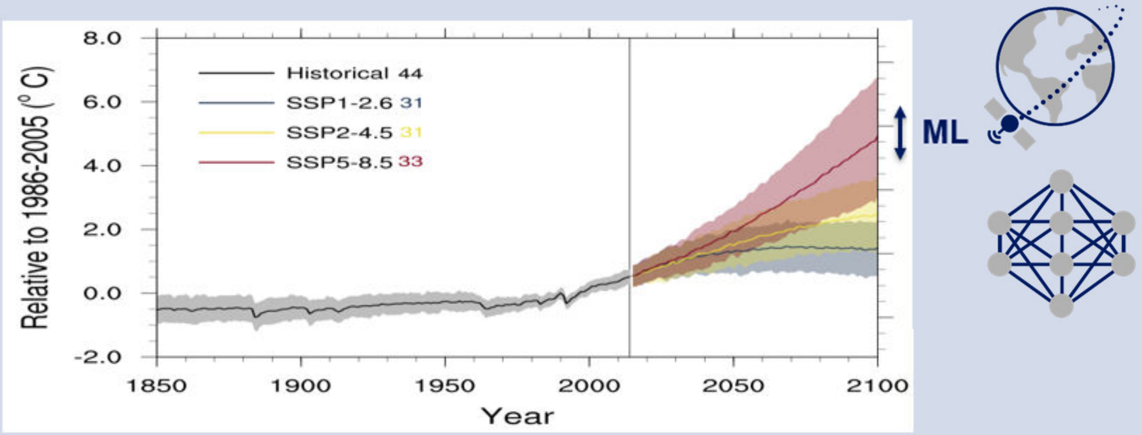
[1] Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für Physik der Atmosphäre, Oberpfaffenhofen, Germany
[2] University of Bremen, Institute of Environmental Physics (IUP), Bremen, Germany

Acknowledgments:

Group Members: Mierk Schwabe, Pauline Bonnet, Max Bouman, Arthur Grundner, Helge Heuer, Lorenzo Pastori, Manuel Schlund et al.

USMILE PIs: Pierre Gentine, Gustau Camps-Valls, Markus Reichstein

Collaborators: Tom Beucler, Marco Giorgetta, Dave Lawrence, Jakob Runge



CESM Workshop 2024, 10 June 2024, Boulder, CO, USA

Outline

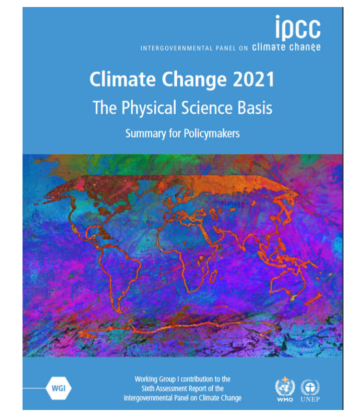
Motivation

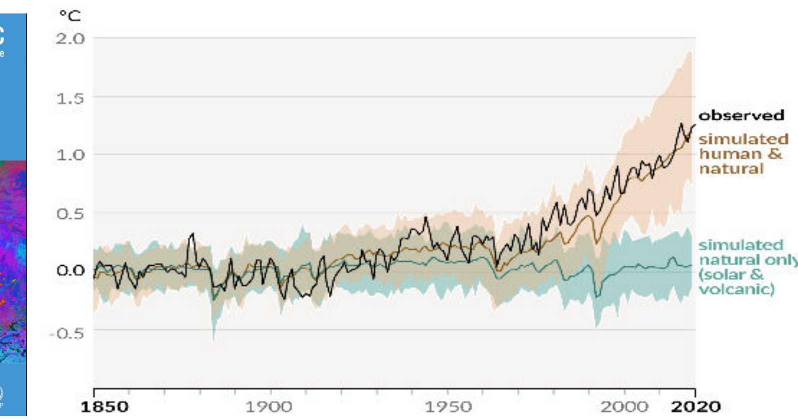
Part 1: ML-based Parametrizations for Cloud Cover
- Feedforward NN in “real world” settings (ICON-A)

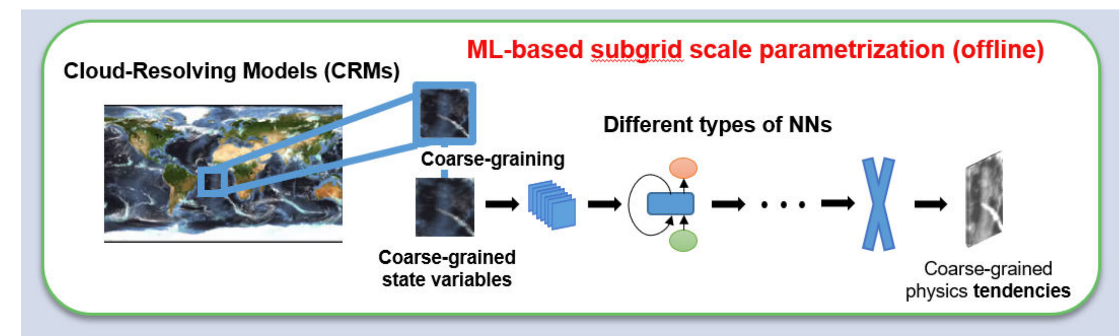
Part 2: Improved Trust in ML Models and Generalization
- Equation Discovery & Physical constraints (ICON-A)
- Causal Deep Learning & Stochastic Neural Nets (SPCAM/CESM)
- Reduction of Systematic Errors in Hybrid ESMs promising
- ML Challenges remain (stability, generalization)

Part 3: ML-based Model Tuning and Evaluation

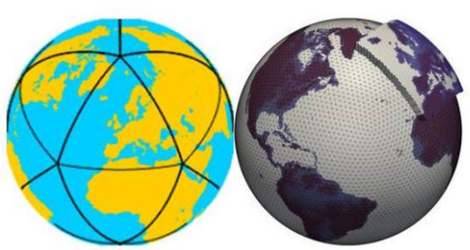
Summary & Vision



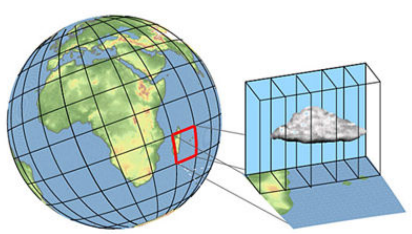




ICON-A / -ESM

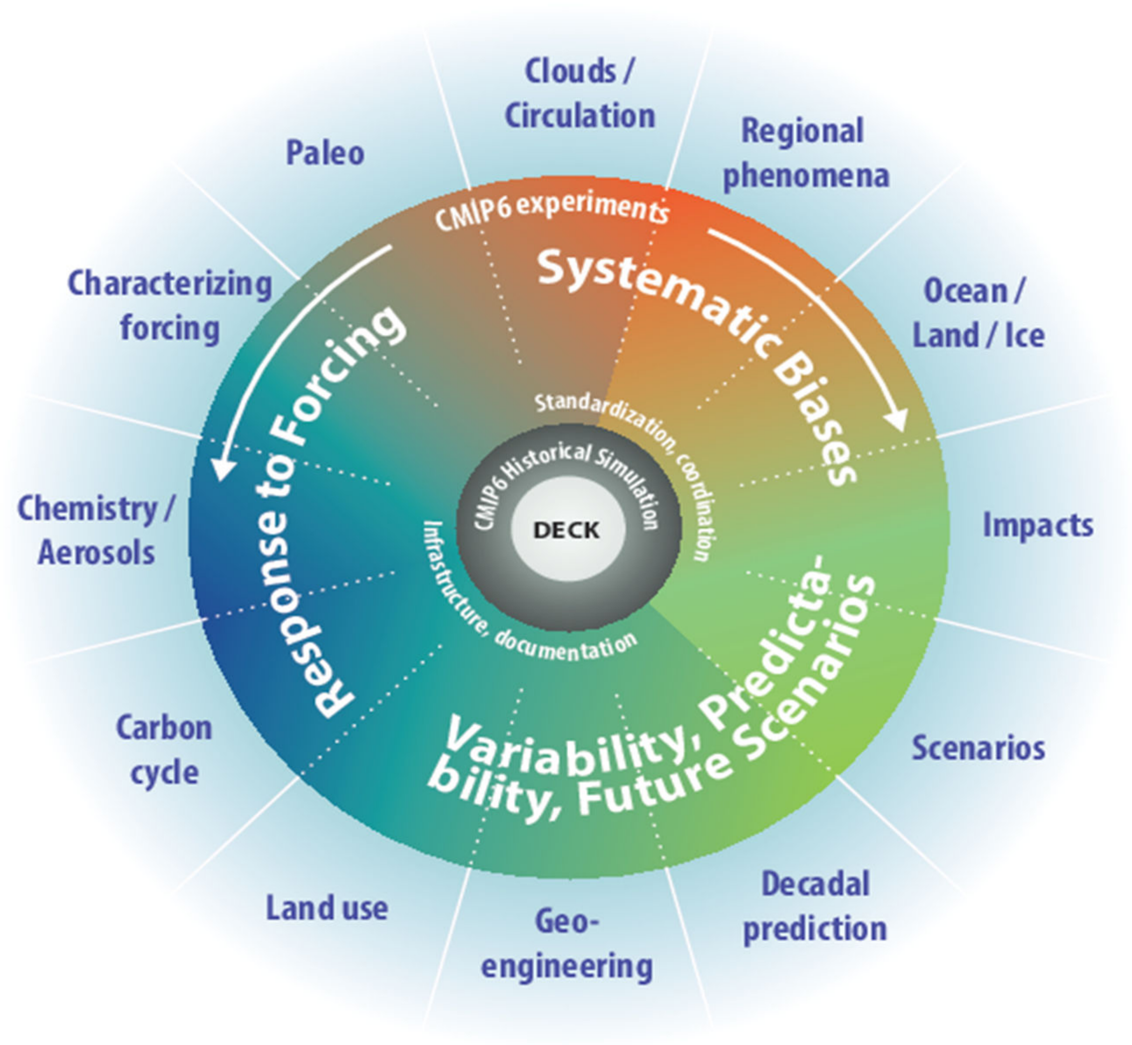


SPCAM

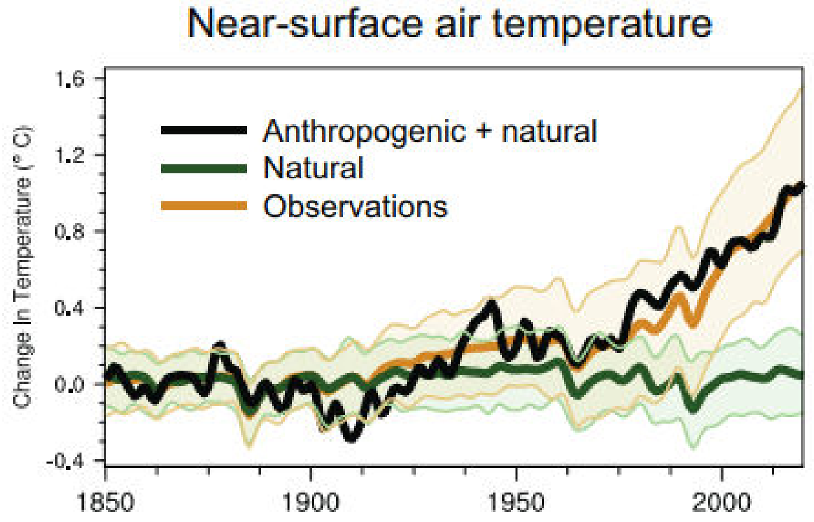


ICON: Icosahedral Non-Hydrostatic (MPI-M, Giorgetta et al. 2018); SPCAM: Superparameterized Community Atmosphere Model

World Climate Research Programme's (WCRP) Coupled Model Intercomparison Project (CMIP)

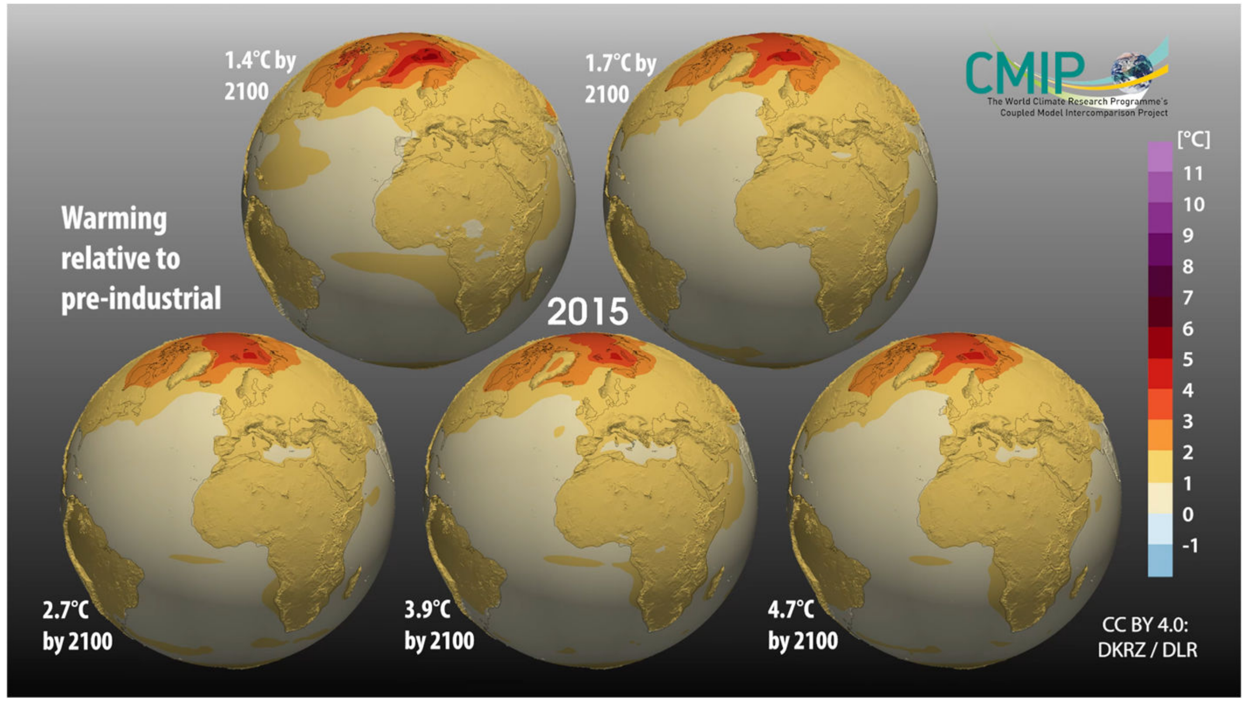


Eyring et al., Overview CMIP6, GMD, 2016



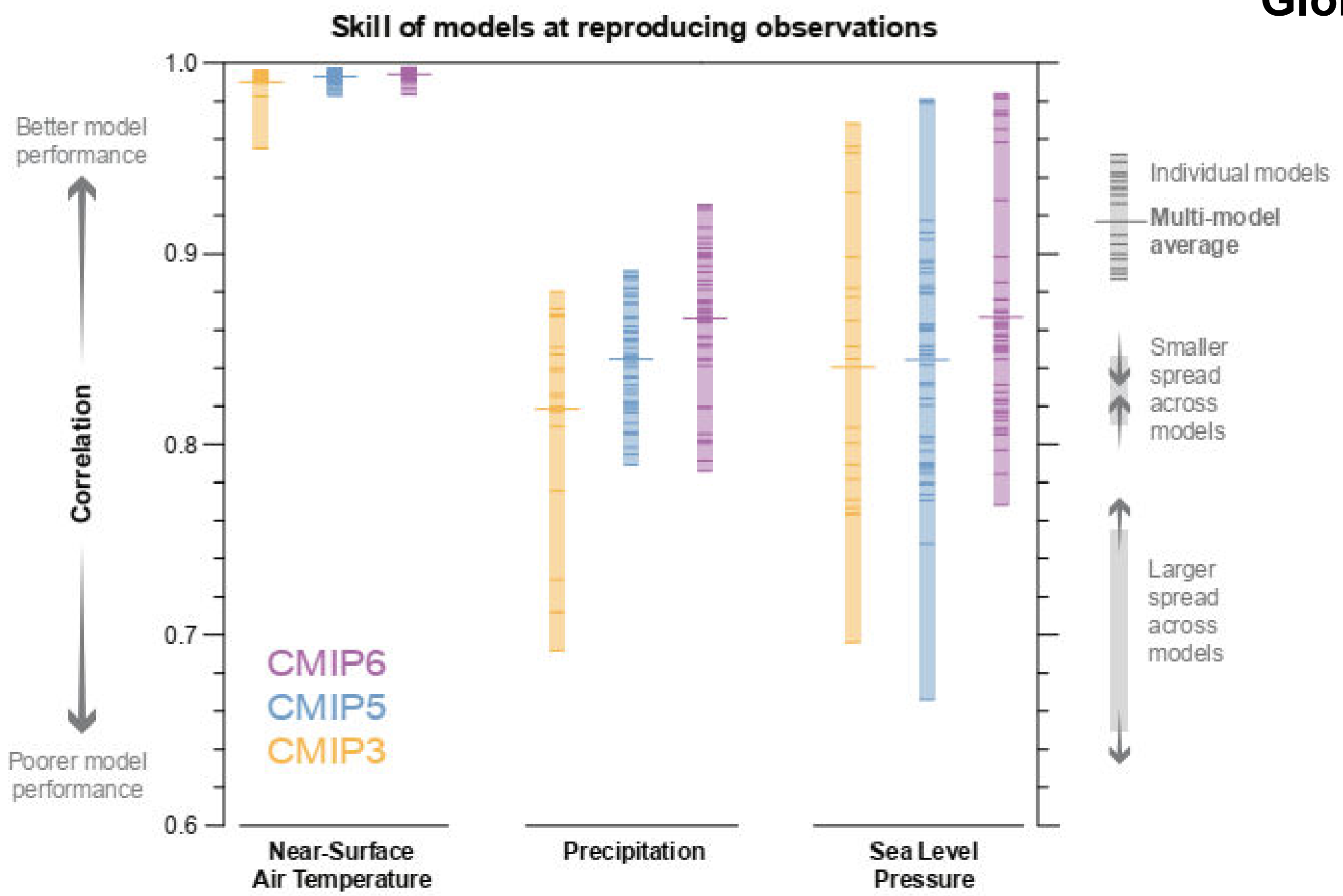
Eyring et al., IPCC WGI AR6 Ch3, 2021

It is **unequivocal** that human influence has warmed the atmosphere, ocean and land.

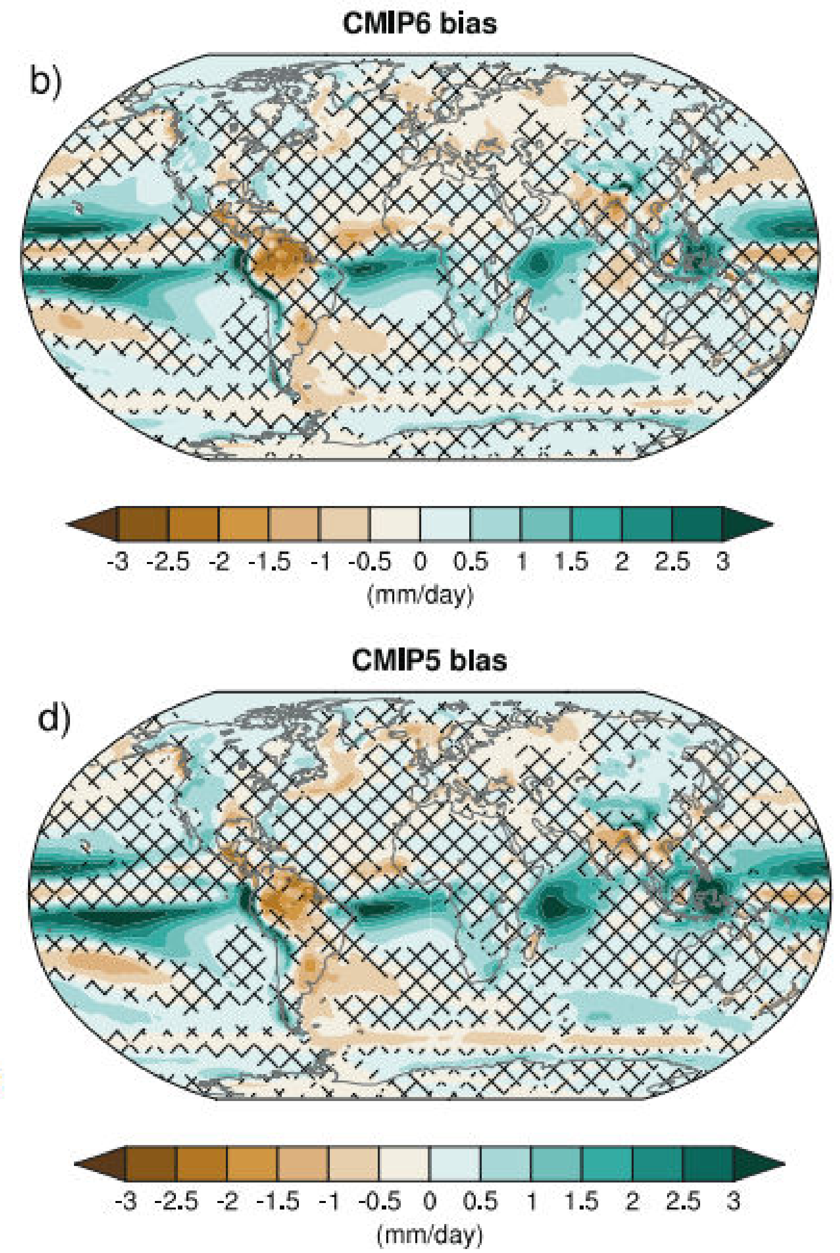


based on Lee et al., IPCC WGI AR6 Ch4, 2021

Climate models are improving, yet systematic biases remain

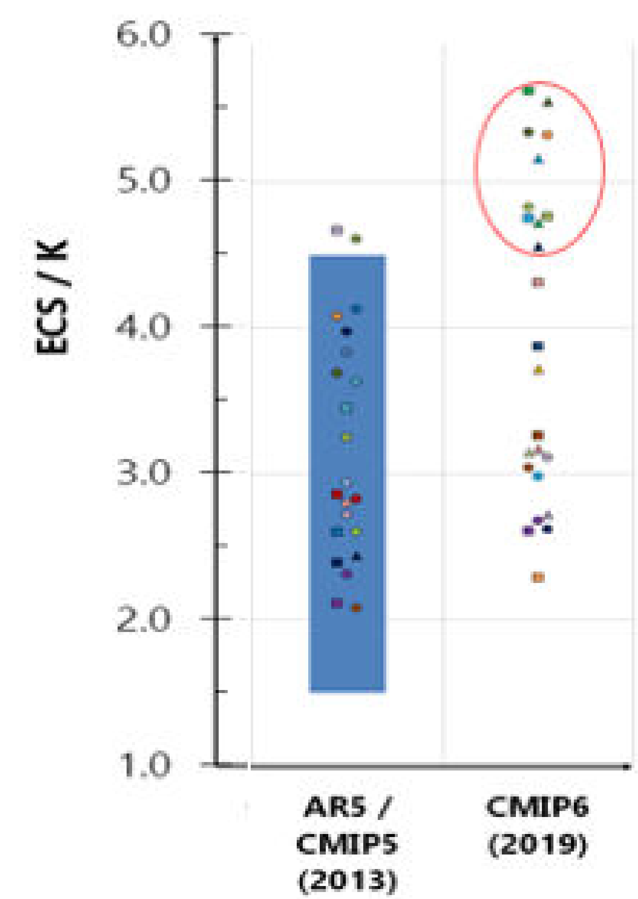


Precipitation bias (1995–2014) to Global Precipitation Climatology Project (GPCP)



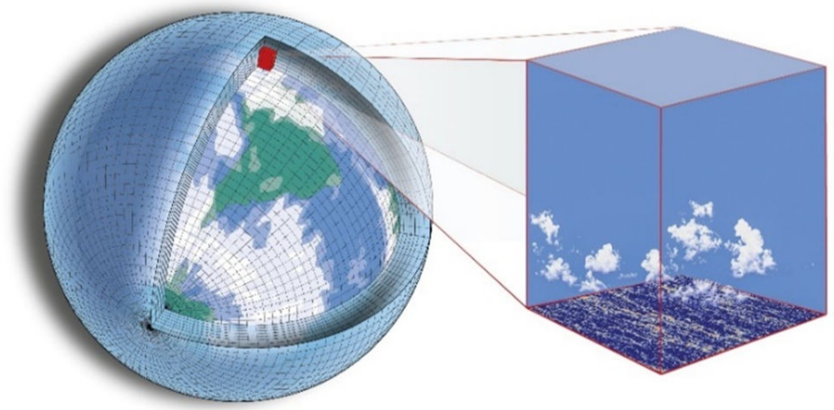
Colour Robust bias Conflicting signals

Climate Sensitivity



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

Problem: subgrid scale parametrizations

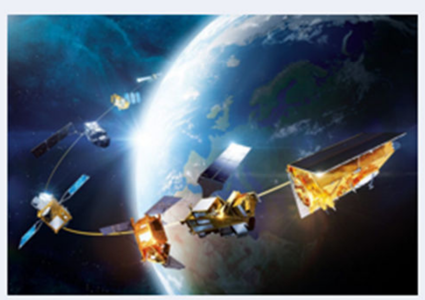


~50-150 km

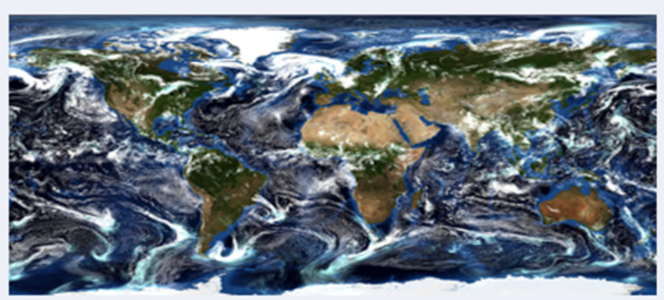
Improved Climate Projections and Understanding

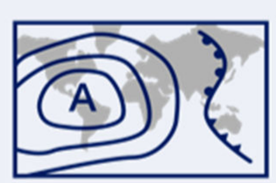
… our approach

1. Massive data from Earth observation



2. High-resolution cloud resolving models

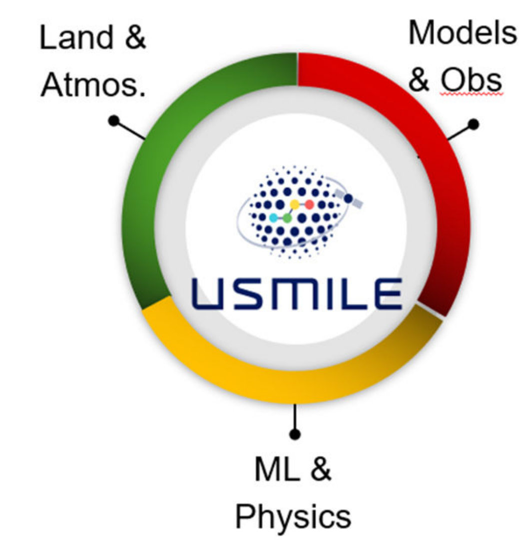




3. Progress in machine learning

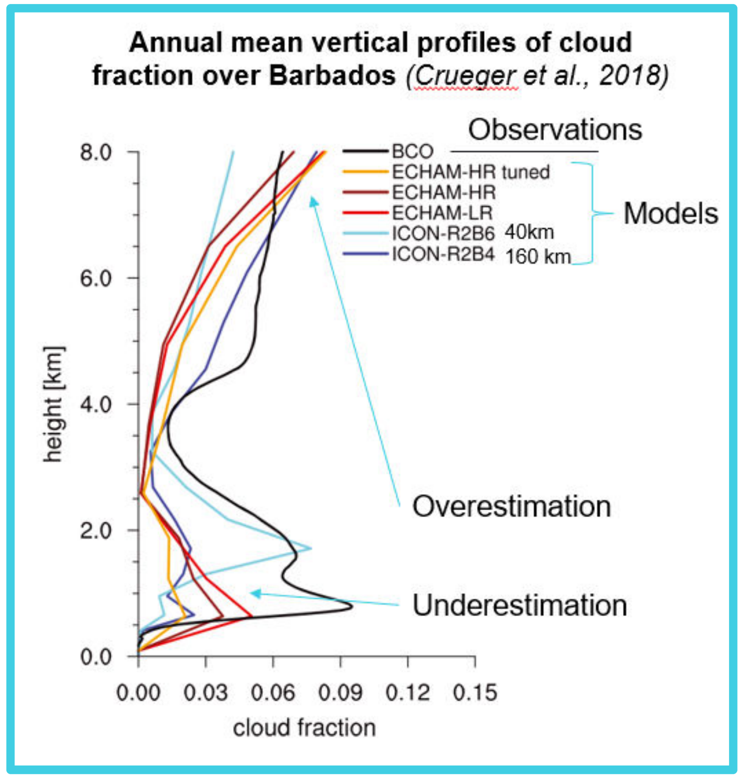
Coupled hybrid model

(ICON-ML-ESM)

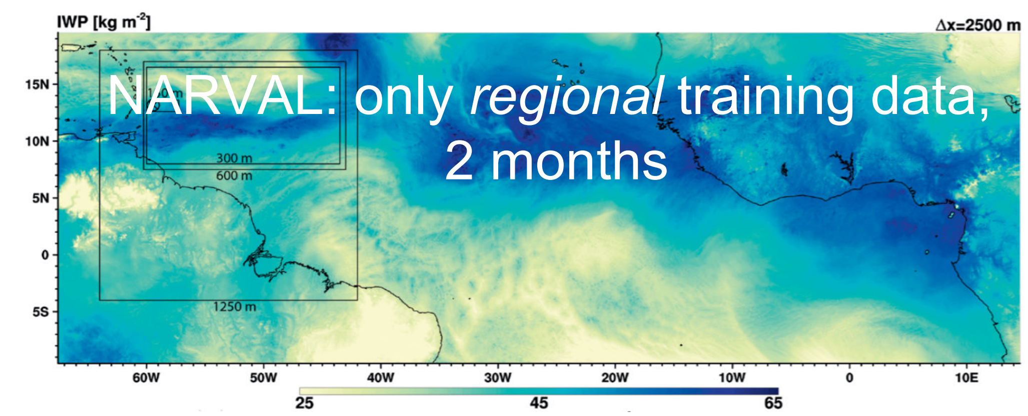


Feedforward NN for Cloud cover parametrization in ICON

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)

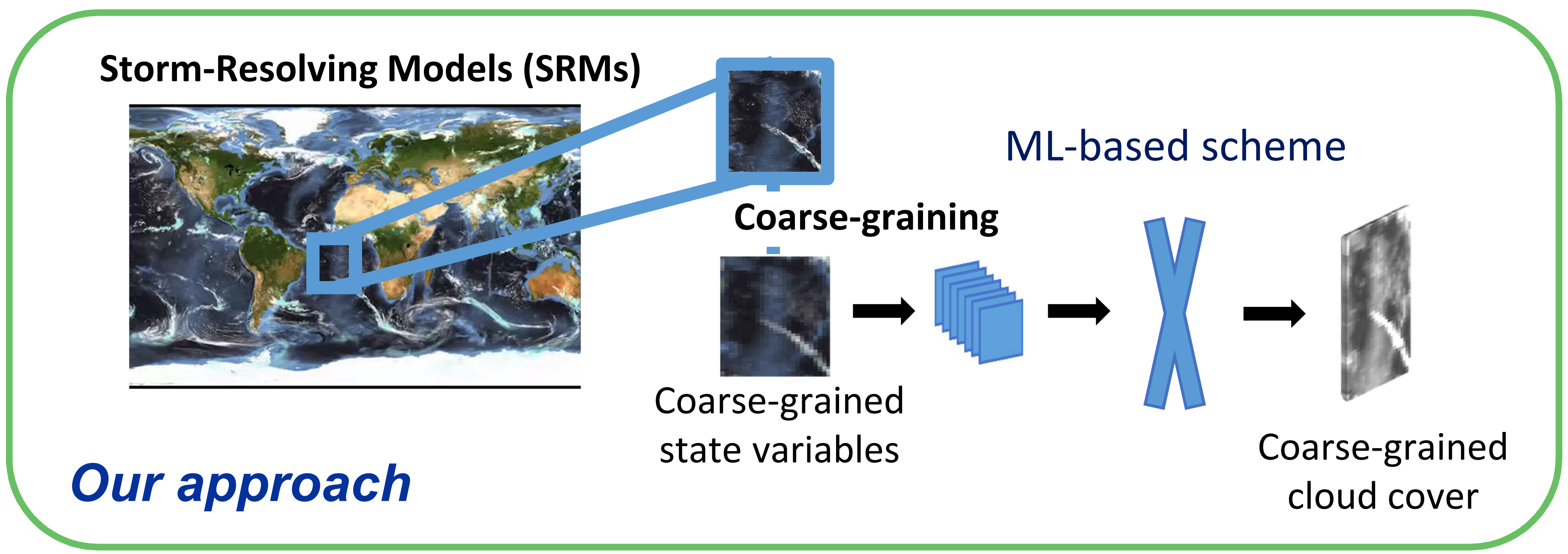


ICON Storm Resolving Model Simulations NARVAL, QUBICC, DYAMOND (~2-5 km)
- Explicit treatment of (deep) convection
- Improved representation of clouds & convection (Stevens et al. 2020, Hohenegger et al. 2020)

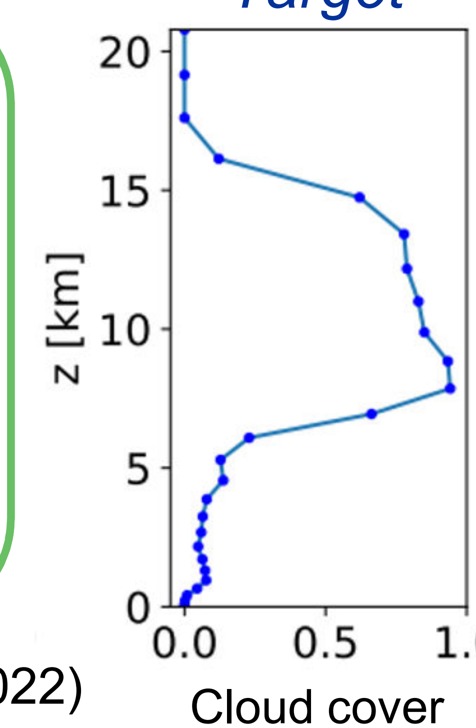


Potential features

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



Target



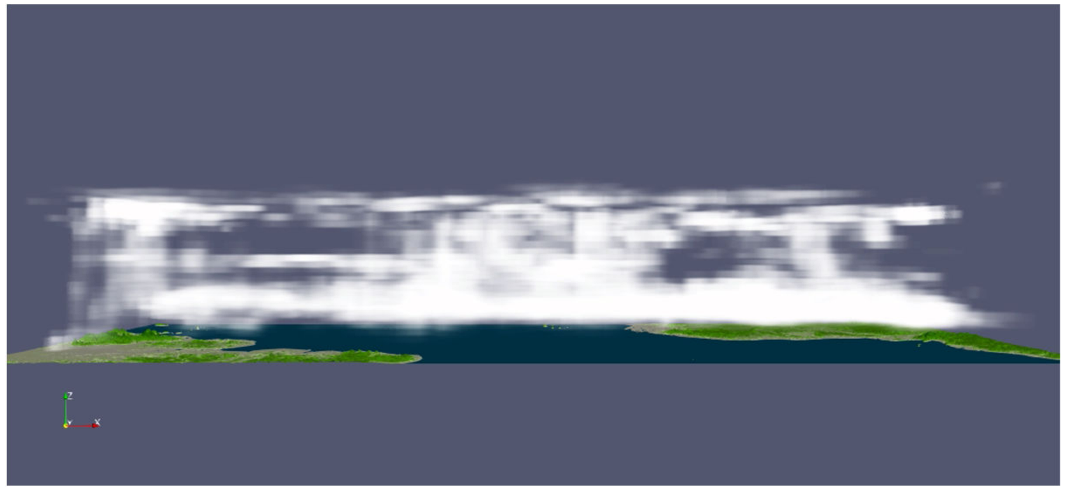
Grundner et al., DL Based Cloud Cover Parameterization for ICON, https://doi.org/10.1029/2021MS002959 (2022)

Neighborhood-based NN clearly outperforms Sundqvist

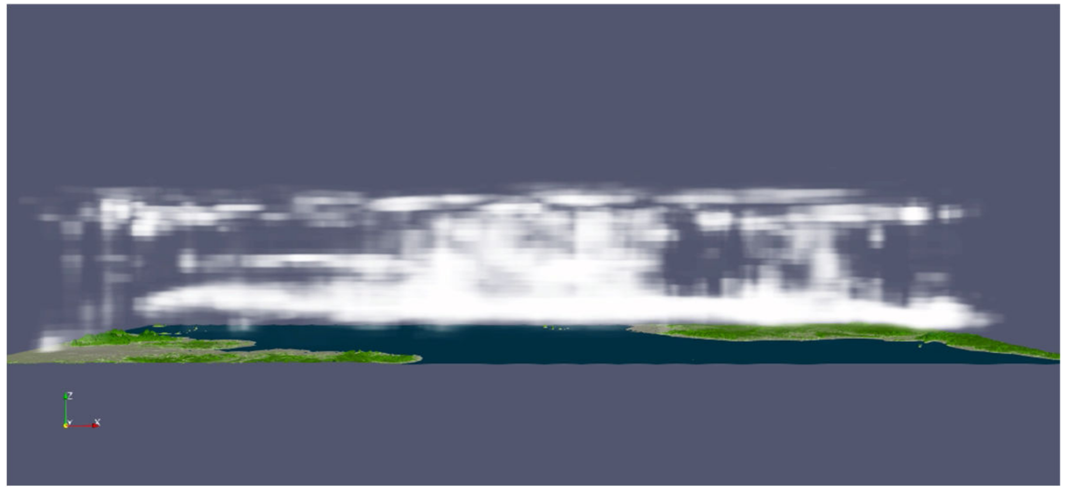
<u>Conclusion:</u>

- **Neighborhood-based NN performs best**
  - R2-values generally well above 0.8 below 15 km
  - Clearly outperforms the Sundqvist scheme currently used in ICON
- **The neural networks accurately learn cloud cover from regional and global storm-resolving model simulations**
- **Generalization Tests:**
  - Globally trained NNs can reproduce sub-grid scale cloud cover of the regional storm resolving model simulation.
  - However, NNs trained on NARVAL region have problems

Reference (Coarse-grained)

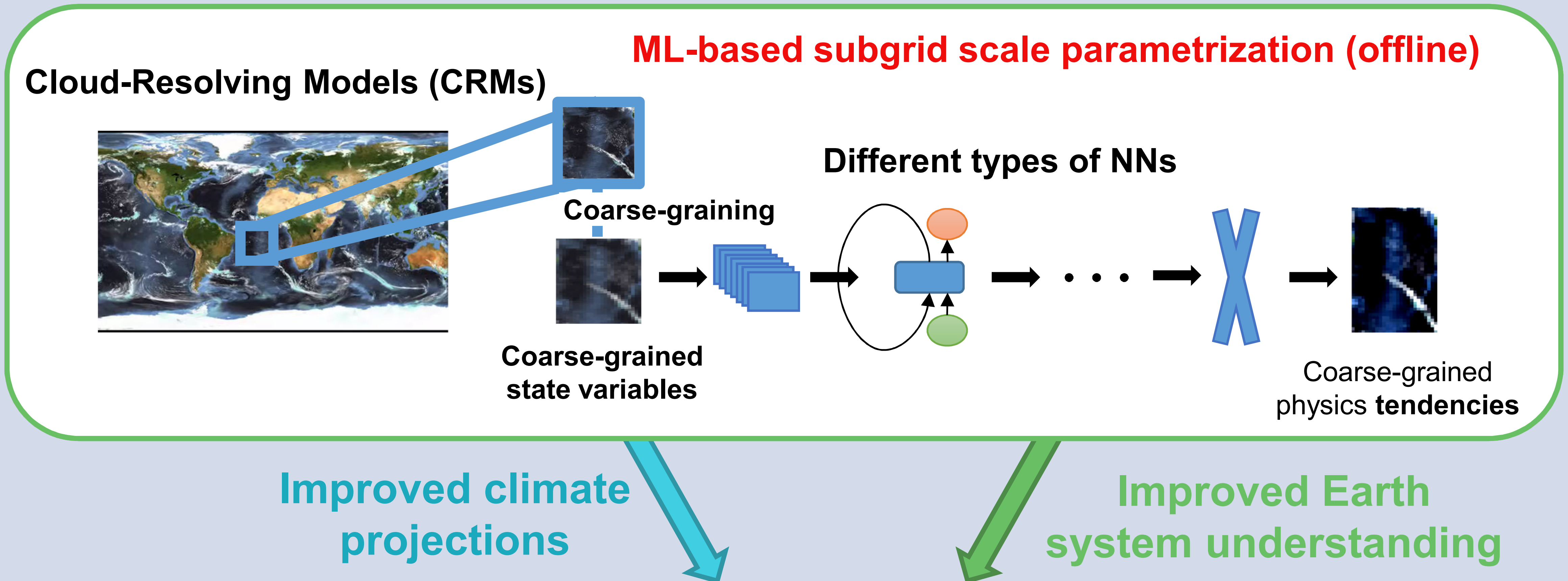


ML simulation

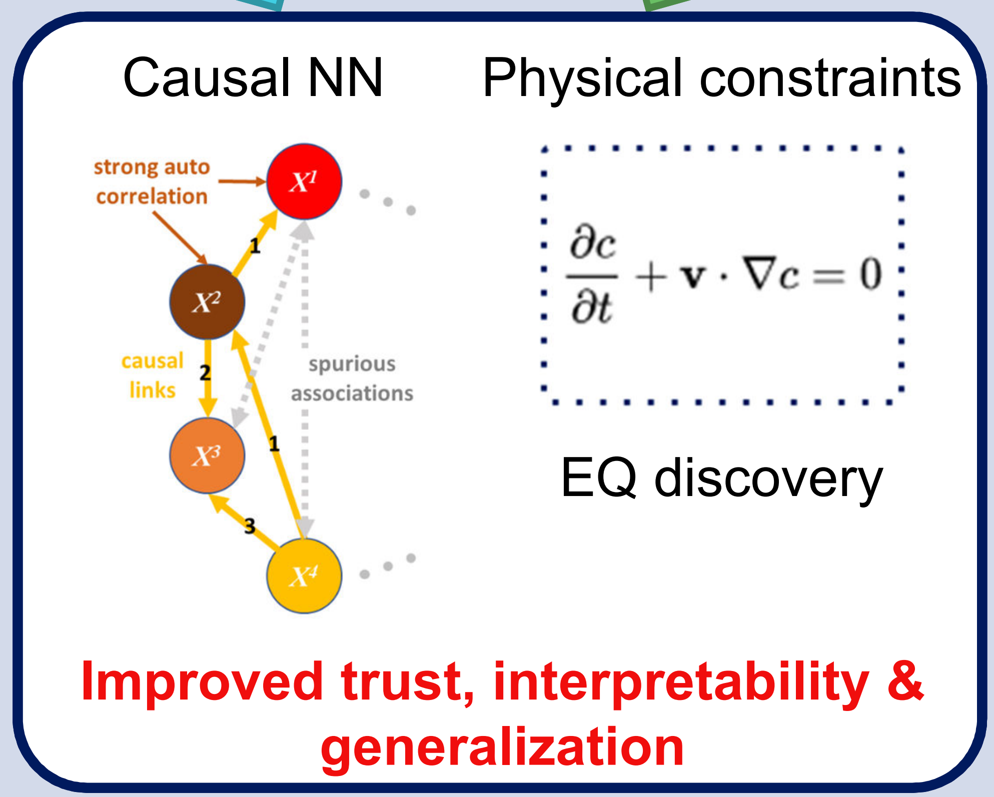


$$R_l^2 = 1 - \frac{mse_l}{var_l}$$

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



- **ML Equation Discovery for Cloud Cover** (Grundner et al., 2024, https://doi.org/10.48550/arXiv.2304.08063)
- **Interpretable multiscale ML-based Convection for ICON** (Heuer et al., 2023, in review; pre-print https://arxiv.org/abs/2311.03251v2)
- **Causally-informed ML parameterizations** (Iglesias-Suarez et al., 2024, https://doi.org/10.1029/2023JD039202)
- **Causal Neural Networks** (Kühbacher et al., submitted to ECAI 2024
- **Stochastic NN** (Behrens et al., submitted, https://doi.org/10.48550/arXiv.2402.03079)



Data-Driven Equation Discovery of a Cloud Cover Parameterization

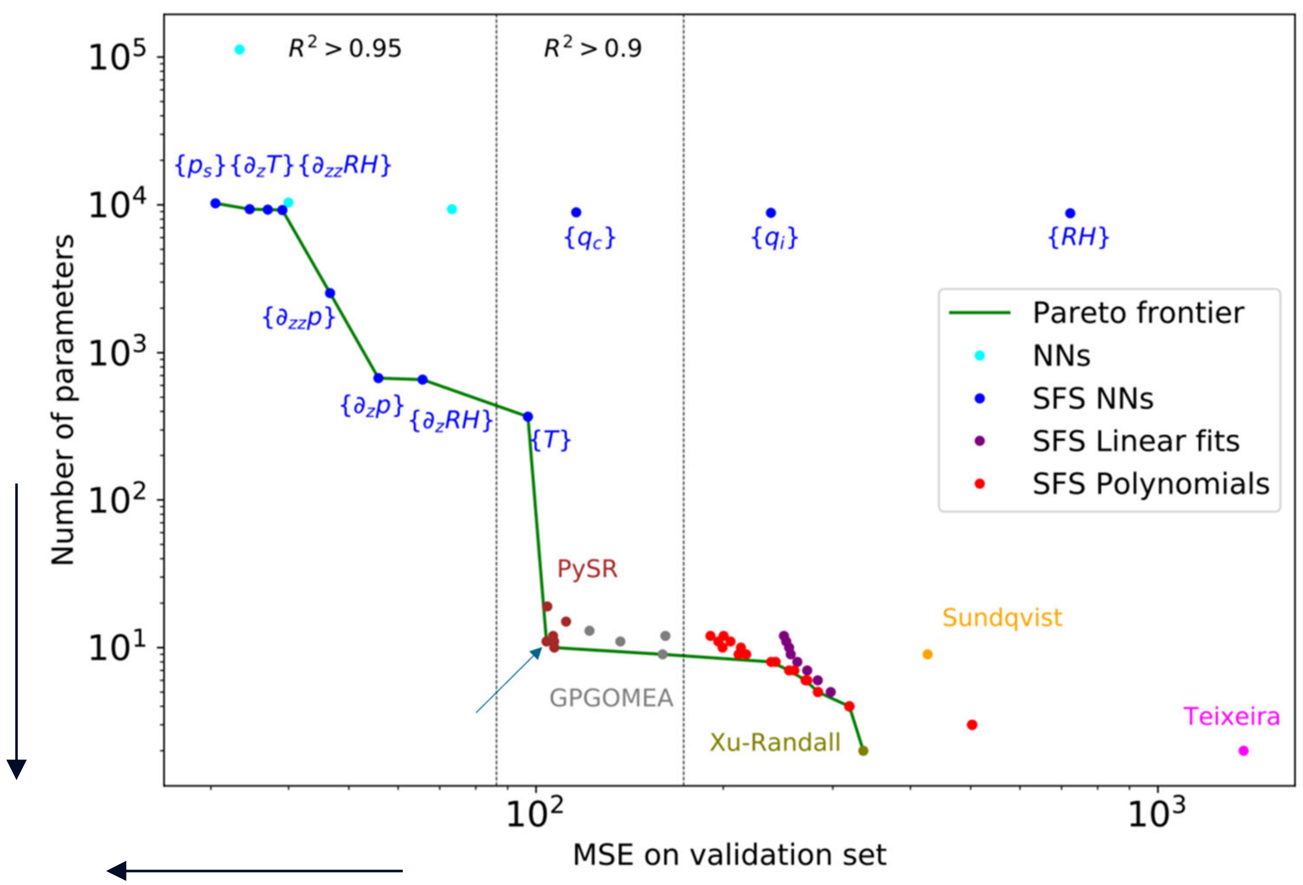
USMILE

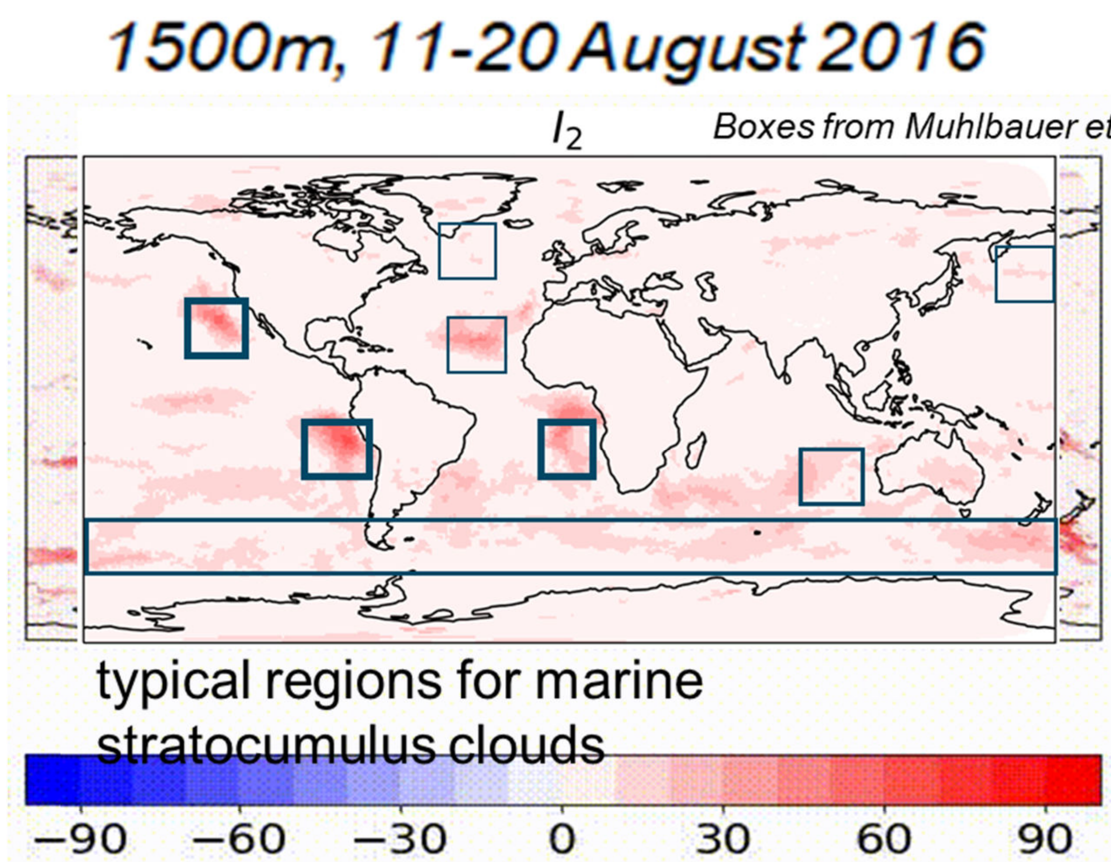
- Novel highly accurate, physically consistent, interpretable data-driven equation for cloud cover
- Both NNs and EQ run stable in online ICON simulations

$$f(RH, T, \partial_z \mathrm{RH}, q_c, q_i) = I_1(RH, T) + I_2(\partial_z \mathrm{RH}) + I_3(q_c, q_i),$$

$$I_2(\partial_z \mathrm{RH}) \stackrel{\mathrm{def}}{=} a_6^3 \left(\partial_z \mathrm{RH} + \frac{3a_7}{2}\right)(\partial_z \mathrm{RH})^2$$

Jointly minimizing error & complexity in a well-defined plane





Physical Constraints

PC_1: $\mathcal{C}(X) \in [0, 100]\%$
PC_2: $(q_c, q_i) = 0 \Rightarrow \mathcal{C}(X) = 0$
PC_3: $\partial \mathcal{C}(X)/\partial \mathrm{RH} \geq 0$
PC_4: $\partial \mathcal{C}(X)/\partial q_c \geq 0$
PC_5: $\partial \mathcal{C}(X)/\partial q_i \geq 0$
PC_6: $\partial \mathcal{C}(X)/\partial T \leq 0$
PC_7: $\mathcal{C}(X)$ is a smooth function

C: cloud cover
RH: Relative Humidity
qc: cloud water
qi: cloud ice

Grundner et al., JAMES (2024)

DLR

Convection: Model Explainability - SHAP Values

Interpretable multiscale ML-based Convection for ICON

- We used **SH**apley **A**dditive ex**P**lanations for best found architecture: U-Net
- $shap(x = x_0, y)_{X_b}$ indicates change from average prediction in y for background data X_b when $x = x_0$
- U-Net focuses mainly on the precipitating tracer species for rain and snow, qr and qs, so learns non-causal relations

Ablated U-NET

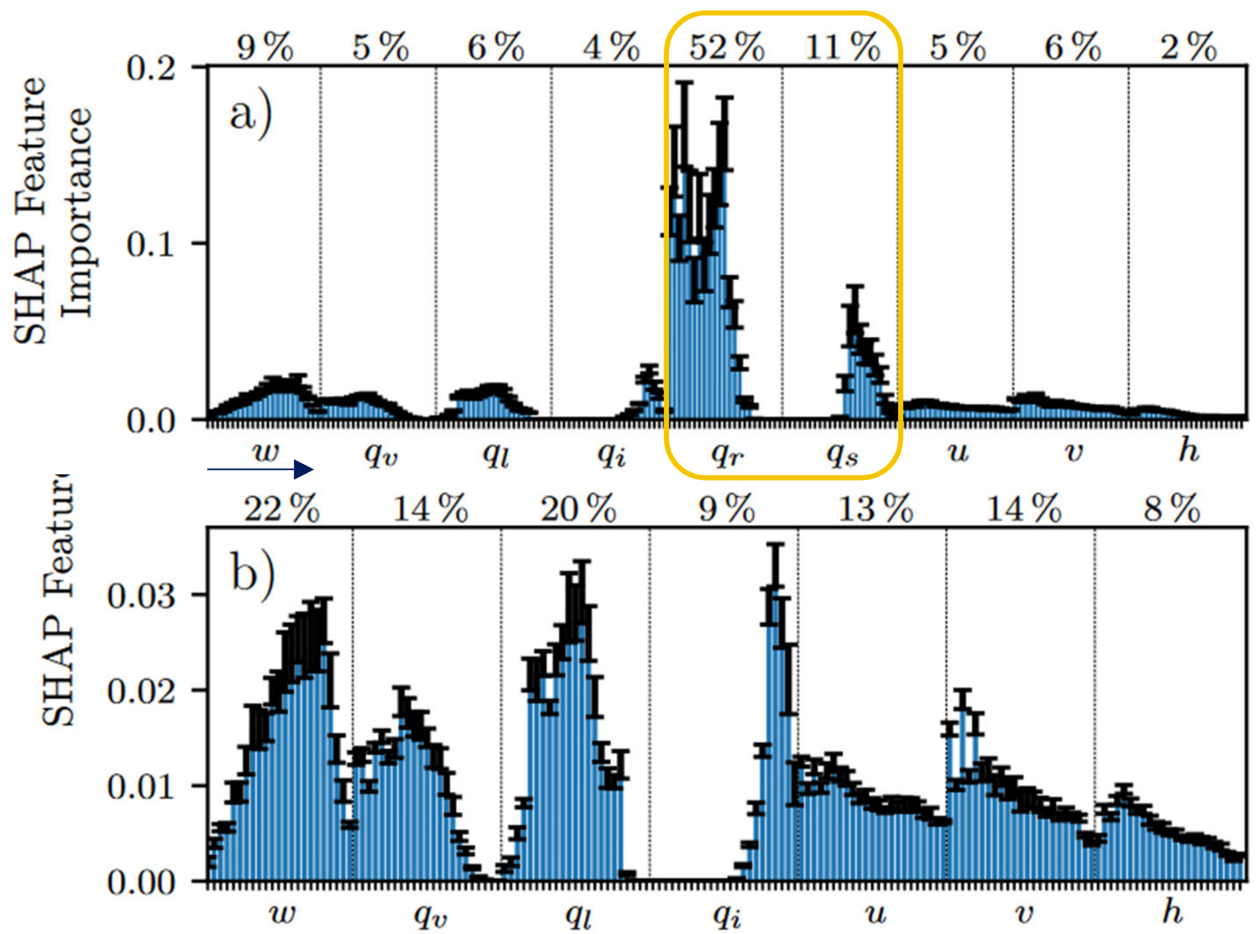
- Excludes precipitating tracer species.
- learned relations connected to physical processes
- Improves online ICON simulations compared to U-NET

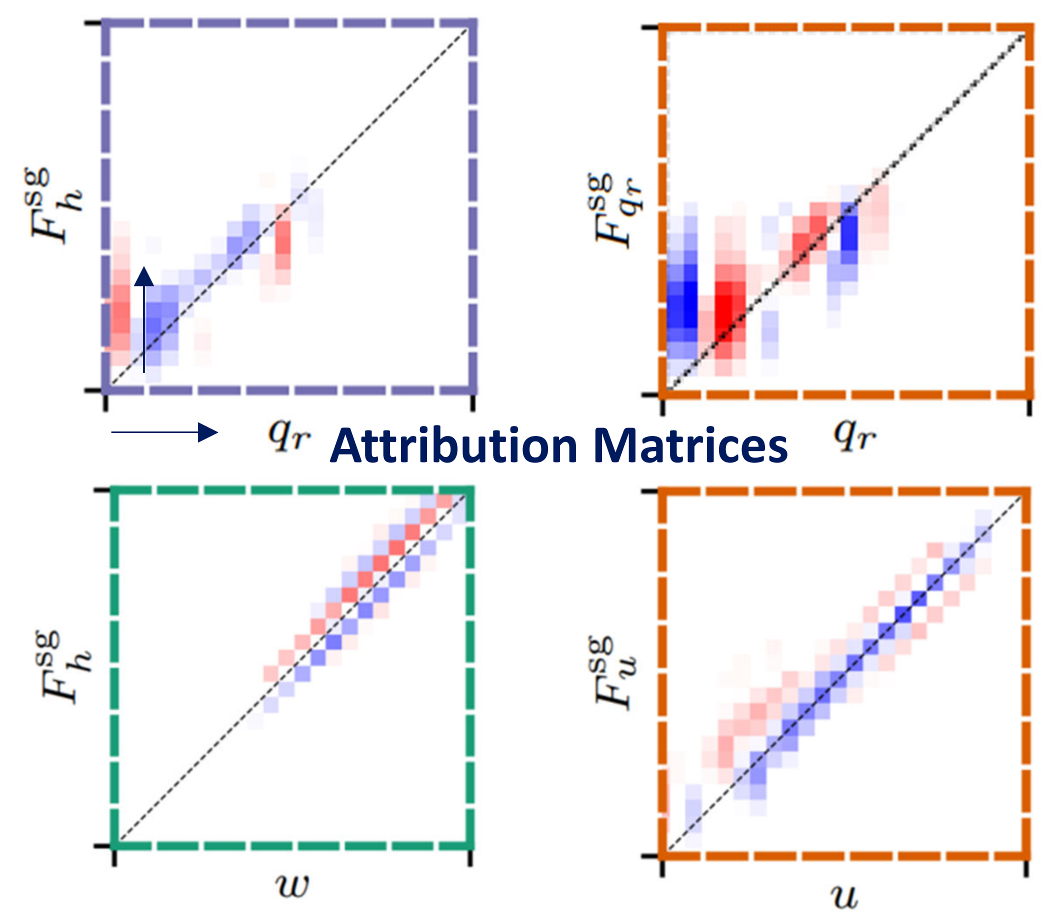
Full U-Net

Learns reversal of causality, so when the ML model sees precipitation it guesses that convection is responsible for rain and snow.

Ablated U-Net

Precipitation tracer species for rain and snow ablated.



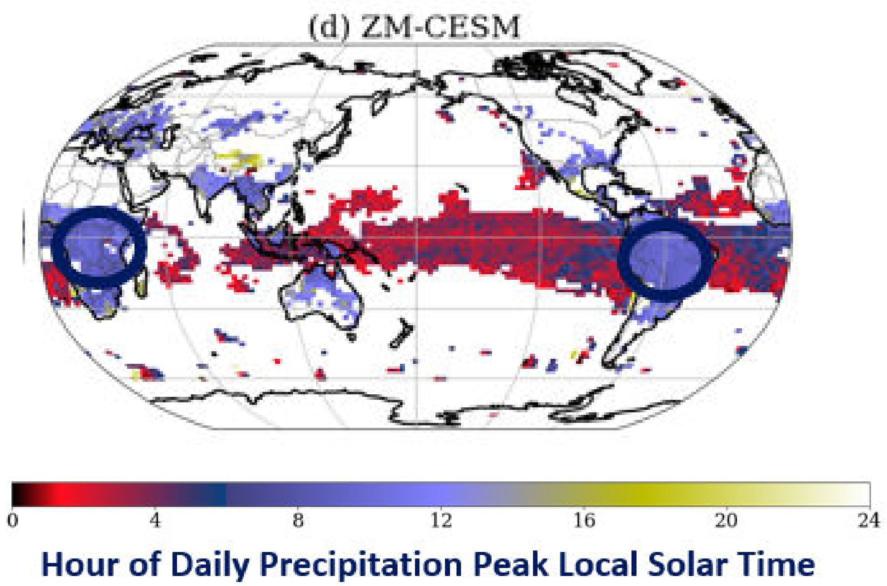


Quantify how each input influences each output variable foreach level

Heuer et al., JAMES, subm., https://arxiv.org/abs/2311.03251

Online: ML-based Climate Models Reduce Systematic Errors

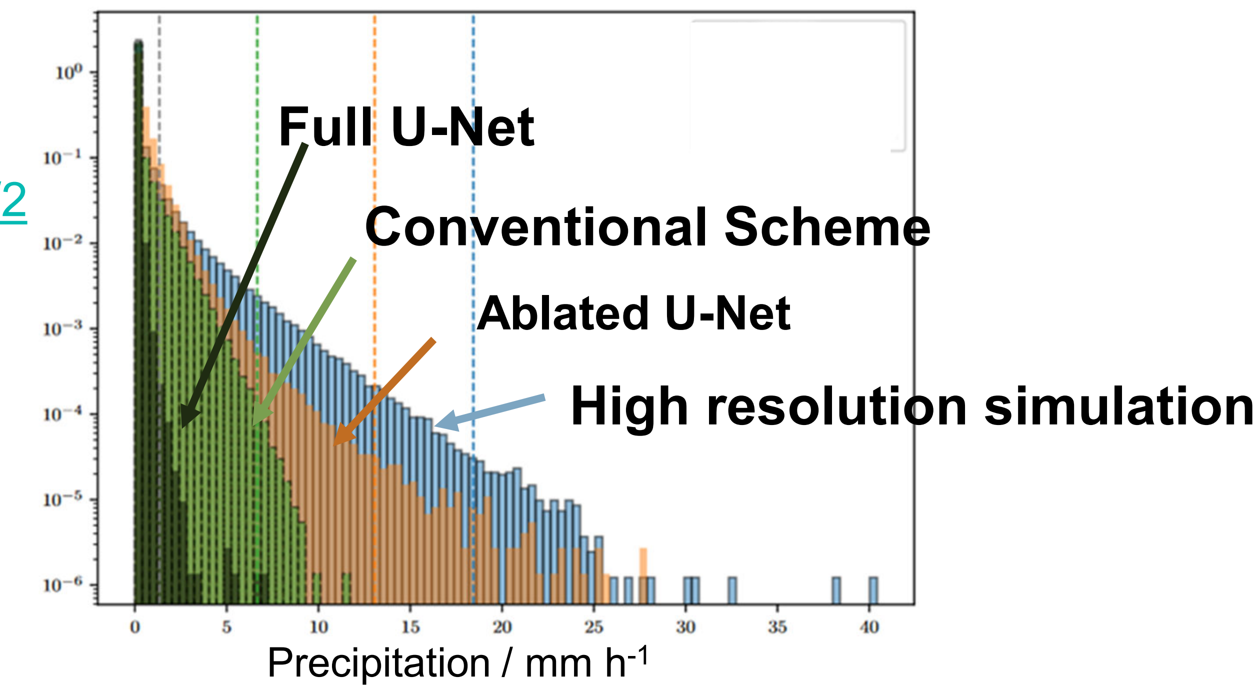
ML-based stochastic parametrizations
=> Improved diurnal cycle of precipitation (CESM)



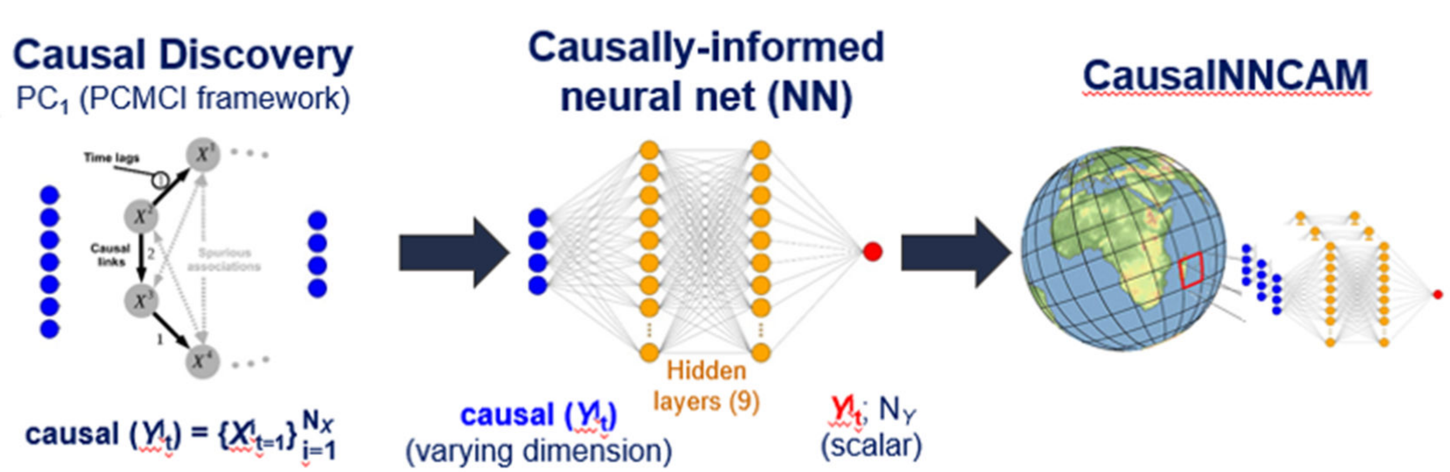
Behrens et al., JAMES, subm. https://arxiv.org/abs/2402.03079

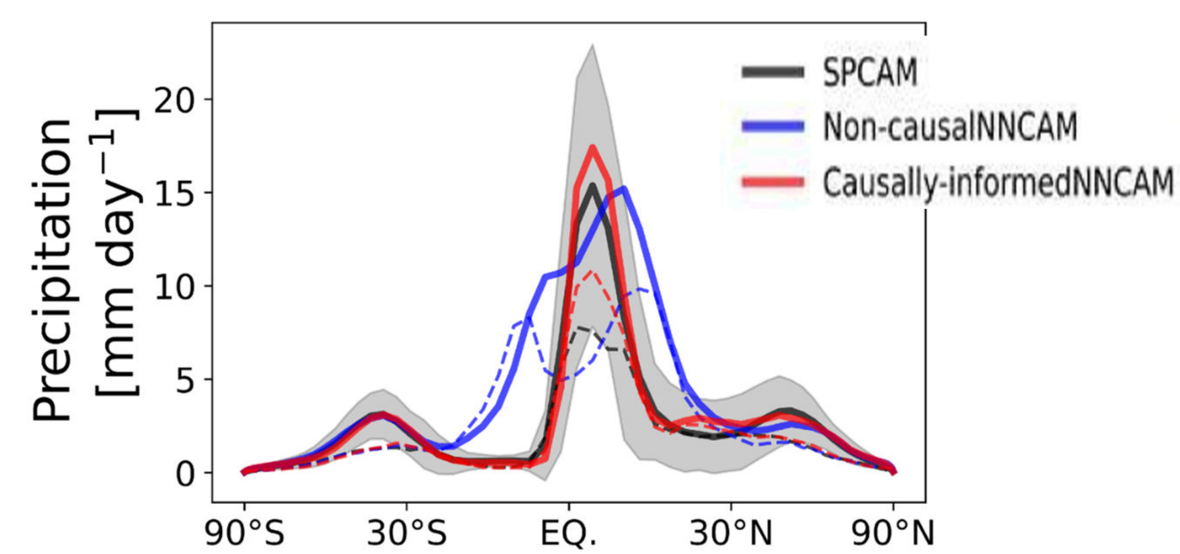
ML-based convection parmetrizations Ablated UNET
=> Improved extreme precipitation (ICON-A)

Heuer et al., JAMES, subm. https://arxiv.org/abs/2311.03251



Causally-informed Neural network: Improved simulation of the ITCZ in causally-informed NNCAM aquaplanet

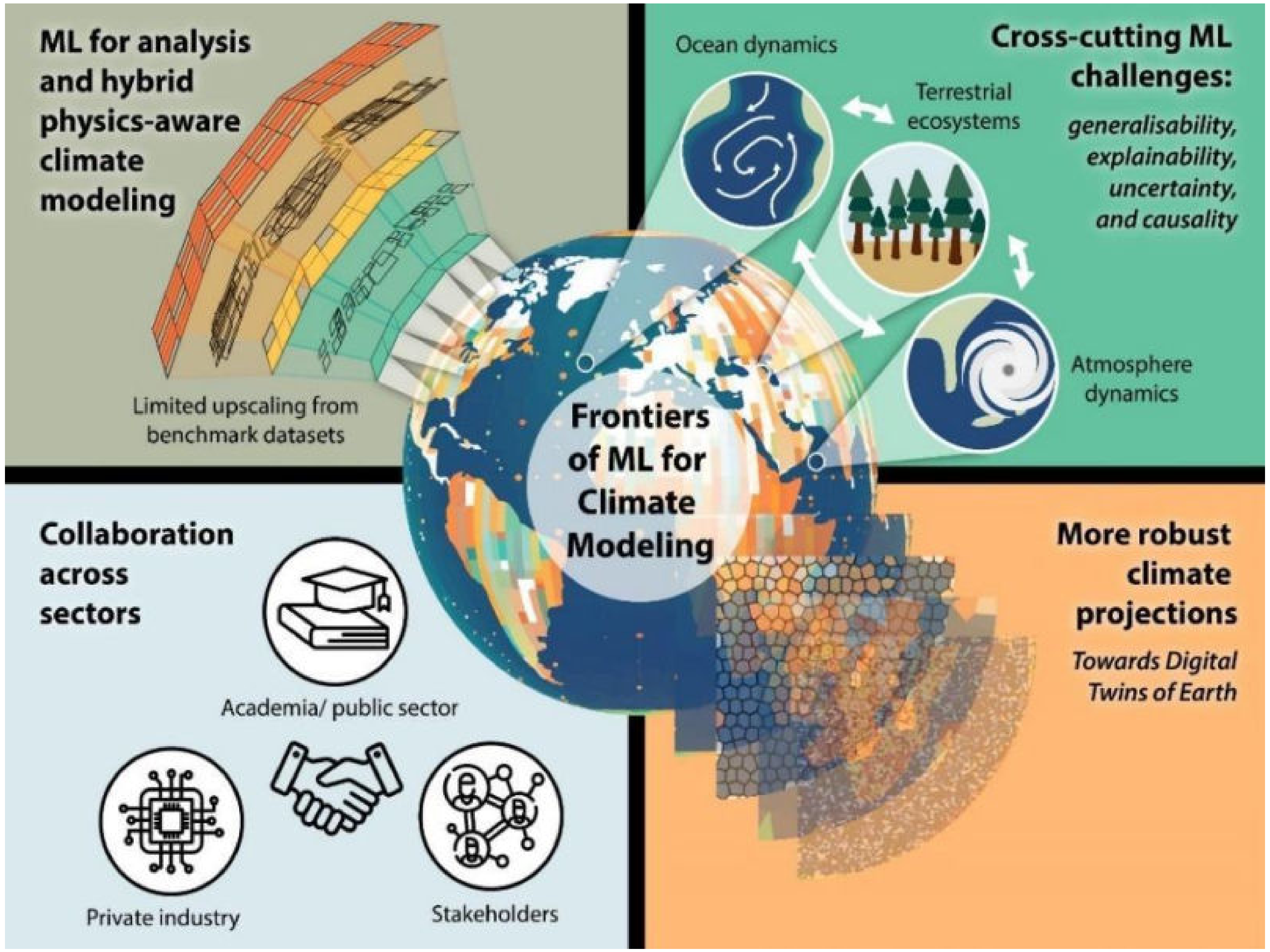




Iglesias-Suarez et al., JGR, 2024

Utilizing this potential requires addressing key ML challenges

Kühbacher, B., F. Iglesias-Suarez, N. Kilbertus & V. Eyring, Towards Physically Consistent Deep Learning For Climate Model Parameterizations, ECAI, submitted, https://arxiv.org/abs/2406.03920



Physical Consistency, Stability, Generalization

- Include physical constraints or other approaches for stable simulations

Uncertainty Quantification

- Stochastic (aka statistical) uncertainty is also present due to noise in the data used for training, and the choice of predictive variables being an incomplete representation of the Earth system

eXplainable Artificial Intelligence

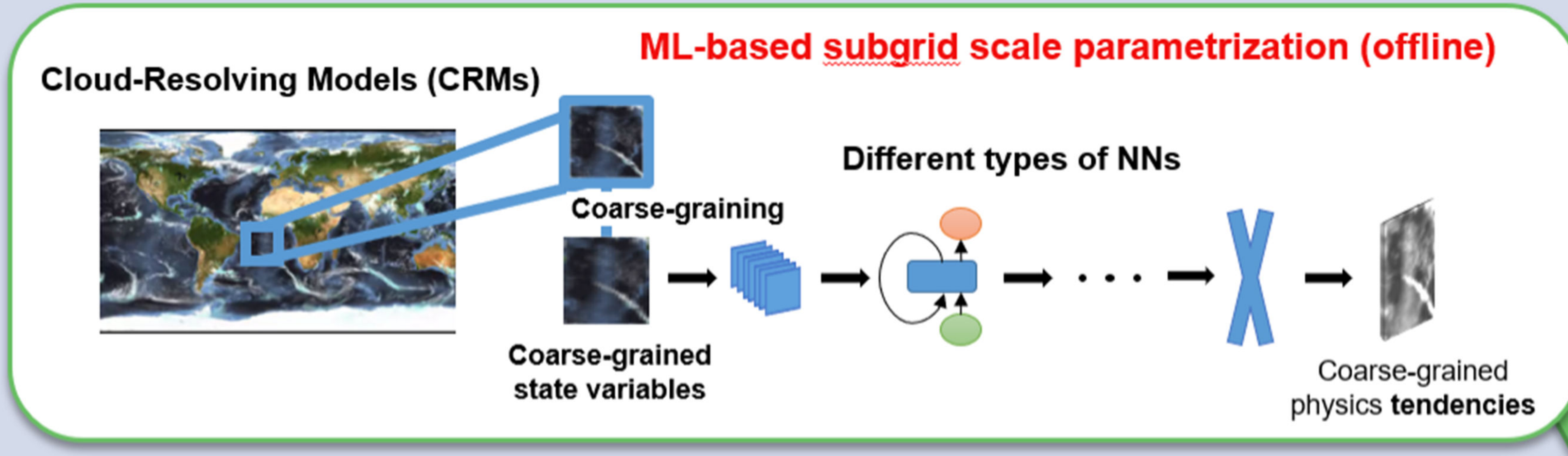
- Assisting scientists to determine whether the ML approach is obtaining the right answers for the right

Causal Inference

- E.g., Data is generated from a causally stationary process when in practice many real-world processes are non-stationary;

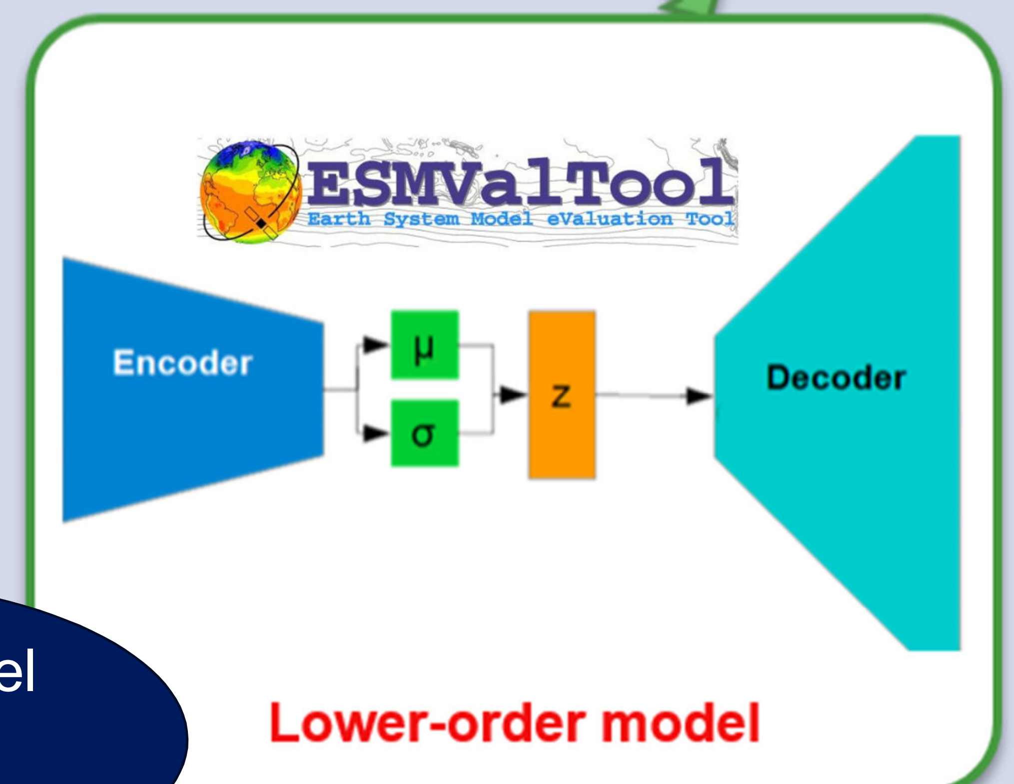
Collaboration across sectors: Academia (ML and climate scientists), **Private sector & Stakeholders**

Eyring, V., W. Collins et al., P. Gentine, Nature Climate Change, Perspective, accepted, 2024



Improved Earth system understanding

- **Learning convection with a VED** (Behrens et al., 2022, https://doi.org/10.1029/2022MS003130)
- **Understanding modes of climate variability with causality** (Karmouche et al., 2022, https://doi.org/10.5194/esd-14-309-2023)
- **Changing effects of external forcing on Atlantic–Pacific interactions** (Karmouche et al., 2024, https://esd.copernicus.org/articles/15/689/2024/)
- **Understanding Arctic teleconnections with causality** (Galytska et al., 2022, https://doi.org/10.1002/essoar.10512569.1)
- **Constraining uncertainty in multi-model climate projections using feature maps** (Schlund et al., 2022, https://doi.org/10.1029/2019JG005619)
- **Benchmarking: Development of ESMValTool** (Schlund et al., 2023, https://doi.org/10.5194/gmd-16-315-2023)



ML-based model tuning and evaluation

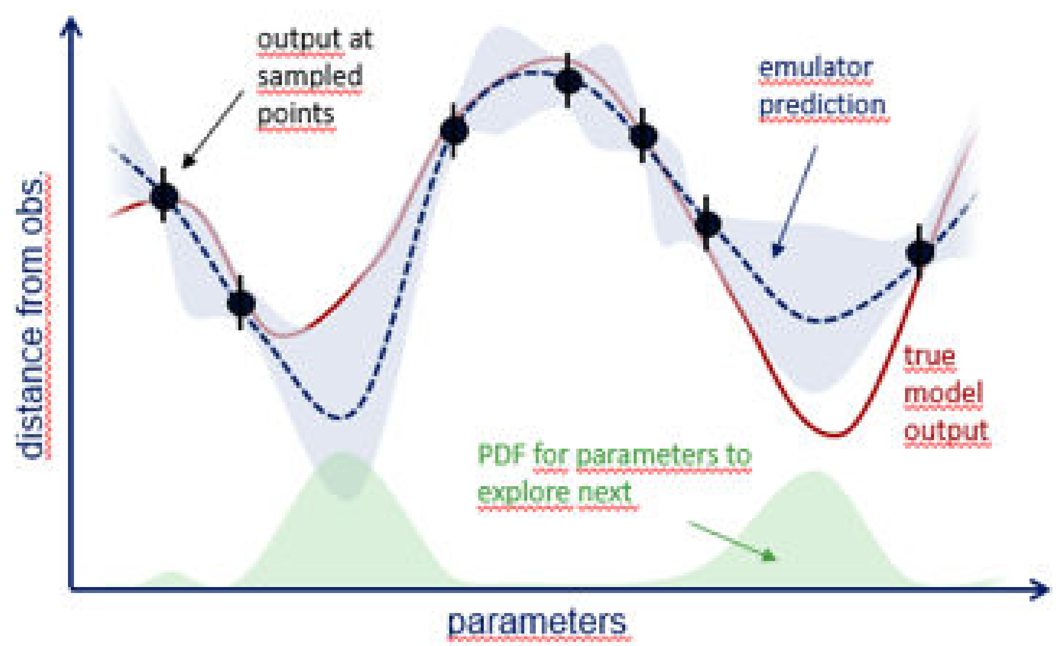
ML-based Automatic Tuning Framework for ICON

- Preliminary step: choose metrics to tune for and identify parameters to tune (e.g., sensitivity analysis)
- **Iterative optimization:** Bayesian scheme applicable to costly ‚black-box' functions

1. Perturbed parameter sensemble (**PPE**): N model runs for randomly sampled parameter
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**.

This e**xploration-exploitation** tradeoff is achieved by shrinking the 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.

Pastori, Bonnet et al., in preparation, 2024 (ICON Atmosphere)

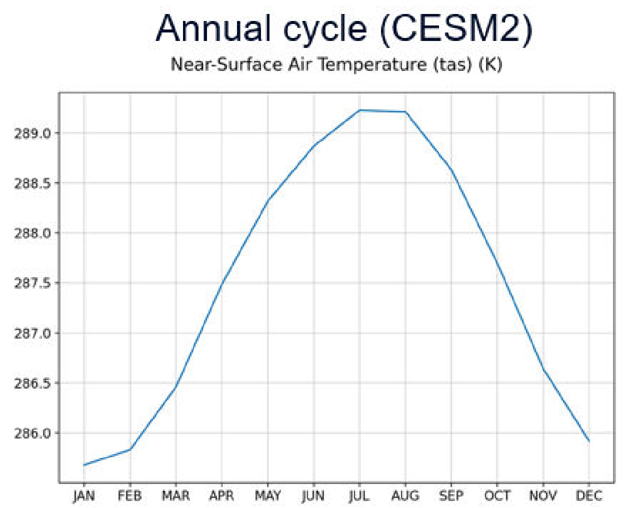
Bouman et al., in preparation, 2024 in collaboration with Katie Dagon and Linnia Hawkins (ICON Land-atm coupling)

Evaluation of Native Model Output with ESMValTool

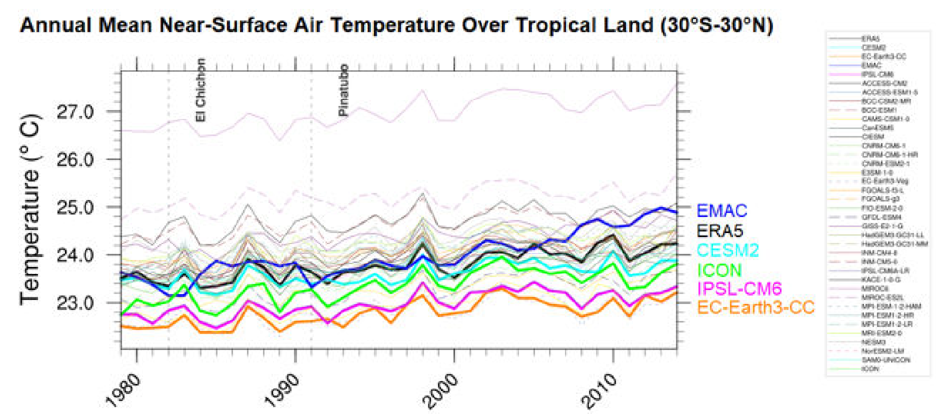
ESMValTool
Earth System Model Evaluation Tool

"Community-developed open-source diagnostic and performance metrics tool for routine evaluation of Earth system models."

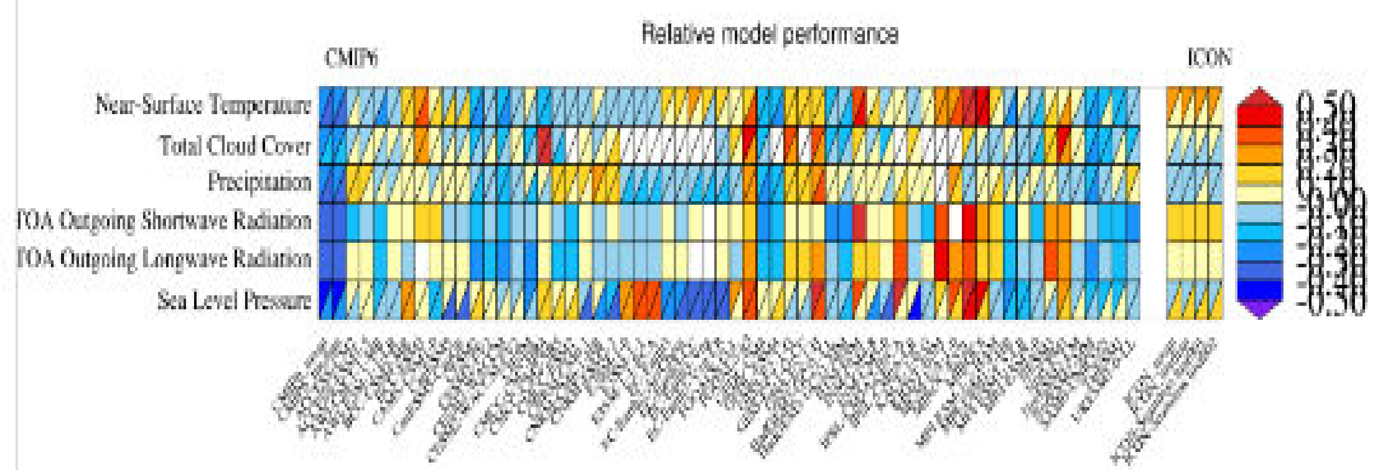
- Reading of native model output, currently: **CESM2**, EC-Earth3, EMAC, **ICON**, and IPSL-CM6.
- No postprocessing (e.g., CMORization) necessary
- This output can be processed like any other CMIP model within ESMValTool
- **Monitoring of simulation available now, but also allows benchmarking of simulations to other CMIP models and observations before submission to the ESGF (or other CMIP archives)**



Single model analysis

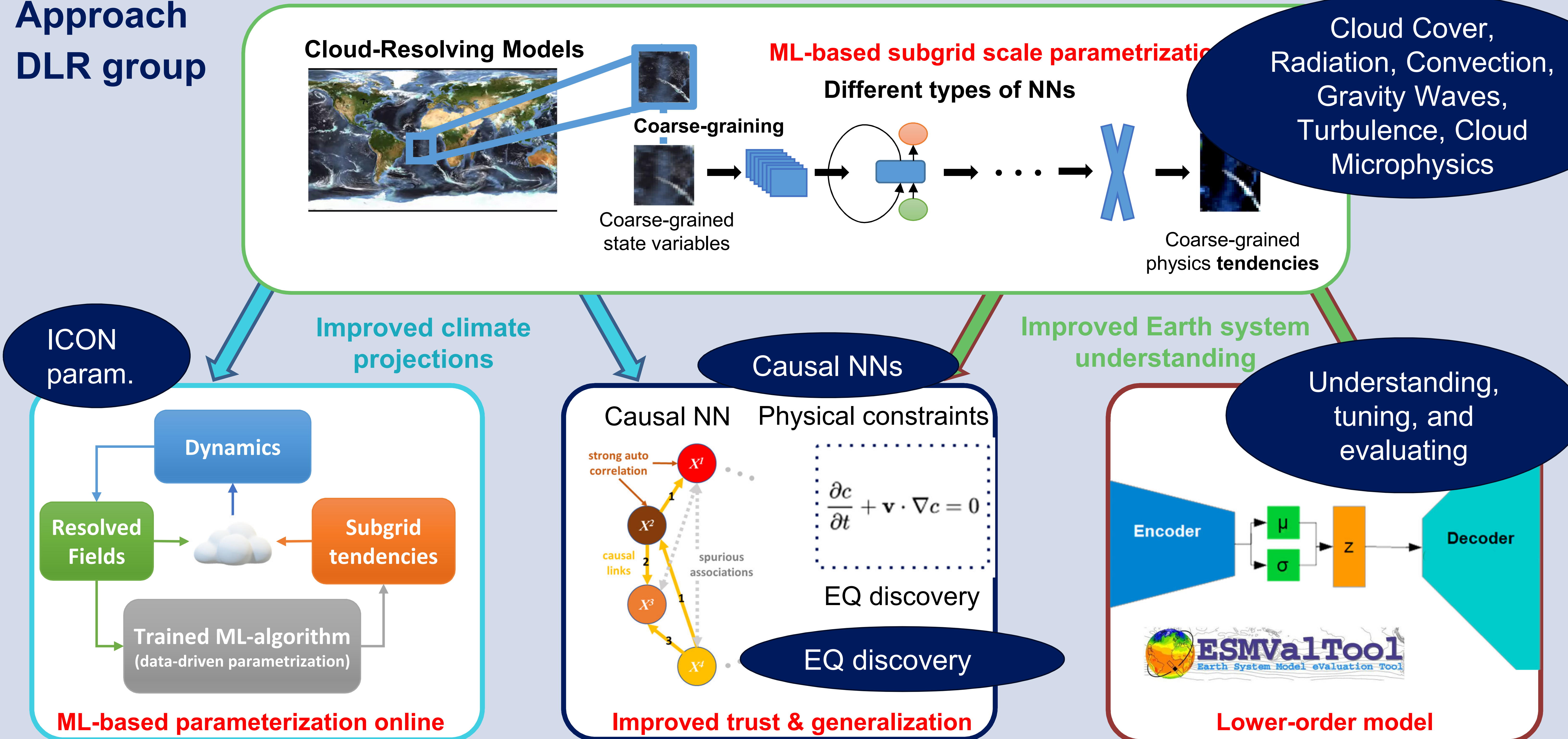


Multi model analysis



Schlund et al. (incl. B. Medeiros), GMD, 2023

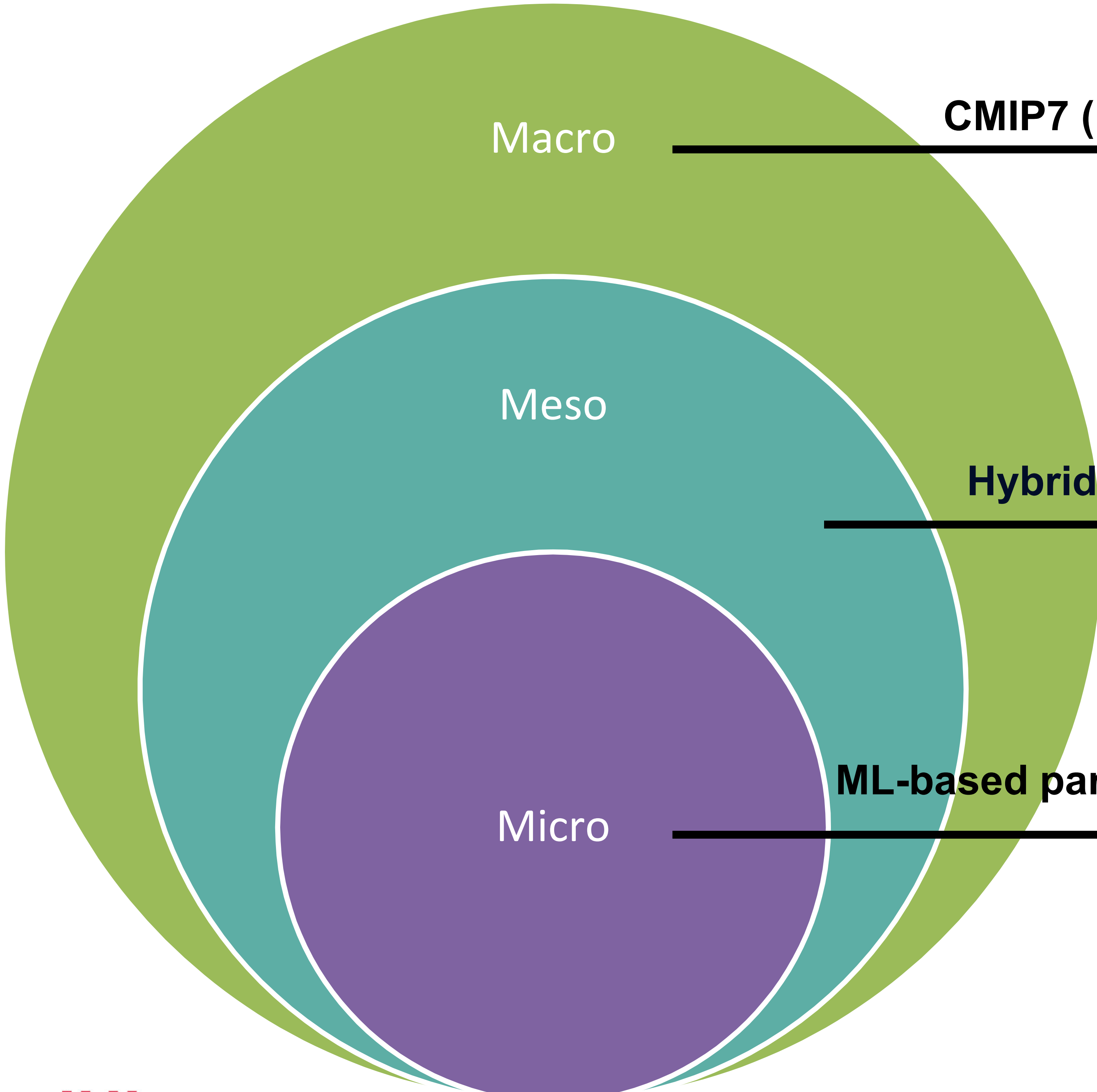
Approach DLR group



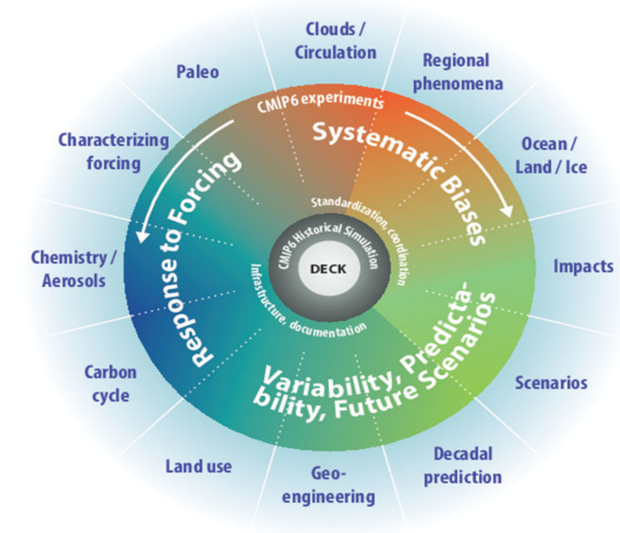
ML-based automatic tuning
(parameter estimation)

Code released open source at
https://github.com/EyringMLClimateGroup/

USMILE Goals

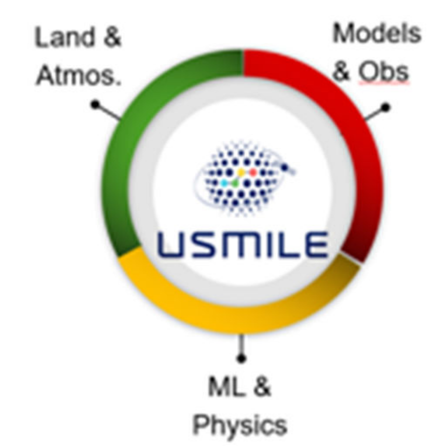


CMIP7 (DECK + historical)



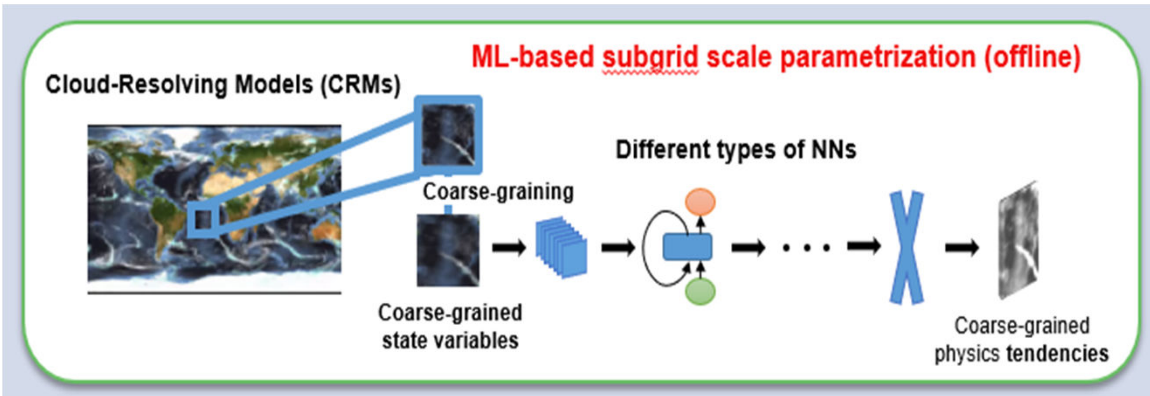
Coupled hybrid model
ICON-XPP-ML
Better & faster Ensembles

Hybrid ICON-ML atm / land

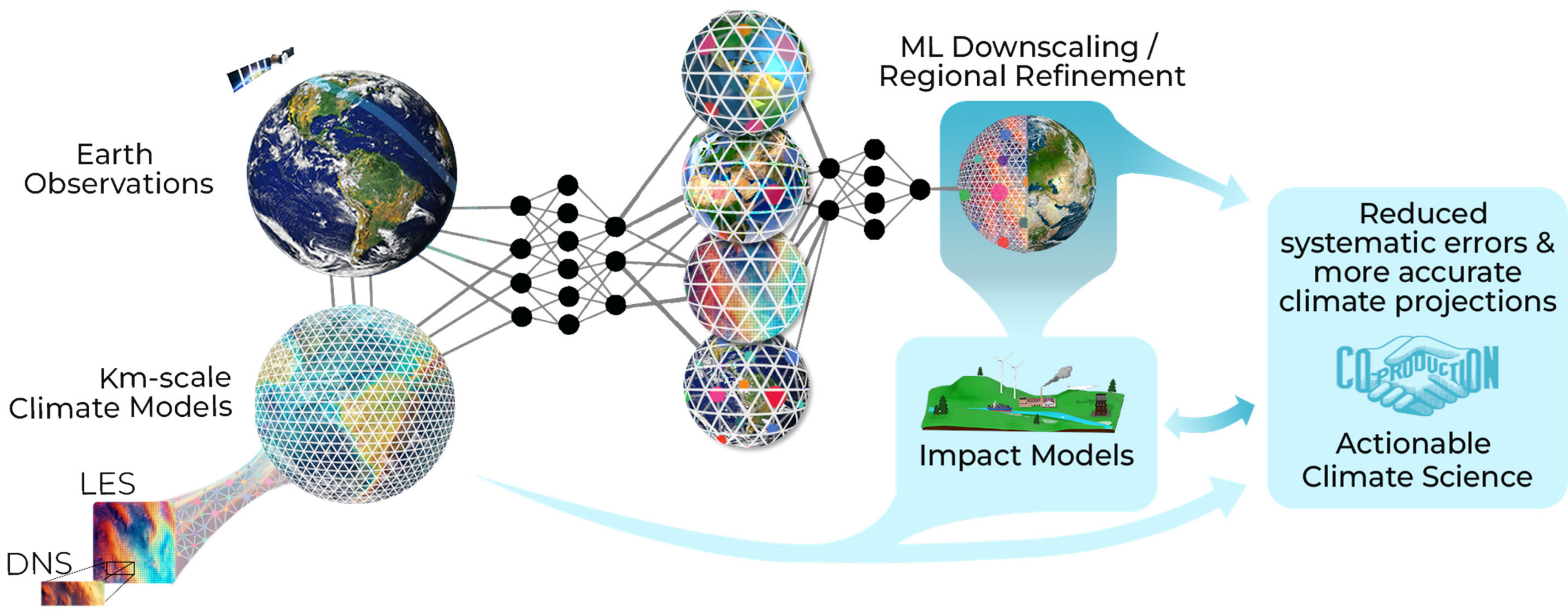


Hybrid model
ICON-ML-A
ICON-ML-land

ML-based parametrizations



Hybrid (physics+ML) ESMs



Bridging across scales

- Higher resolution with new computing opportunities
- Improved with physics-aware ML
- Constrained and benchmarked with Earth observations
- Modern and operational science infrastructures

Eyring, V., P. Gentine, G. Camps-Valls, D. M. Lawrence, M. Reichstein, Nature Geoscience, accepted, 2024

Summary & Vision

1

CMIP

- Provides **scientific understanding** and an **important source for IPCC Assessment Reports** since decades.
- However, **large errors** and **climate projection uncertainties** remain and the **slow pace** of updated climate information through the CMIP cycles deters policy decisions.

2

Development of hybrid (physics + ML) Earth System Models

- ML trained against **short km-scale climate model simulation**s has been successfully substituted for conventional parameterizations (e.g. deep convection, cloud cover), thereby enhancing the **fidelity of the host ESM.**
- Through **innovative ML methods**, ML is no longer a black box, rather can help understanding physical processes

3

Challenges

- **ML Challenges:** physical constraints and generalization, uncertainty quantification, XAI, causality
- **Other Barriers: operationalization of policy-relevant simulations** and **annual updates of forcing datasets** as well as the broad an inclusive accessibility of climate model data.

4

Bridging across scales and complexity

- This approach complements **km-scale modeling** activities with **models that include important Earth system processes and feedbacks, yet are still fast enough to deliver large ensembles for better quantification of internal variability and extreme events**.
- Could form an integral part of international activities such as **CMIP and Digital Twin Initiatives.**
- Together, this can form a step change in the **accuracy and utility of climate projections**, meeting the urgent mitigation and adaptation needs of society and ecosystems also on the **regional scale** in a rapidly changing world.

Eyring, V., P. Gentine, G. Camps-Valls, D. M. Lawrence, M. Reichstein, Nature Geoscience, accepted, 2024

Contact: veronika.eyring@dlr.de
Project information: https://www.usmile-erc.eu/
Code availability: https://github.com/EyringMLClimateGroup/
https://github.com/ESMValGroup

USMILE

DLR