AI-empowered Next-generation Multiscale Climate Modeling for Mitigation and Adaptation

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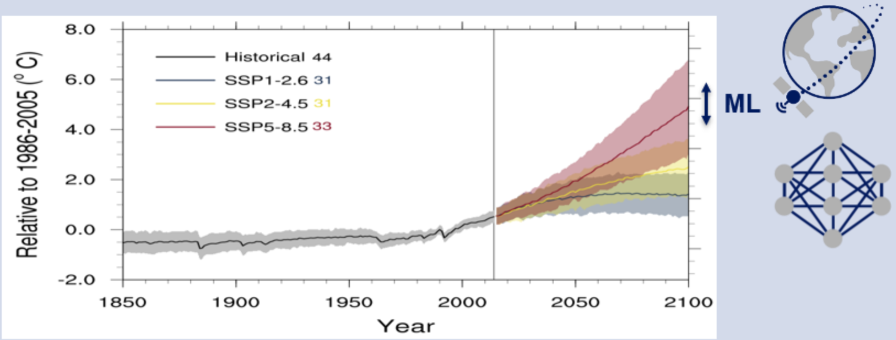


Acknowledgments:

Group Members: Mierk Schwabe, Max Bouman, Arthur Grundner, Katharina Hafner, Helge Heuer, Janis Klamt, Lorenzo Pastori, Julien Savre, Manuel Schlund et al.

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

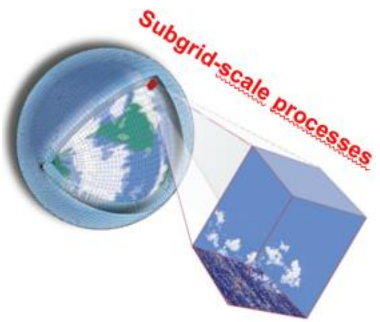
Collaborators: Tom Beucler, Marco Giorgetta, Dave Lawrence, Robert Pincus, Jakob Runge, Sara Shamekh

CESM Group Workshops, NCAR, Boulder, CO, 4 February 2025

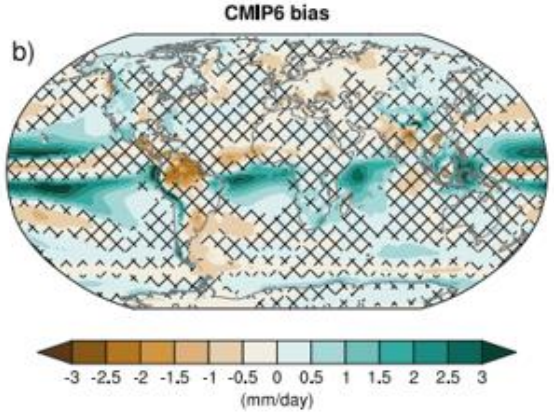
Hybrid (Physics + Machine Learning) Earth System Models (ESM)

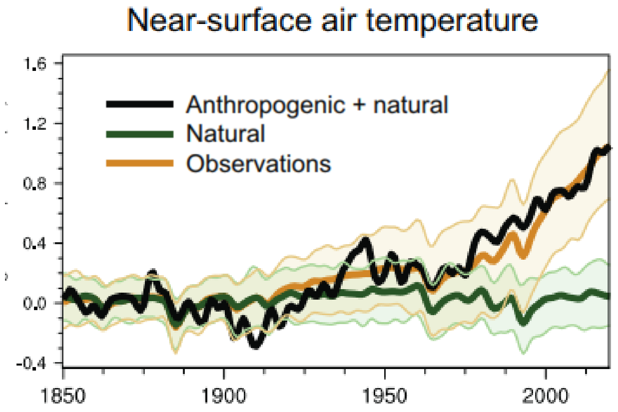
Coupled Model Intercomparison Project (CMIP)

Systematic Errors



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

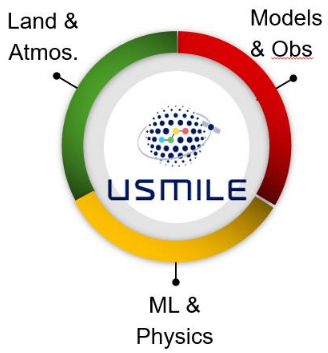


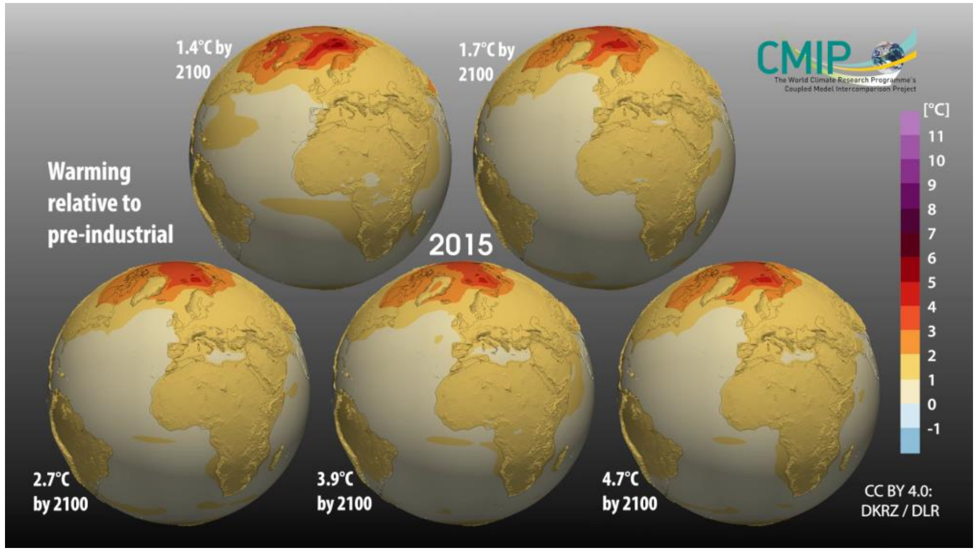


- Research tool for understanding Earth system processes and feedbacks
- Detection and Attribution
- Climate Projections

Eyring et al., IPCC WGI AR6 Ch3, 2021

Hybrid (physics + ML) ESM
ICON-XPP-ML



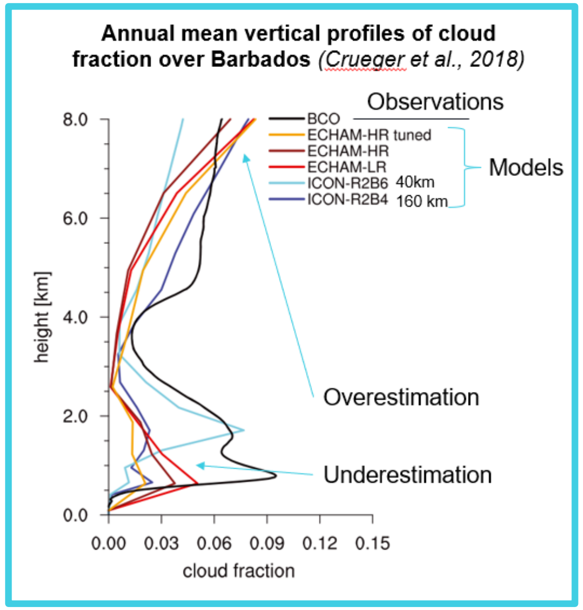


based on Lee et al., IPCC WGI AR6 Ch4, 2021

1. Cloud cover parameterization: Feedforward NN for ICON

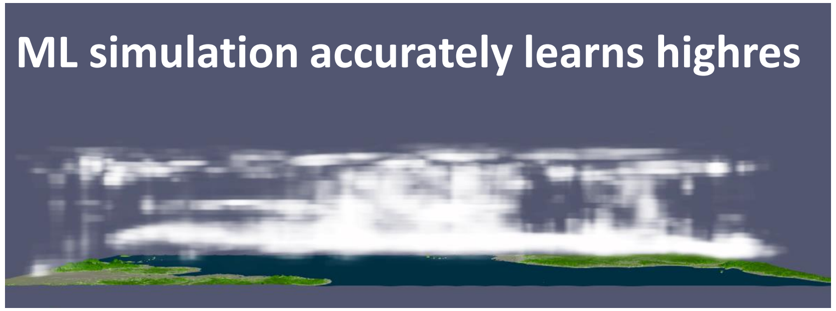
Estimated as a diagnostic (Sundqvist et al., 1989)

- 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)



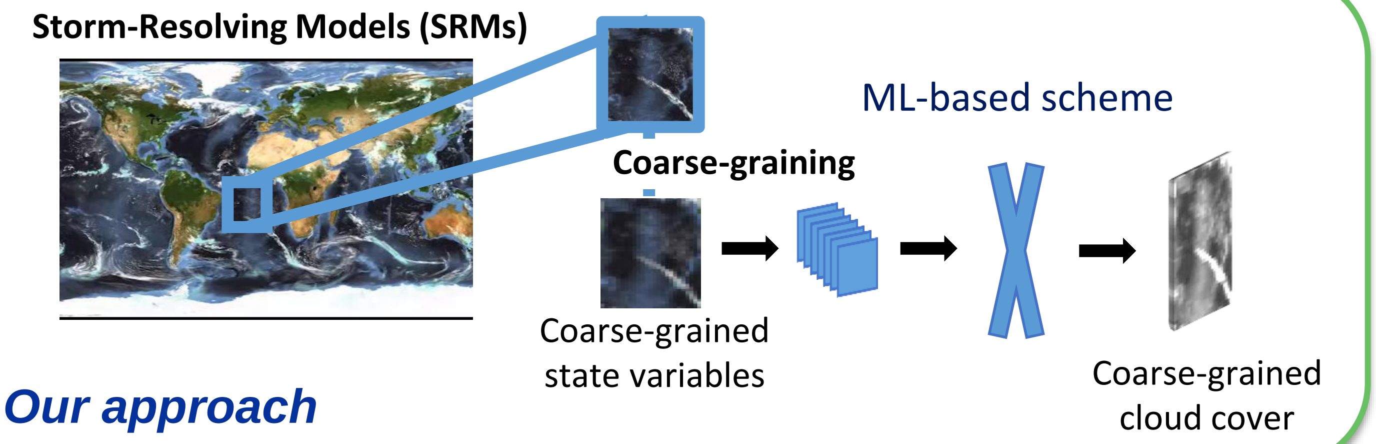
ICON Storm Resolving Model Simulations NARVAL, QUBICC, DYAMOND (~2-5 km)

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



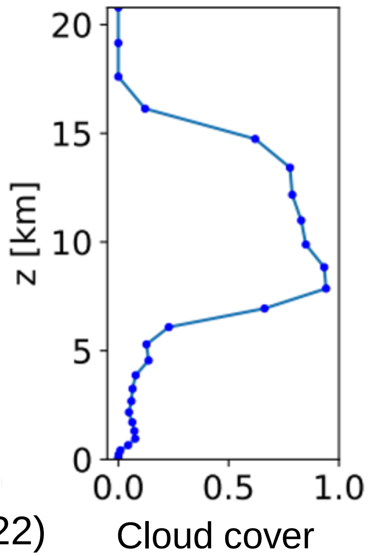
Potential features

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



Our approach

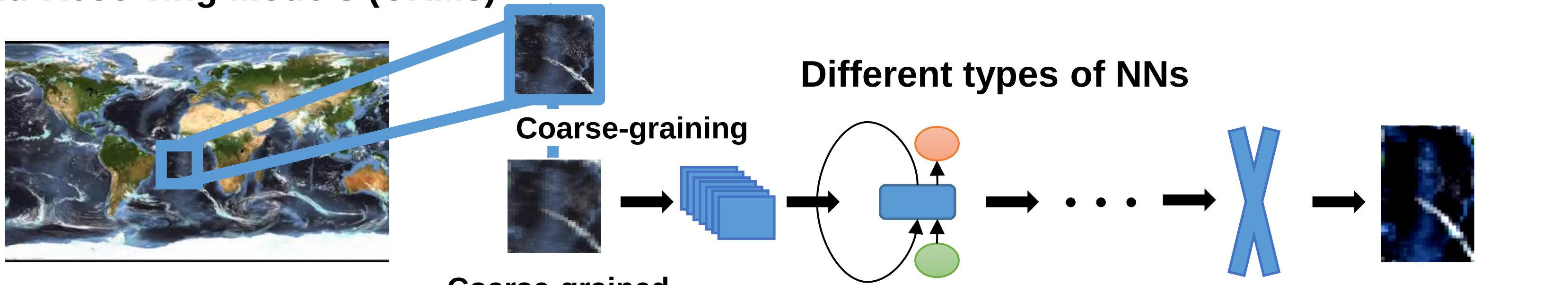
Target



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

ML-based subgrid scale parametrization (offline)

Cloud-Resolving Models (CRMs)



Coarse-grained state variables

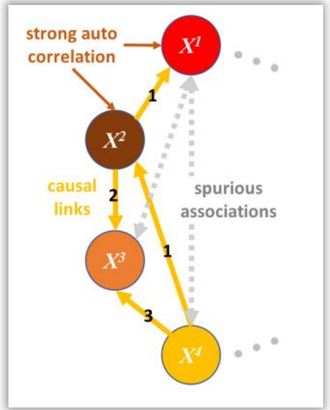
Coarse-grained physics **tendencies**

Improved climate projections

Improved Earth system understanding

- **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, https://doi.org/10.1029/2024MS004398)
- **Causally-informed ML parameterizations** (Iglesias-Suarez et al., 2024, https://doi.org/10.1029/2023JD039202)
- **Causal Neural Networks** (Kühbacher et al., ECAI 2024, https://arxiv.org/abs/2406.03920)
- **Stochastic NN** (Behrens et al., submitted, https://doi.org/10.48550/arXiv.2402.03079)
- **ML-based Radiation Emulation** (Hafner et al., submitted, https://doi.org/10.22541/essoar.173169996.65100750/v1)

Causal NN



Physical constraints

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = 0$$

EQ discovery

Improved trust, interpretability & generalization, acceleration

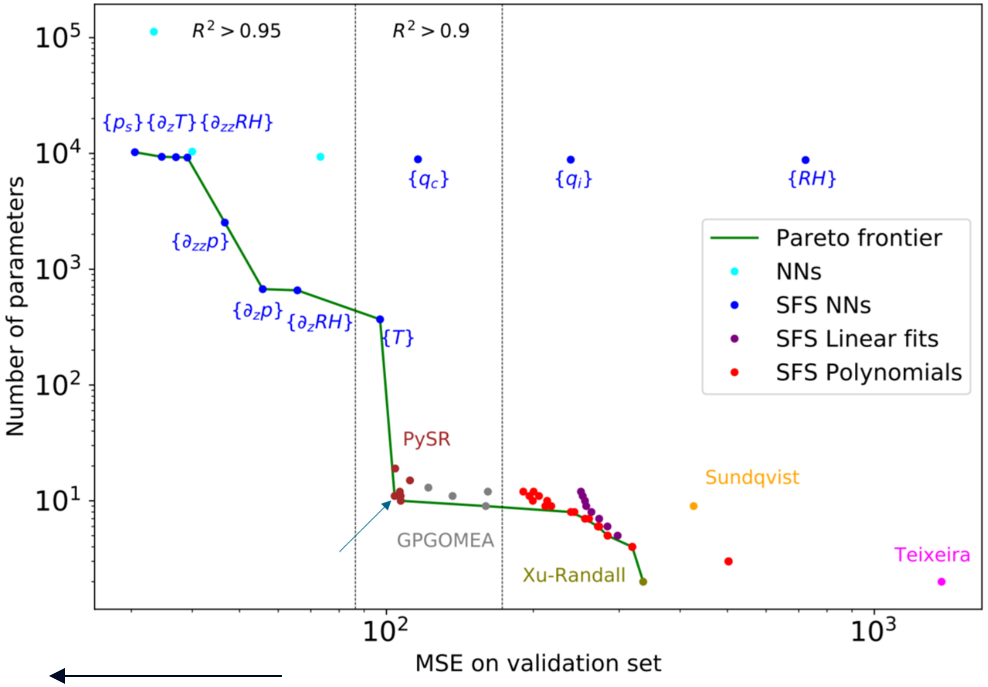
2. Cloud cover parameterization: Data-Driven Equation Discovery

- Novel highly accurate, physically consistent, interpretable data-driven equation for cloud cover
- Retune. Both NNs and EQ run stable in online ICON simulations, significantly reducing biases in cloud cover compared to Sundqvist

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

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

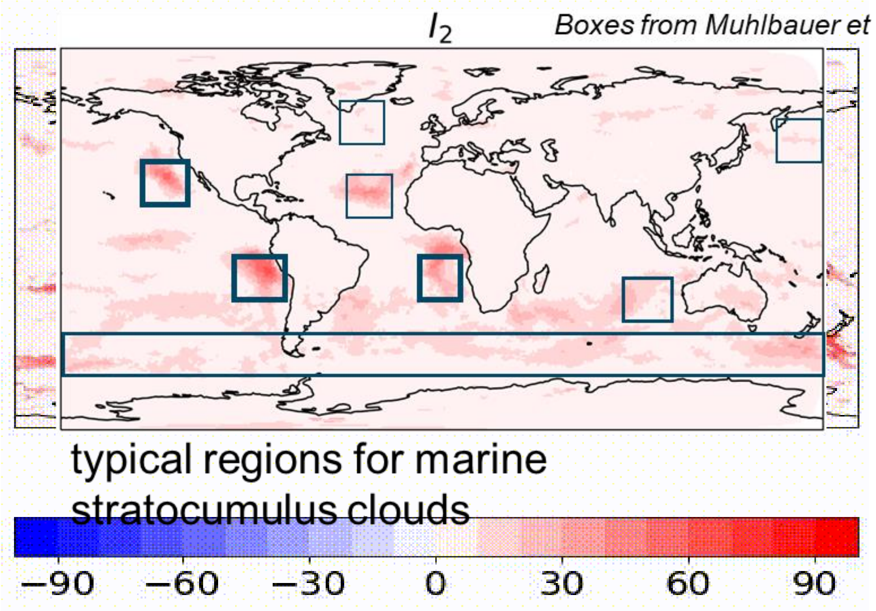
Jointly minimizing error & complexity in a well-defined plane



simpler

More accurate

1500m, 11-20 August 2016



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

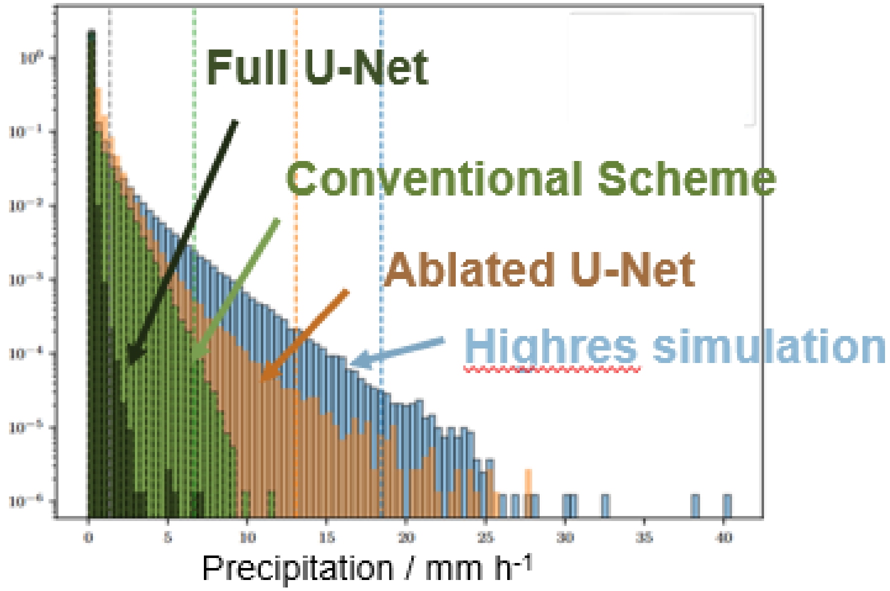
C: cloud cover
RH: Relative Humidity
qc: cloud water
qi: cloud ice

Grundner et al., JAMES (2024) https://doi.org/10.48550/arXiv.2304.08063

3. Convection parameterization: Interpretable multiscale UNET, Bi-LSTM

OFFLINE ICON

- We benchmarked different ML models and **U-Net outperformed other ML models**
- SHAP values identified non-causal connections for U-Net to precipitating tracer species
- **Ablated U-Net** (excludes precipitating tracer species) shows better extreme precipitation predictions



Heuer et al., JAMES, 2024; https://doi.org/10.1029/2024MS004398

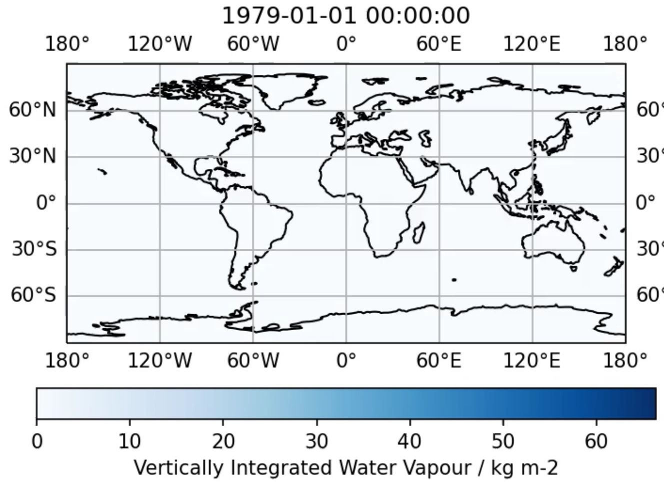
OFFLINE ClimSim *(Yu et al., CliimSim, NeurIPS 2024)*

- **Bidirectional Long Short-Term Memory (Bi-LSTM)** inspired from Kaggle Competition
- Substract radiative tendencies from other CRM tendencies
- Introduce memory to the two last timesteps
- Also include pressure as input as ICON has different height levels compared to ClimSim

ONLINE ClimSim Bi-LSTM coupled to ICON:

- 1 year stable ICON simulation is already possible, smoothing effect substantially reduced compared to ablated U-Net

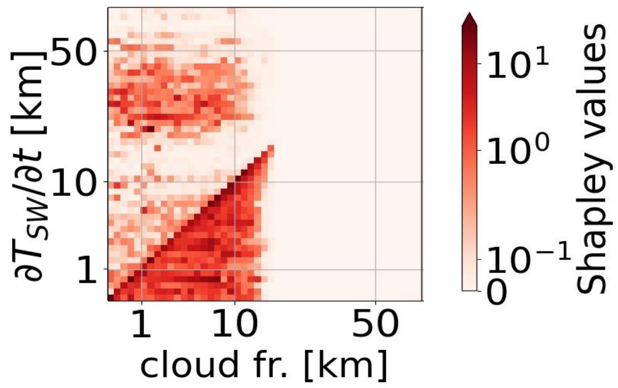
Heuer et al., in prep.



4. Radiation emulation & Boundary Layer Height scheme

Interpretable ML-based radiation emulation for ICON

– Neural Networks can efficiently and **accurately** emulate ICON's radiation scheme RTE+RRTMGP (Pincus et al. 2019)
– Neural networks are **statistically energy consistent** without explicitly enforcing it during training
– BiLSTMs **learn physically meaningful relationships** related to locality such as thermal emission and non-locality such as reflection by clouds

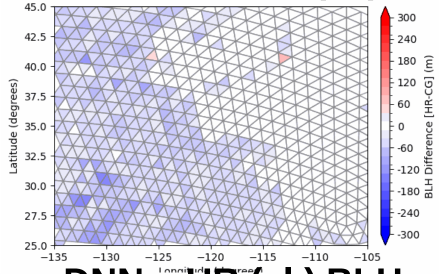


Hafner et al., JGR: MLC subm., Preprint: https://doi.org/10.22541/essoar.173169996.65100750/v1

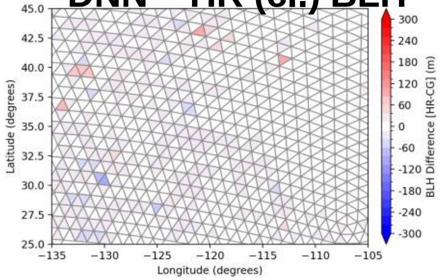
DL-based Boundary Layer Height (BLH)

- Reduced biases and numerical artifacts
- Diurnal BLH cycle improved, BLH higher in DNN
- Stable Long-Term Runs: *35-year AMIP*
- Stat. significant difference for various key indicators of climate change (e.g. BLH, surface T)
- Could reduce ICON's cloud cover bias together with ML-cloud cover parameterization

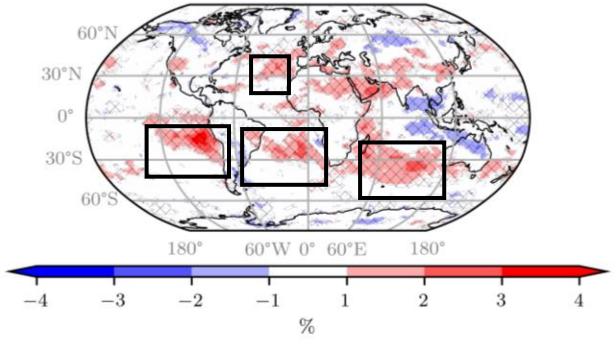
LR – HR BLH (cl.)



DNN – HR (cl.) BLH



Mean differences (DNN– cl. BLH scheme)

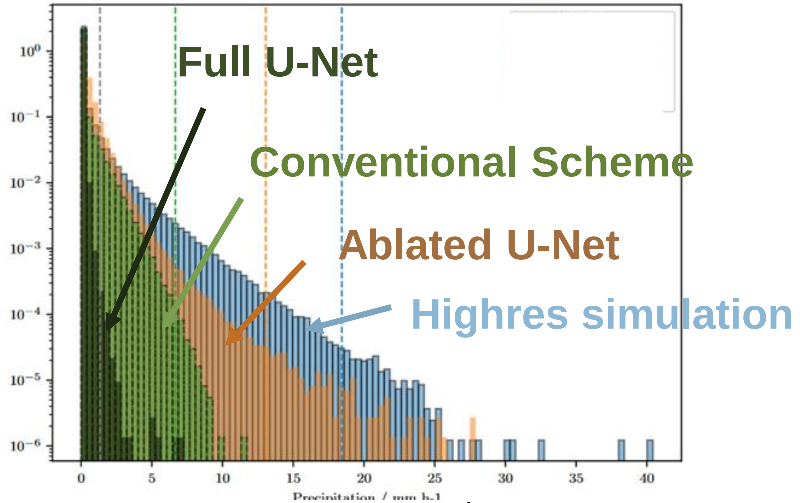


ML-based hybrid Earth System Models show reduced systematic errors

ML-based convection parmetrizations Ablated UNET

=> Improved extreme precipitation (ICON-A)

Heuer et al., JAMES, 2024

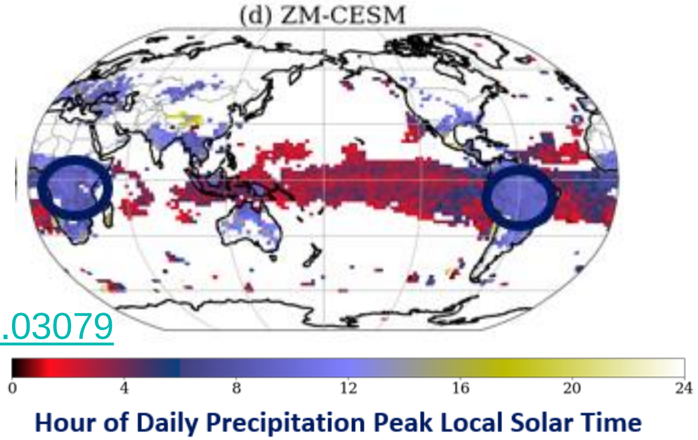


Precipitation / mm h^{-1}

ML-based stochastic parametrizations

=> Improved diurnal cycle of precipitation (CESM)

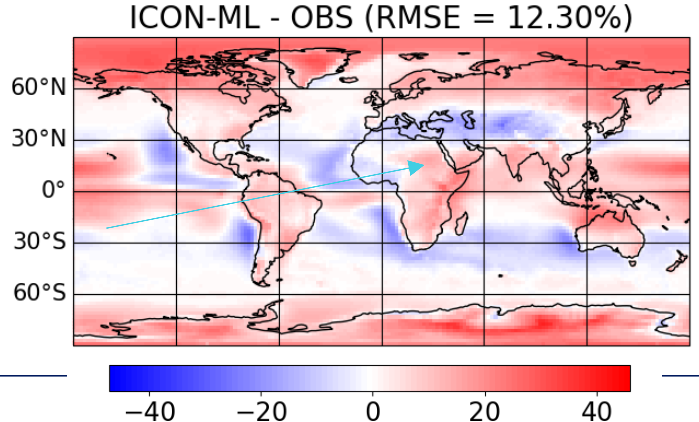
Behrens et al., JAMES, subm.
https://arxiv.org/abs/2402.03079



ML-based cloud cover & BLH in ICON-ML

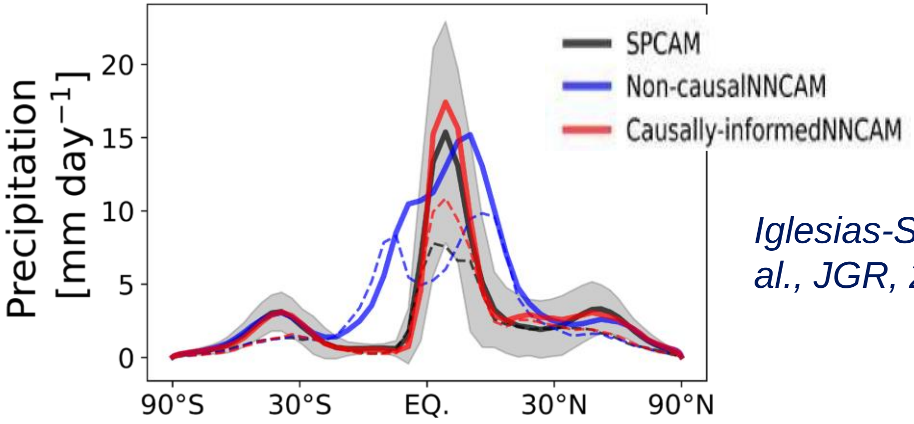
=> Improved cloud cover (ICON-A)

Grundner et al., in prep.
Klamt et al., in prep.



Causally-informed Neural network SPCAM:

Improved simulation of the ITCZ



Iglesias-Suarez et al., JGR, 2024

20-year ICON-ML AMIP with data-driven cloud cover equation

Problem: far off from observations and CMIP6 models

Implement data-driven cloud cover equation $\boldsymbol{f}$ in ICON-A

'ICON-ML' model

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

$$I_1(\mathrm{RH}, T) \overset{\mathrm{def}}{=} a_1 + a_2(\mathrm{RH} - \overline{\mathrm{RH}}) + a_3(T - \overline{T}) + \frac{a_4}{2}(\mathrm{RH} - \overline{\mathrm{RH}})^2 + \frac{a_5}{2}(T - \overline{T})^2(\mathrm{RH} - \overline{\mathrm{RH}})$$

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

$$I_3(q_c, q_i) \overset{\mathrm{def}}{=} \frac{-1}{q_c/a_8 + q_i/a_9 + \epsilon}.$$

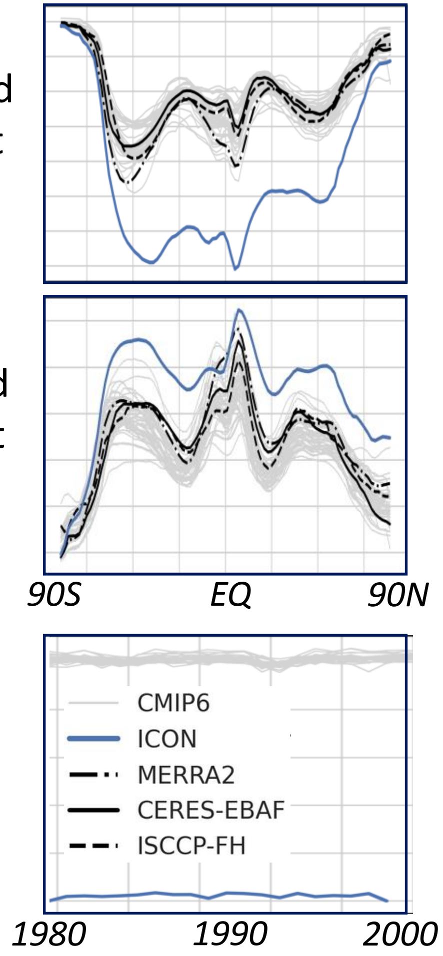
Grundner et al., JAMES, 2024

$$\{a_1, \ldots, a_9, \epsilon\} = \{0.4435, 1.1593, -0.0145\,\mathrm{K}^{-1}, 4.06, 1.3176 \cdot 10^{-3}\,\mathrm{K}^{-2}, 584.8036\,\mathrm{m}, 2\,\mathrm{km}^{-1}, 1.1573\,\mathrm{mg/kg}, 0.3073\,\mathrm{mg/kg}, 1.06\}$$

Shortwave cloud radiative effect zonal means

Longwave cloud radiative effect zonal means

Radiative balance timeseries



Tuning ICON-XPP-MIe with Nelder-Mead Algorithm

Nelder-Mead (also called downhill simplex method) uses a simplex shape (vertices = dimensions +1)

1. Forms triangle around $\boldsymbol{f}(Param_{init})$
2. Evaluates function that is to be minimized
3. Iteratively modifies placement of vertices (several options)
4. Until stopping criteria

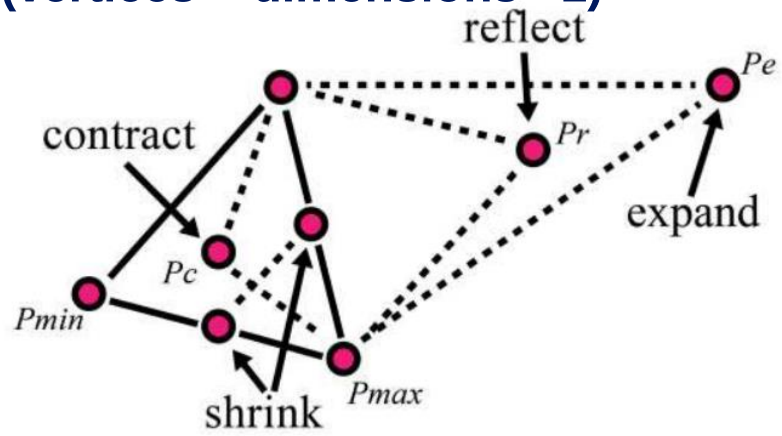


Figure taken from Mishra et al. (2023)

Advantages

- Relatively fast and computationally cheap method for tuning
- Doesn't need to know the gradient of the function that is to be minimized
- Yields good results after few iterations (compared to other methods).
- Efficient for low-dimensional problems.

Disadvantages

- Can get stuck in a local minimum
- Depends strongly on initial parameters.
- Can spend a lot of time for negligible improvements in later iterations

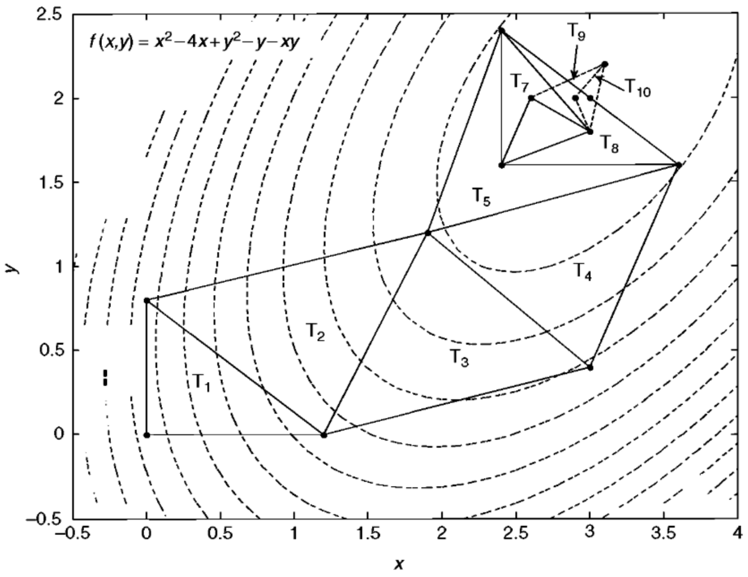


Figure taken from Krishnadasan et al. (2010)

Grundner, A., in prep., 2025

ONLINE: Tune the ICON-ML model in simulations of increasing length!

Grundner, A., T. Beucler, J. Savre & V. Eyring, Reduced cloud cover errors in hybrid climate models through a novel combination of data-driven parameterizations and automatic tuning, in prep., 2025

Implement data-driven cloud cover equation $\boldsymbol{f}$ in ICON-A

'ICON-ML' model

Typical ICON-A tuning parameters P_{ICON} **+** Metrics **M** that ought to be satisfied by the tuning process

Online tuning

Nelder-Mead optimizes tunable parameters P_f and P_{ICON} such that ICON-ML($P_f \cup P_{ICON}$) satisfies all metrics M in T-long simulations.

Begin with T = two days, set to a week/month/year in subsequent iterations.

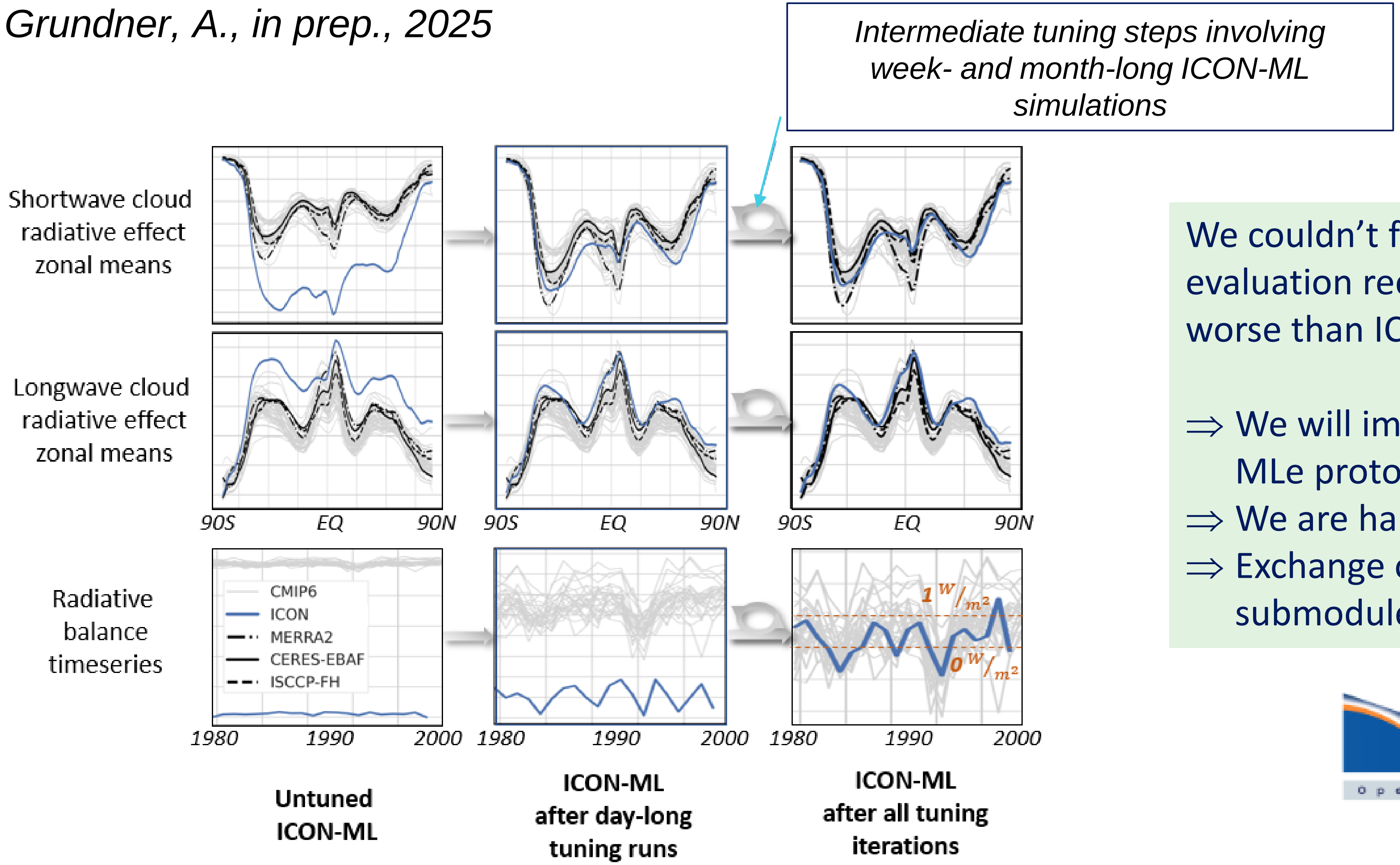
Final ICON-ML model. Test in 20-year simulations.

→ Efficient, easily extendible, automatic tuning pipeline (could also be a good method to tune km-scale models)

Tuning cloud cover equation discovery

Results improve drastically following the tuning pipeline

Grundner, A., in prep., 2025



We couldn't find any diagnostics in our large evaluation recipe in which ICON-ML did worse than ICON-A.

⇒ We will implement this in our ICON-XPP-MLe prototype for CMIP7
⇒ We are happy to share with CESM
⇒ Exchange other ML parametrizations or submodules with CESM

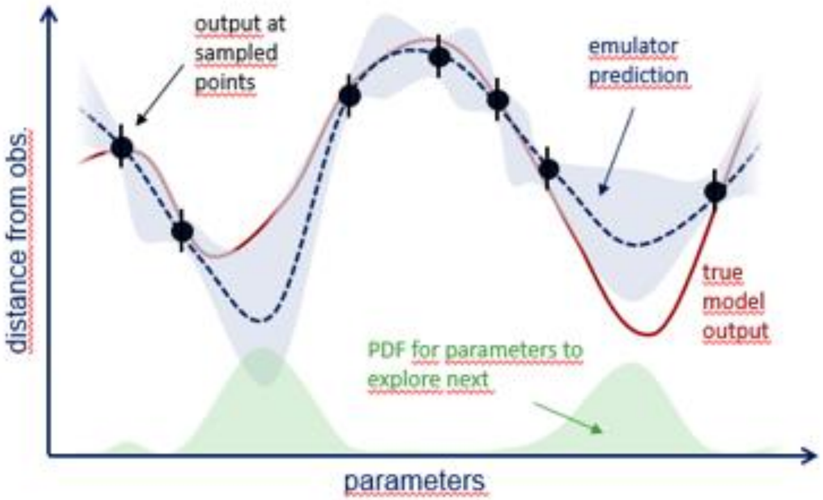
ML-based Automatic Tuning Framework for ICON

- 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.

Bonnet & Pastori et al., EGUsphere [preprint], https://doi.org/10.5194/egusphere-2024-2508, 2024 *(ICON Atmosphere)*

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

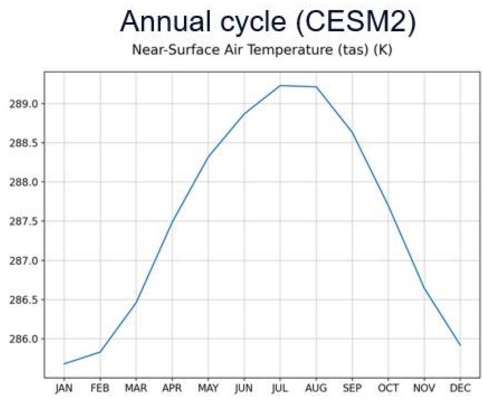
Evaluation of Native Model Output with ESMValTool, also compared to CMIP

ESMValTool
Earth System Model Evaluation Tool

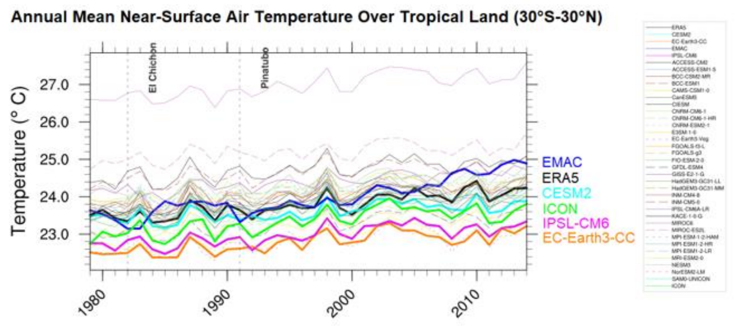
"Community-developed open-source diagnostic and performance metrics tool for routine evaluation of Earth system models."

GitHub: https://github.com/ESMValGroup/ESMValTool

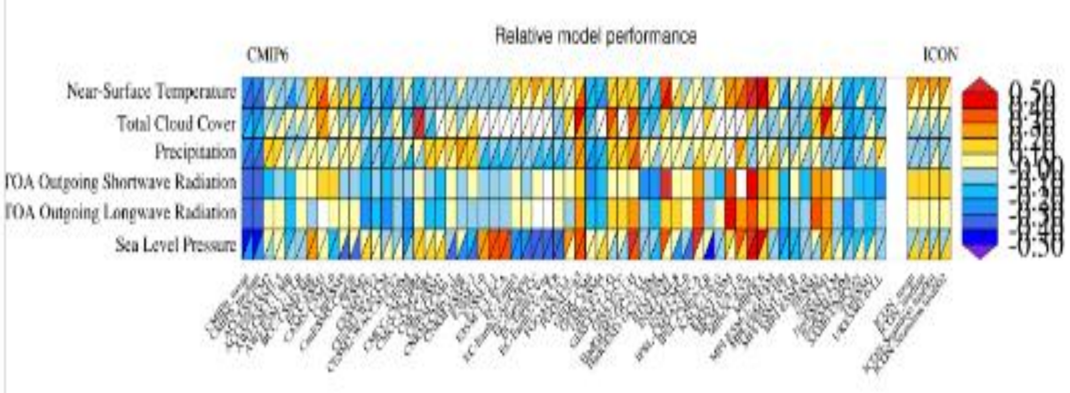
- Reading of native model output, currently: **CESM2**, EC-Earth3, EMAC, **ICON**, and IPSL-CM6.
- No postprocessing (e.g., CMORization) necessary
- This output can be processed like any other CMIP model within ESMValTool
- **Monitoring of simulation available now, but also allows benchmarking of simulations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



Single model analysis



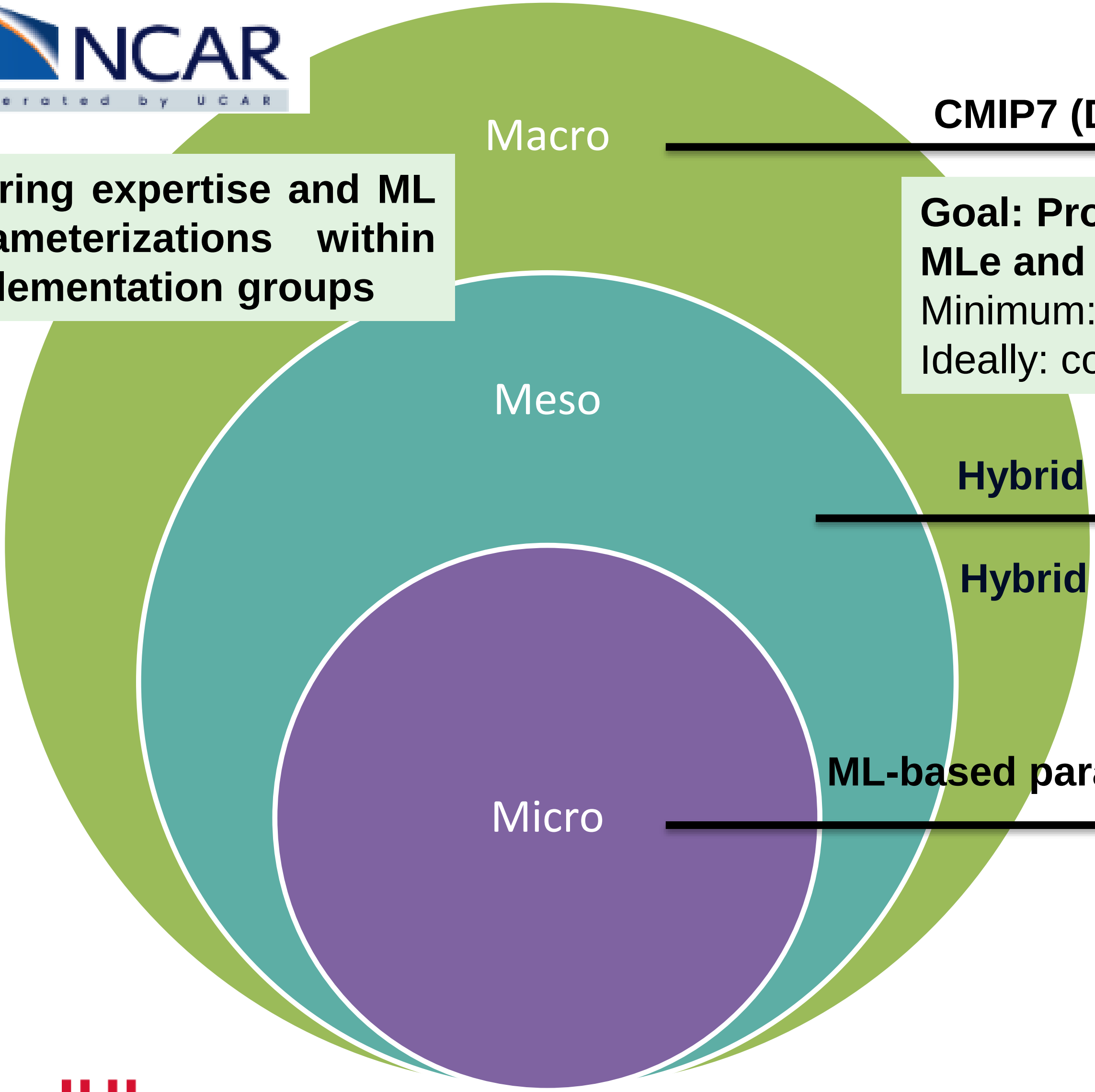
Multi model analysis



Schlund et al., GMD, 2023

Contact: Manuel.Schlund@dlr.de

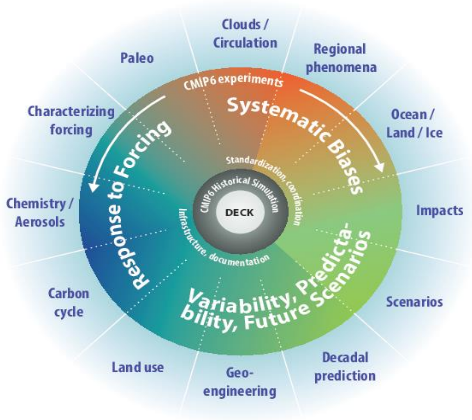
USMILE Goal for CMIP7



Sharing expertise and ML parameterizations within implementation groups

CMIP7 (DECK + historical)

Goal: Protoytpes CESM-MLe and ICON-XPP-MLe
Minimum: AMIP
Ideally: coupled



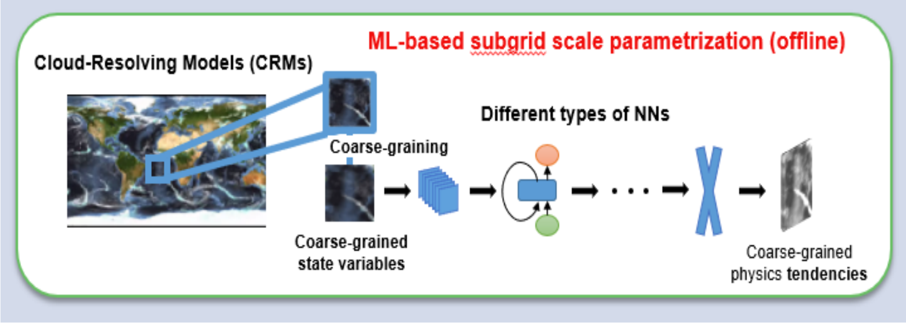
Coupled hybrid model
ICON-XPP-ML
Better & faster Ensembles

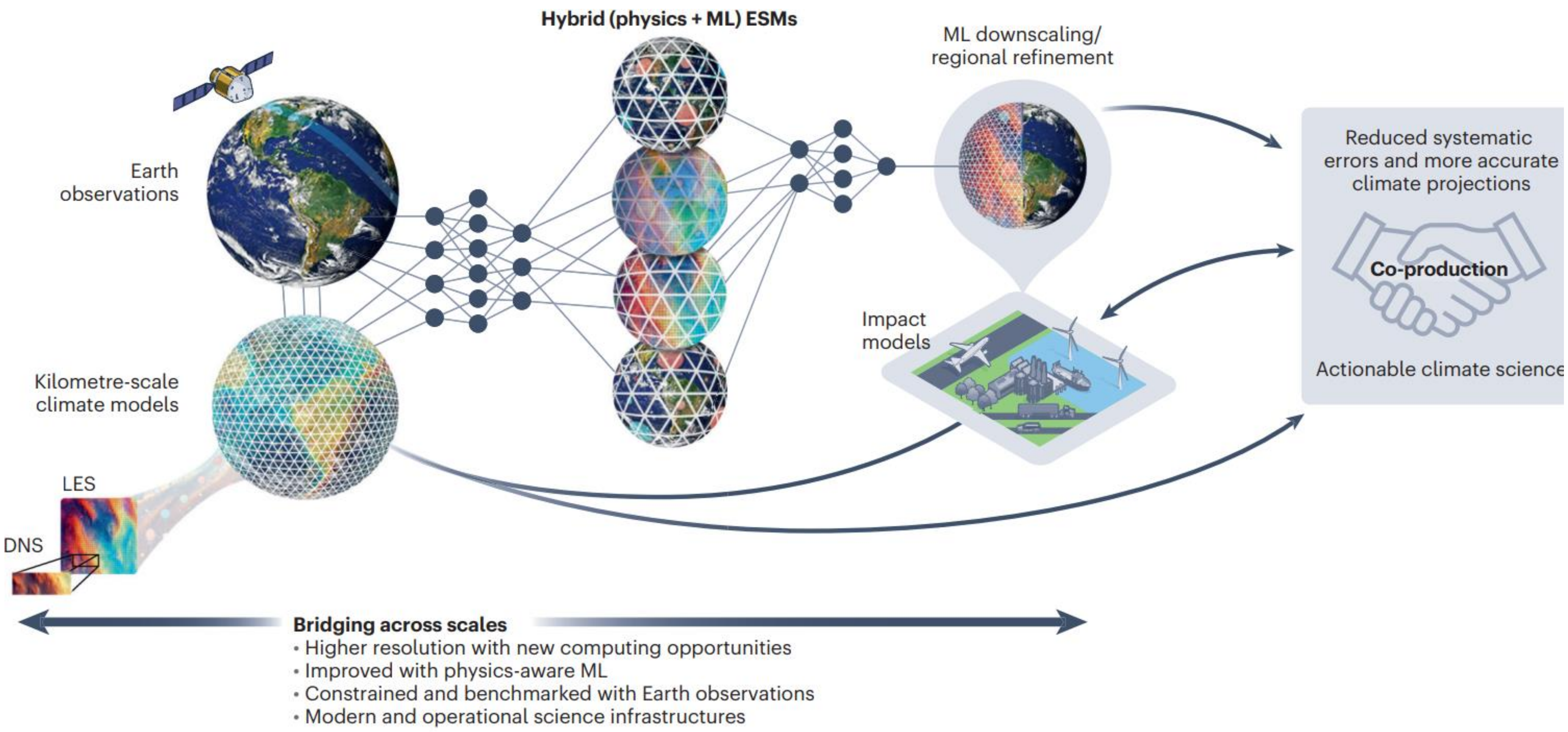
Hybrid ICON-MLe

Hybrid CESM-MLe

Hybrid model
ICON-XPP-ML Atm.
ICON-XPP-ML Land

ML-based parametrizations





Eyring, V., P. Gentine, G. Camps-Valls, D. M. Lawrence, M. Reichstein, Nat. Geosci., https://doi.org/10.1038/s41561-024-01527-w, *2024*

Recommendations

- **To fully embrace hybrid Machine Learning Earth system modelling**
  - does not mean that Earth system modelling developments disappears, in contrast
  - Provides ESM with significantly reduced systematic errors that are just in the way for everybody
- **To make ML an integral part of your Earth system modelling strategy**
  - fully integrate in CESM developments alongside enhancements in Earth system processes / components
  - work across scales and complexity
    - ML for acceleration so to also run coarser-ESMs at higher resolution as we move forward
    - offers regionalization through ML-based downscaling and regional refinement of hybrid models
    - allows creation of large ensembles
    - Also allows to enhance km-scale models with a similar approach (e.g., turbulence, shallow clouds)
- **Prototype hybrid model for CMIP7 (or on this timescale)**
  - to jointly develop prototype hybrid models (CESM-MLe and ICON-XPP-MLe)
  - at least AMIP / LMIP / OMIP, but ideally coupled
- **To secure some of the AI funds** (while aiming high and thinking big)
- **To move ML forward, we organize**
  - Gordon Research Conference Machine Learning for Actionable Climate Science, 22-27 June, Bryant U
  - Planning on AGCI workshop proposal on **ML for Earth system predictability** or **ML for hazard management** together with NCAR CGD

Eyring, V., P. Gentine, G. Camps-Valls, D. M. Lawrence, M. Reichstein, Nat. Geosci., https://doi.org/10.1038/s41561-024-01527-w, *2024*