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Assessing Machine Learning Techniques as Emulators for Simple Physics in the Community Atmosphere Model

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Working Groups Meeting

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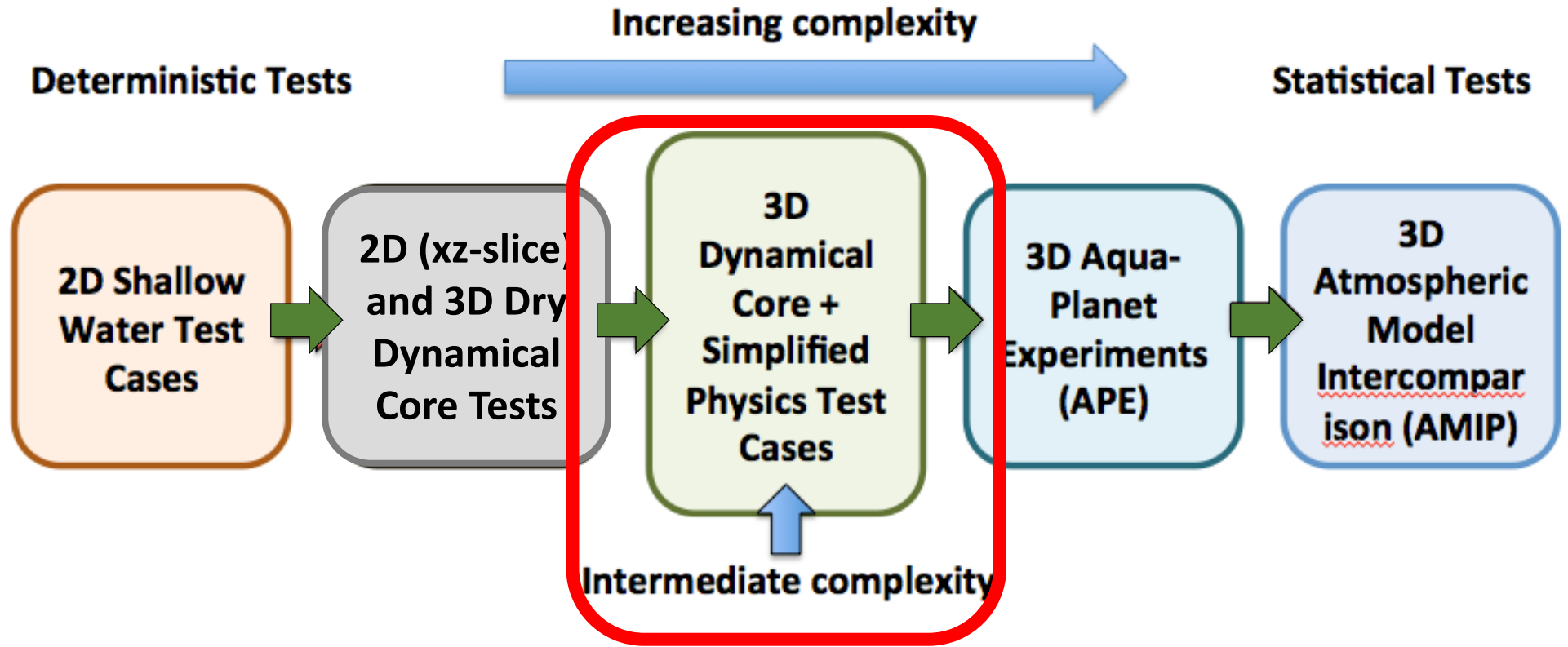


Overarching Questions

- Can Machine Learning (ML) methods replace or augment physical parameterizations in atmospheric GCMs?
- How well can ML methods capture the parameterization scheme?
 - Physical realism
 - Dynamic range
 - Computational complexity/efficiency & data availability
- How does the ML performance depend on the data selection & preparation, ML technique, and the architecture/hyperparameter choices?
 - We utilize an ML tuning tool called Sherpa
- How can we embed physical constraints?

 Answer some of these questions with the help of a GCM model hierarchy

Bridging the Gap: Model Hierarchy with Increasing Complexity



GCMs with Simplified Physics (for climate time scales)

- Dry Held-Suarez test (Held and Suarez, BAMS 1994)
- Moist version of the Held-Suarez test (Thatcher and Jablonowski, GMD 2016)

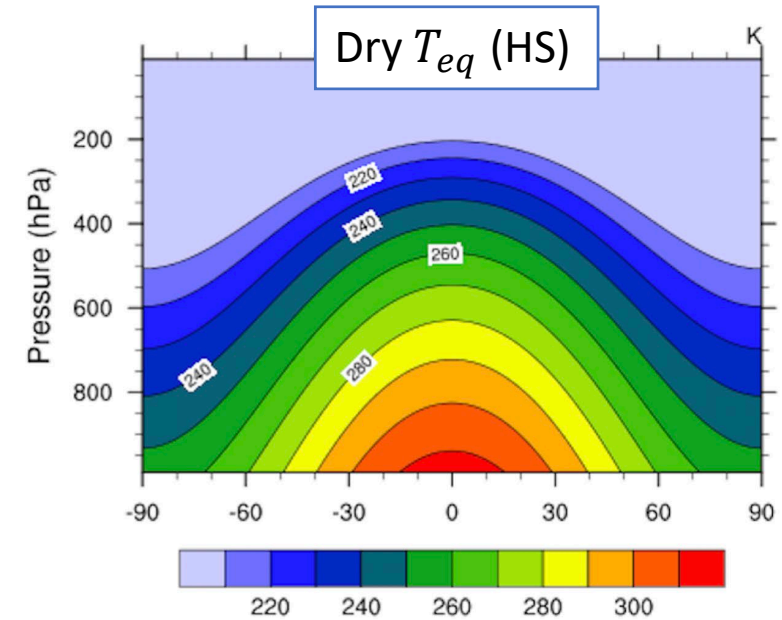
Idealized Model Setups: Dry Held-Suarez (HS)

- Simplified HS forcings are Rayleigh friction and a Newtonian temperature relaxation:

Linear:
$$\frac{\vec{v}_h}{\partial t} = -\frac{1}{k_v(p)} \vec{v}_h$$

k_v and k_T are spatially-dependent relaxation coefficients

$$\frac{\partial T}{\partial t} = -\frac{1}{k_T(\phi, p)} [T - T_{eq}(\phi, p)]$$



- Focus here: **Can ML mimic the physics time tendency of the temperature T ?**

Moist Version of the Held-Suarez test (MHS)

- Simplified MHS forcings (moist) are Rayleigh friction, a Newtonian temperature relaxation, PBL mixing (Laplacian), surface fluxes & rain

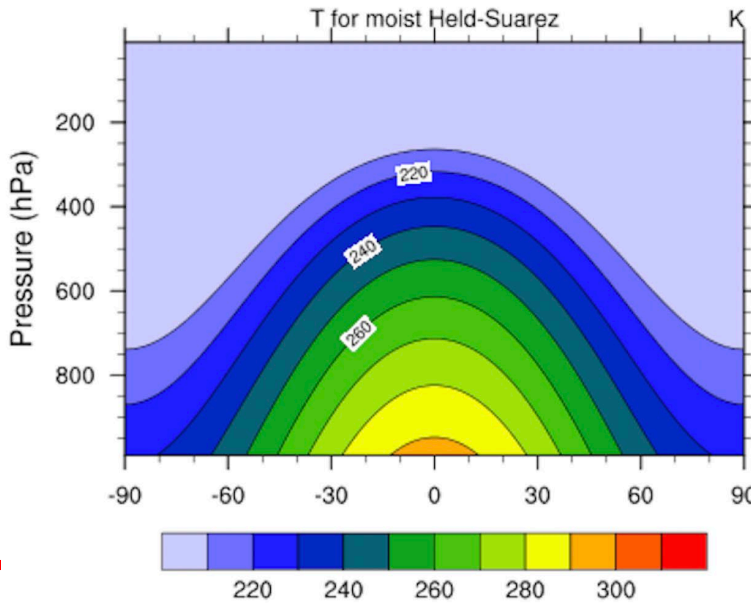
$$\frac{\vec{v}_h}{\partial t} = -\frac{1}{k_v(p)} \vec{v}_h$$

PBL mixing (Laplacian),
surface fluxes & rain

$$\frac{\partial q}{\partial t} = -C + \text{PBL diffusion} + \text{surface latent heat flux}$$

$$\frac{\partial T}{\partial t} = -\frac{1}{k_T(\phi, p)} [T - T_{eq}(\phi, p)] + \frac{L}{c_p} C + \text{PBL diffusion} + \text{surface sensible heat flux}$$

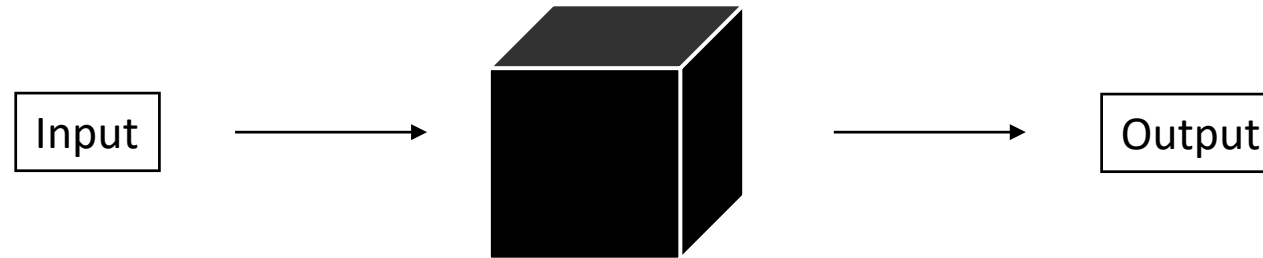
$$\text{Precipitation rate} = \frac{1}{\rho_{water} g} \int_0^{p_s} C dp$$



L: Latent heat of vaporization
C: Condensation rate

- Focus here: Can ML (neural network & random forests) mimic the **physics time tendency of T?** The **precipitation rate?**

Machine Learning



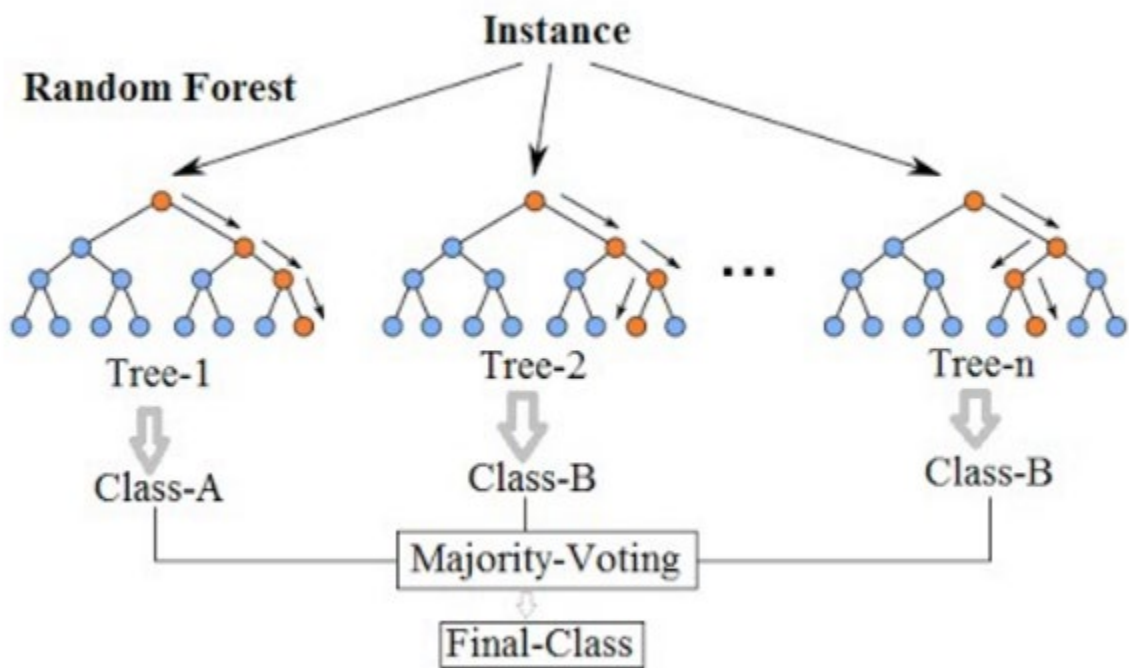
- Determines a functional relationship within a given dataset without being programmed to do so
- Requires a lot of data
- Our focus: Neural Network (NN) and Random Forest models
- Built using Keras (TensorFlow) & Scikit-Learn
- Optimized with Sherpa (ML hyperparameter optimization tool)

SHERPA

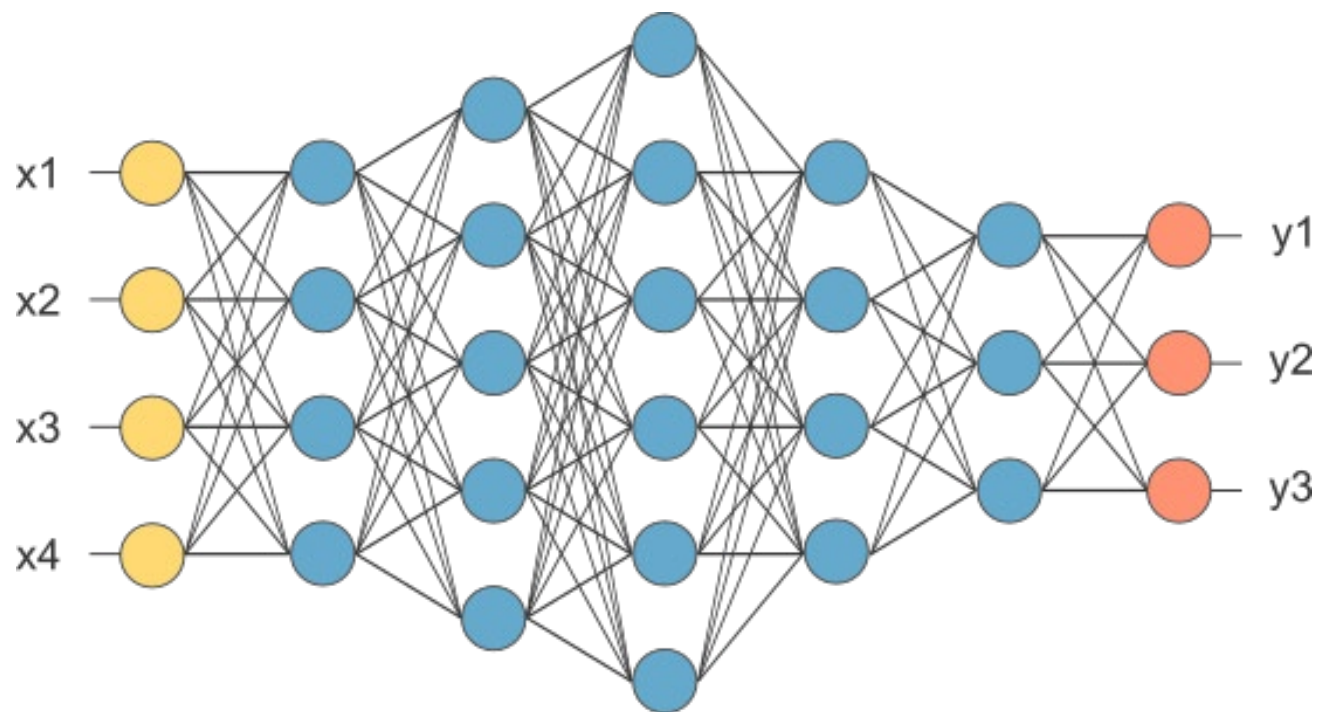
Hertel et al. (2020): <https://arxiv.org/abs/2005.04048>
<https://github.com/sherpa-ai/sherpa>

Random Forests & Neural Networks

Random Forest Simplified



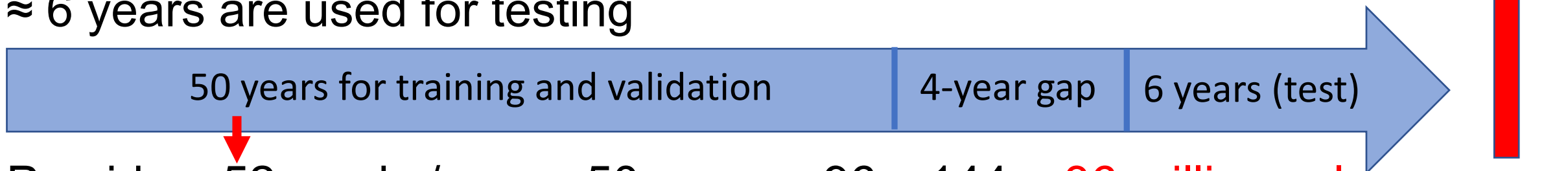
RF image by Venkata Jagannath – [Wikipedia](#)



NN image from [WhyAxis](#)

GCM Configuration

- NCAR's Community Earth System Model (CESM) version 2.1
- Finite-Volume (FV) CAM6 dynamical core at the resolution 1.9 x 2.5 (96 x 144 grid points) with 30 vertical levels (from now on: **2 degree**)
- Model is run for about 60 model years
- Output is collected every week: u, v, p_s, T, **Q, LHFLX, SHFLX**, du/dt, dT/dt, **dq/dt, PRECL**
- 40 years is used for training, ~10 years for validation (total of 50)
- ≈ 6 years are used for testing

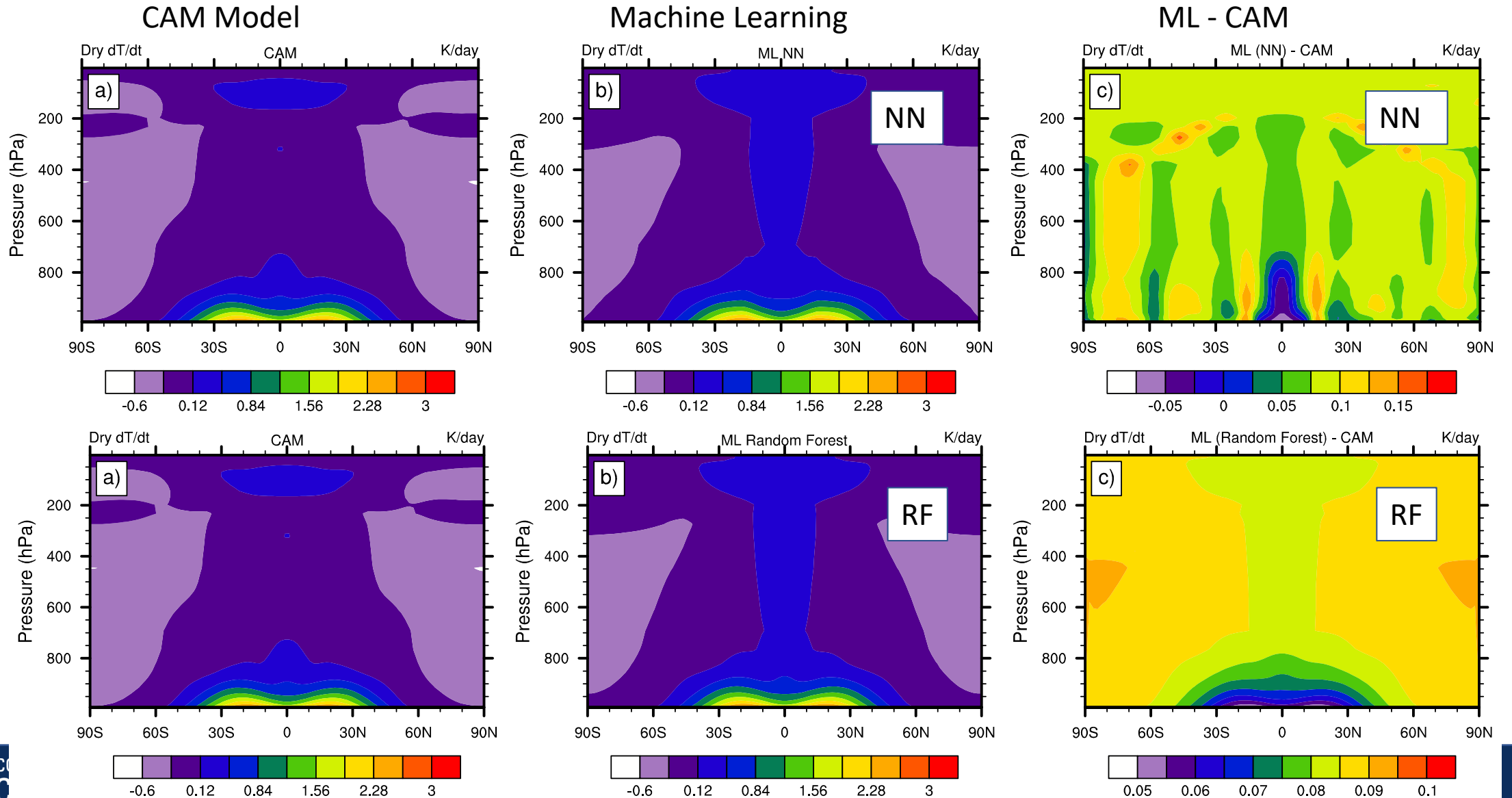


- Provides: $52 \text{ weeks/year} \times 50 \text{ years} \times 96 \times 144 = 36 \text{ million columns}$

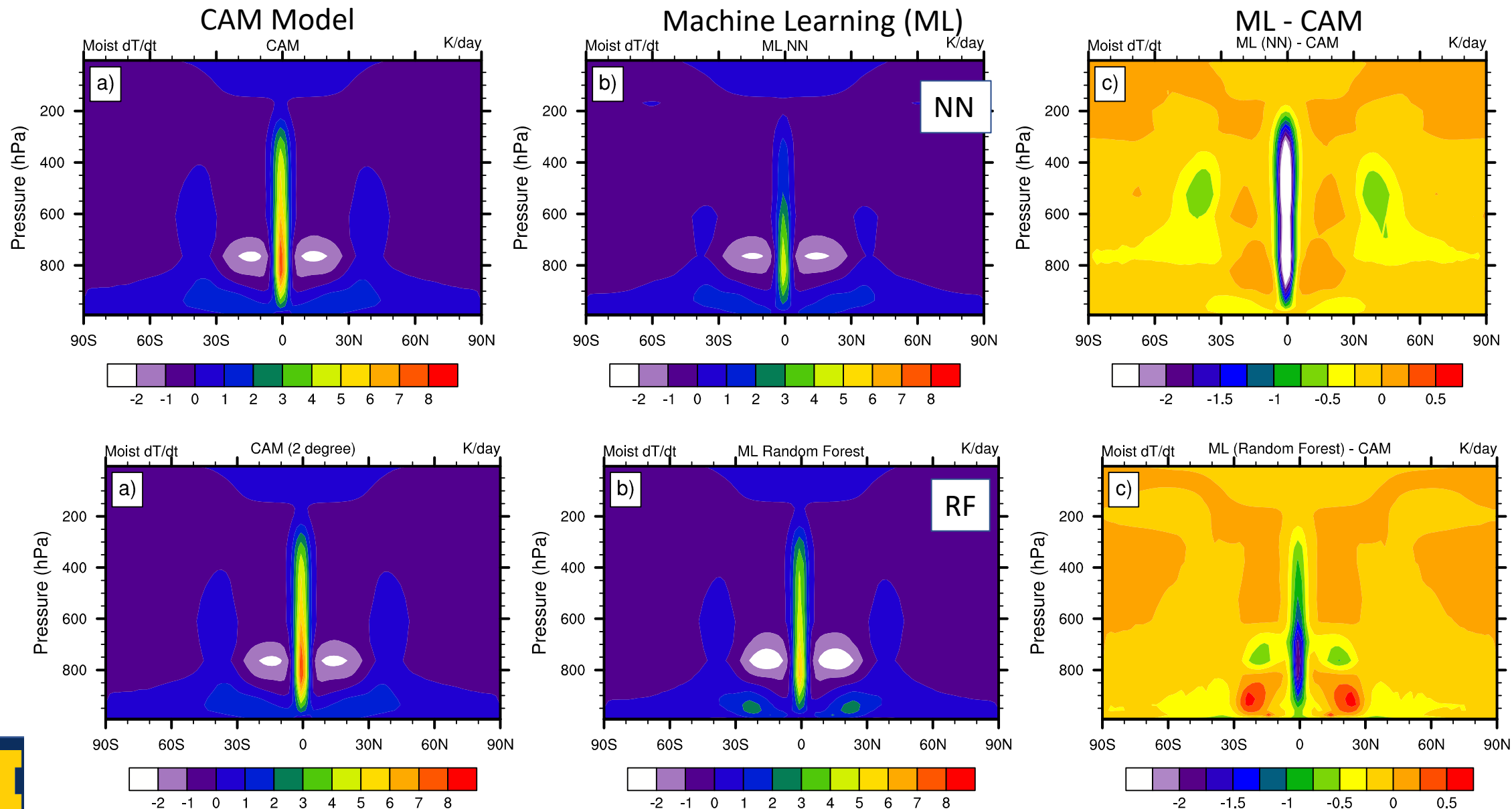
Data & Preparation

- Training and testing is currently done 'offline'
- Different ML models are trained for
 - dT/dt (temperature tendency)
 - Precipitation rate
- Data Preparation:
 - Samples grouped into vertical columns:
 - reshape from (time, lev, lat, lon) -> (time*lat*lon, lev, nfeatures)
 - Normalized to be unitarily invariant (subtract the mean at each level, divide by standard deviation), scaled to range $[-1,1]$
 - Data are shuffled during training

Closer Look at **Dry** HS Results: dT/dt (HS)

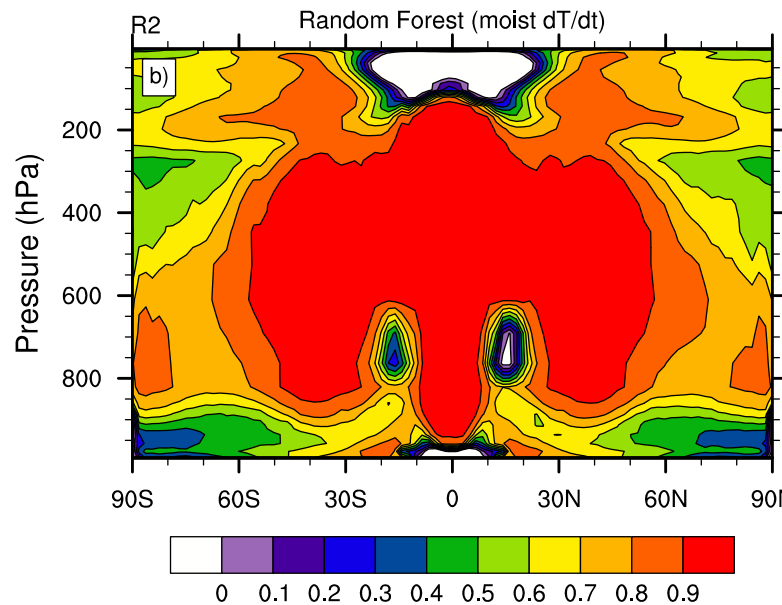
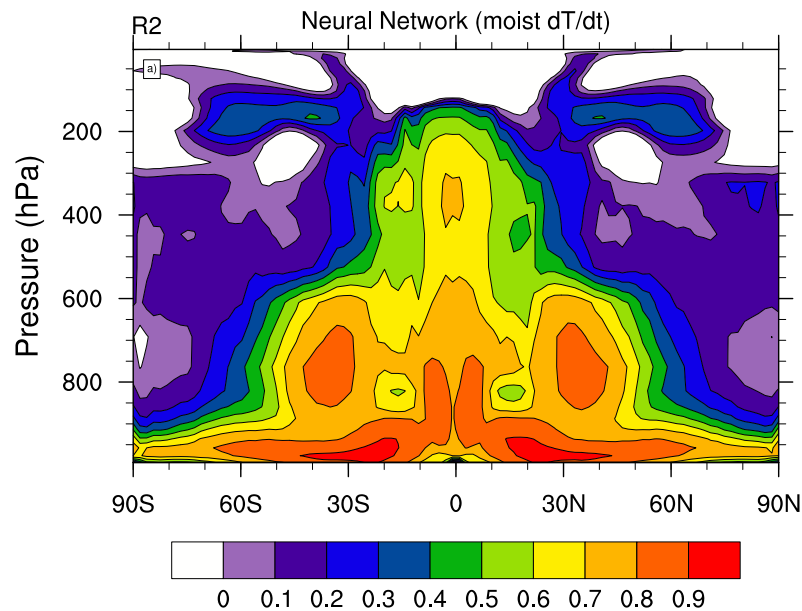


Increasing Complexity: Moist dT/dt (MHS)



Analysis of the 2-deg Test Data: Moist dT/dt

- R^2 (Coefficient of Determination) assessment reveals problem zones for both
- RF outperforms NN (higher correlations)



$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

Residual sum of squares
Variance of the data

High R^2 (close to 1) desired.
If R^2 negative (white regime):
unexplained variance of the ML model
exceeds the total variance of the
original data.

$$R^2 = 1 - \frac{\sum_{time} \sum_{lon} [\text{CAM}(time, :, :, lon) - \text{ML}(time, :, :, lon)]^2}{\sum_{time} \sum_{lon} [\text{CAM}(time, :, :, lon) - \overline{\text{CAM}(:, :, :)}]_{\text{time-mean zonal-mean}}^2}$$

Promising NN performance Precipitation (1 degree)

- 30 day animation of the precipitation rate based on 3-hourly data***
- Comparison: CAM (1 deg) versus ML (NN)
- Precipitation bands are captured well by the NN model
- Difficult problem: Precipitation relies on 3D T, p, q and the flow field in order to generate supersaturation (relative humidity > 100%)
- Supersaturation leads to condensation C which needs to be integrated:

$$\text{Precipitation rate} = \frac{1}{\rho_{water} g} \int_0^{p_s} C dp$$



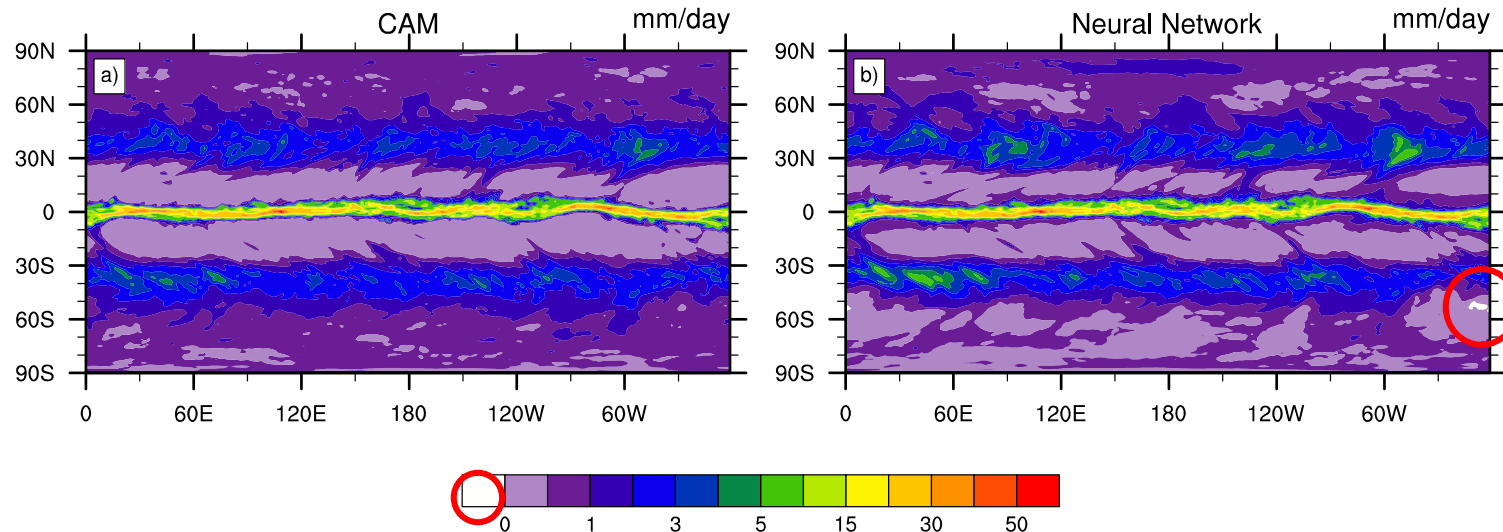
Precipitation Rate (large-scale condensation, 1 degree)

- Time-mean zonal-means of the test data (68 days):
- CAM and ML (NN) **closely resemble** each other
- Precipitation peaks are well captured
- However: negative precip rates are possible in NN
- Physical constraints are needed

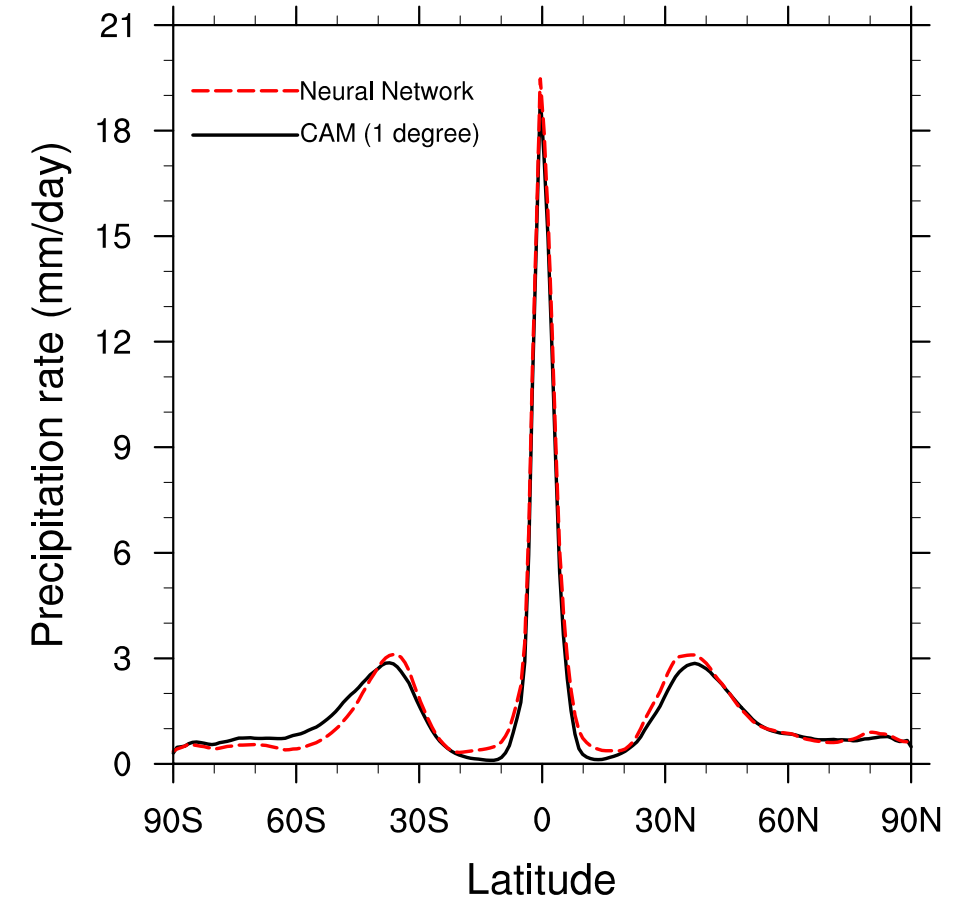
CAM Model

Time-Mean Precipitation Rate

ML Neural Network (NN)



Time-Mean Zonal-Mean (Test Data)



Summary

- Machine learning **can** emulate these simplified physical parameterizations.
- Both Neural Networks and Random Forests show skill.
- **Not** making a claim that our current ML models are optimal (particularly NN).
- Further testing, hyper-parameter tuning and improved data selection are still needed.

Future Work

- Exploring boosted forests (**XGBoost**), Convolutional Neural Nets (**CNN**), and other ML techniques
- Porting these models to be easily **coupled** to CAM6 (Python-Fortran) & investigate numerical **stability** in an online mode
- Enforce **physical constraints**, advance physics-guided ML principles
- **Add additional levels of complexity** to the hierarchy (aquaplanet, full physics, etc).





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Thank You!

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