



CGD Laboratory



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Emulating Water Isotopes in Coupled Earth System Models

Overview & Preliminary Results of an NSF-CAIG Project

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Image by ChatGPT

Motivation

Water isotopes are key tracers of hydrological processes in the Earth system.

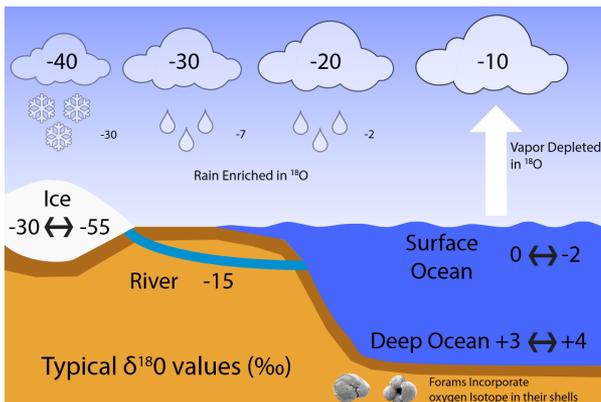


Image Credit: Andreas Schmittner

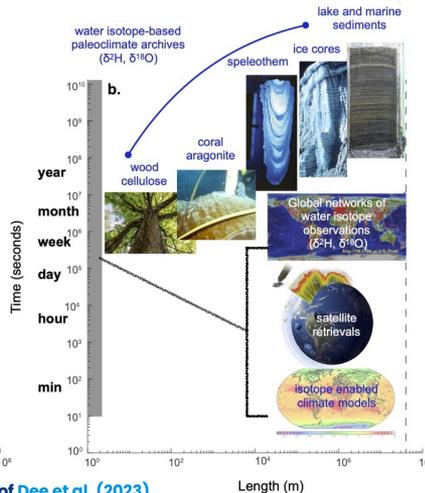
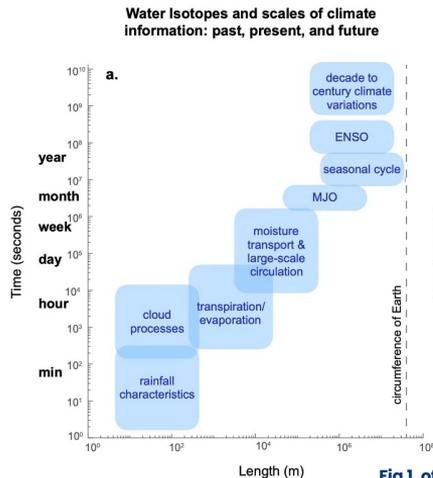


Fig 1. of Dee et al. (2023)

Paleo records of water isotopes can serve as paleo-thermometers and rain gauges, providing real-world constraints for validating Earth System Models (ESMs).

Incorporating water isotopes into ESMs is scientifically and technically challenging.

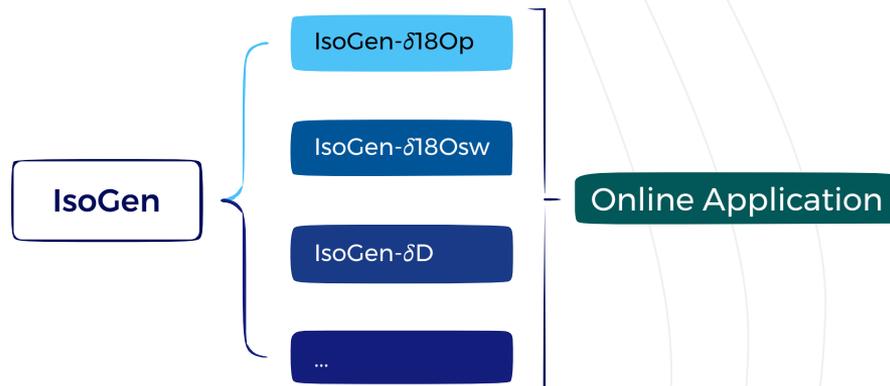
- It requires modifications to the dynamical core and physical parameterizations.
- It adds ~40% higher runtime computational cost.

Project Objectives



This project aims to:

- develop a machine-learning-based emulator for water isotopes (e.g., $\delta^{18}\text{O}$, δD), trained on ESM simulations and observations;
- apply the emulator to non-isotope ESMs to generate their water isotopic fields efficiently and cost-effectively;
- improve **scientific understanding** of the leading drivers of water isotopic variability and support the development of physically based isotope-enabled ESMs;
- contribute to ongoing (paleo)climate data assimilation efforts, where the lack of isotopic prior simulations has been a limiting factor.



Key Scientific Questions



Q1: What are the leading drivers of water isotopic variability in the Earth system?

Q2: Is the underlying climate–isotope mapping relationship stable across different climatologies (i.e., coldhouse, coolhouse, warmhouse, hothouse climates)?

Q3: Is the underlying climate–isotope mapping transferable across different ESMs (i.e., sensitive to specific model physics)?

Preliminary results:

- Single ESM precipitation $\delta^{18}\text{O}$ ($\delta^{18}\text{O}_p$) emulation [Q1]
- Multiple climatologies [Q2]

State of the Art $\{\delta^{18}\text{O}_p\}$ Variability



Dansgaard (1964)

Temperature Effect: the positive $\delta^{18}\text{O}_p$ -T correlation, dominant in mid-to-high latitudes and high altitude mountains.

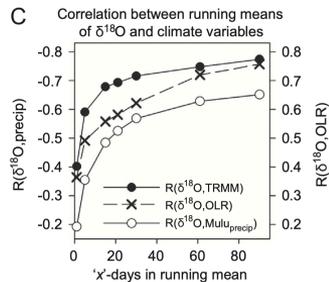
Amount Effect: the negative $\delta^{18}\text{O}_p$ -P correlation, dominant in tropical and monsoon regions.

Bony et al. (2008) & Risi et al. (2008)

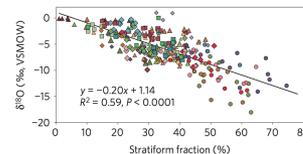
suggest that **amount effect** is tied to large-scale atmospheric circulation that organize convective processes, rather than local rainfall amount per se, and temperature changes not associated with circulation changes lead to an anti-amount effect, highlighting the **non-local nature of isotopic controls**, according to model-data comparisons.

Konecky et al. (2019) suggests that "cloud type is leading influence where stratiform rain is abundant, and moisture transport plays key role along tropical rain belt", and that " $\delta^{18}\text{O}_p$ is a more reliable proxy for **large-scale** hydrological processes than precipitation", based on a conceptual framework and statistical model: $\delta^{18}\text{O}_p = \beta_1 RE_{\text{frac}} + \beta_2 MF + \beta_3 MTD + \beta_4 SRF$

Moerman et al. (2013) studies a $\delta^{18}\text{O}_p$ record (daily, 5-yr-long) from site "Mulu" and suggests that the $\delta^{18}\text{O}_p$ -P correlation increases with increased **temporal and spatial averaging**.



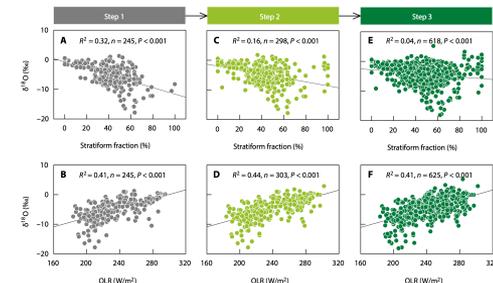
Aggarwal et al. (2016, Nat. Geosci.) proposes a **Stratiform-Fraction (SF) theory** based on obs.



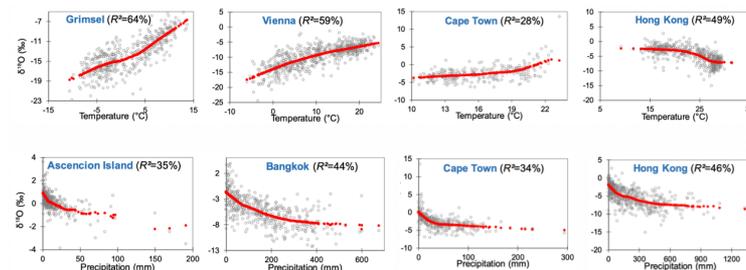
Leading Drivers [Q1]

- Nonlocal
- Nonlinear
- Nontrivial

Yu et al. (2024, Sci. Adv.) denies the SF theory based on more obs and suggests the importance of convection intensity (OLR).



Vystavna et al. (2021) studies 20 GNIP stations (monthly, 60-yr-long) and suggests **nonlinear** climate-isotope relationships.



Experimental Design



- **Goal:** learning the climate–isotope mapping $\delta^{18}\text{O}_p = f(\text{climate})$ and gain scientific insights
- **Strategy:** fitting $\delta^{18}\text{O}_p = f(\text{climate})$ using different input variables
- **Neural network: Fourier Neural Operators (FNOs)** → nonlocal & nonlinear problems
(FNOs learn global interactions in Fourier space, where expensive convolution becomes cheap multiplication: [Li et al., 2021](#))
(A benchmark of multiple deep learning methods for water isotope emulation: [Li et al., 2025](#))
- **Dataset: iCESM1.3 simulations of the 1.5xCO₂ & 3xCO₂ MCO cases**
(Long Simulations of the Miocene Climatic Optimum: [Zhu & Zhu, 2025](#))
(iCAM5 is the only one that can simulate the observed SF– $\delta^{18}\text{O}_p$ correlation among other iGCMs: [Hu et al., 2018](#))
- **Data splitting**
 - Total: 200 yrs x 12 months = 2400 months
 - Train / Valid / Test: 70% / 10% / 20%
- **Experiments**
 - In-distribution (ID) Exps. (Train: 1.5xCO₂, Test: 1.5xCO₂)
 - Out-of-distribution (OOD) Exps. (Train: 1.5xCO₂, Test: 3xCO₂)

Preliminary Results

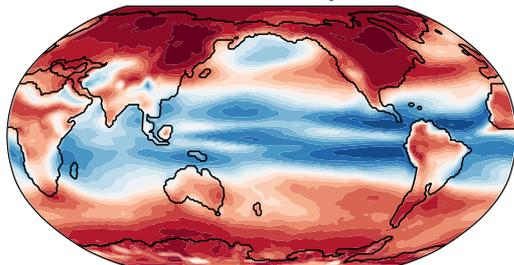
ID Exps.

Train: 1.5xCO₂; Test: 1.5xCO₂



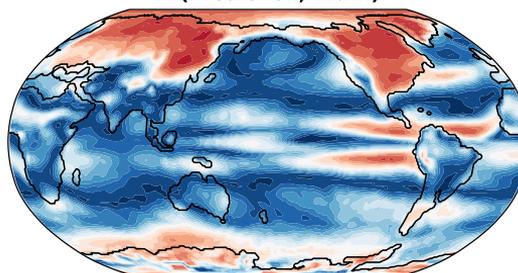
Diagnostics: local correlations

Corr(tas, d18Op)



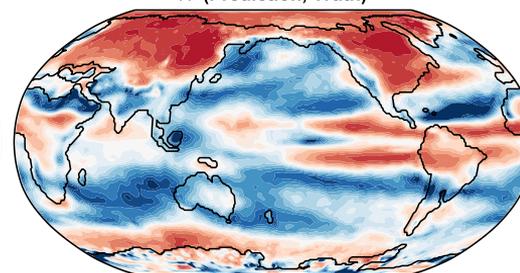
$\delta^{18}\text{O}_p = \text{LinearReg}(\text{tas})$

$R^2(\text{Prediction, Truth})$

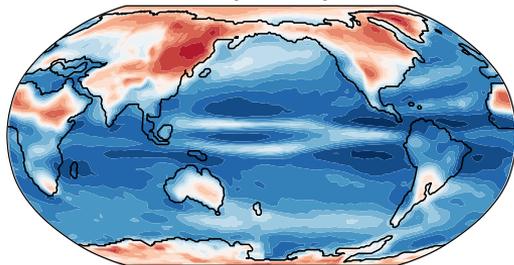


$\delta^{18}\text{O}_p = \text{FNO}(\text{tas})$

$R^2(\text{Prediction, Truth})$

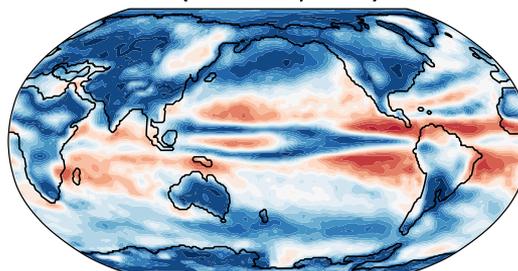


Corr(pr, d18Op)



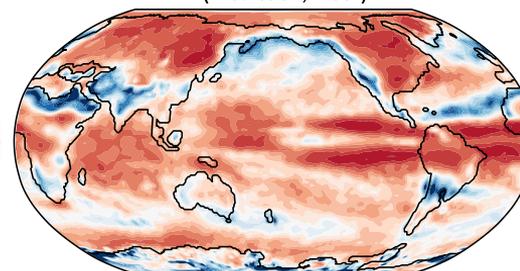
$\delta^{18}\text{O}_p = \text{LinearReg}(\text{pr})$

$R^2(\text{Prediction, Truth})$



$\delta^{18}\text{O}_p = \text{FNO}(\text{pr})$

$R^2(\text{Prediction, Truth})$



Taking nonlinearity and nonlocality into account (FNO fitting) appears to be effective, confirming the previous studies.

Preliminary Results

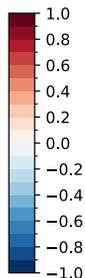
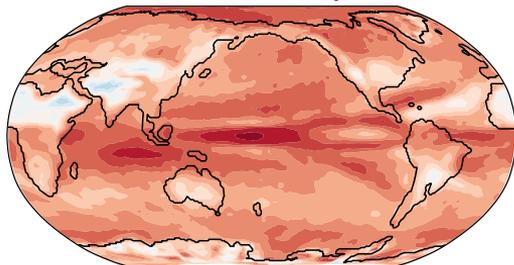
ID Exps.

Train: 1.5xCO₂; Test: 1.5xCO₂



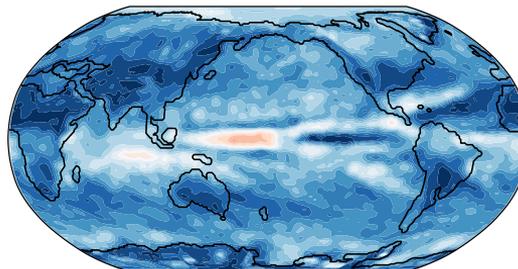
Diagnostics: local correlations

Corr(OLR, d18Op)



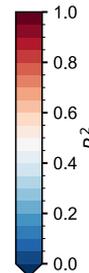
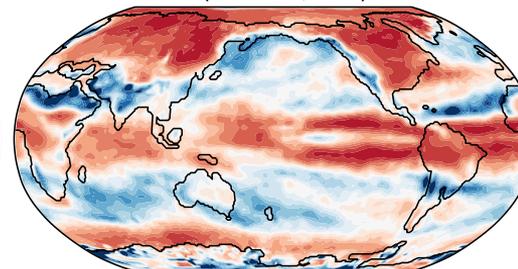
$\delta^{18}\text{O}_p = \text{LinearReg}(\text{OLR})$

$R^2(\text{Prediction, Truth})$

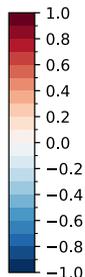
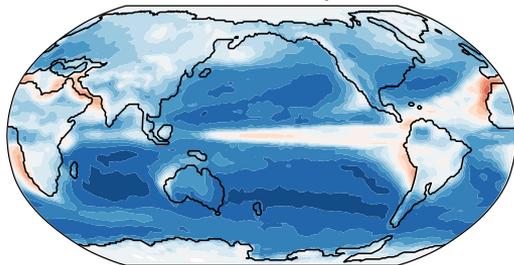


$\delta^{18}\text{O}_p = \text{FNO}(\text{OLR})$

$R^2(\text{Prediction, Truth})$

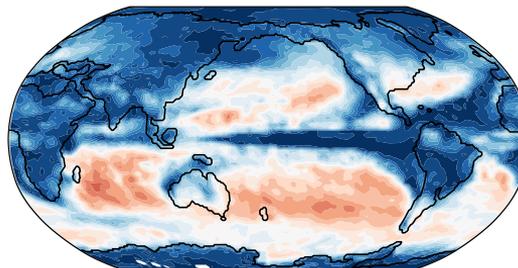


Corr(SF, d18Op)



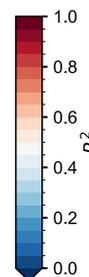
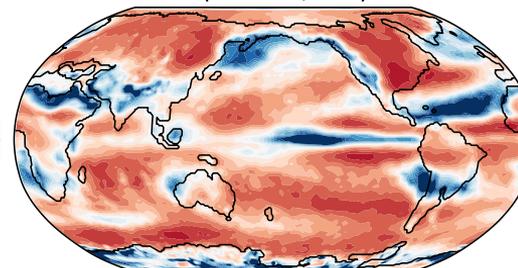
$\delta^{18}\text{O}_p = \text{LinearReg}(\text{SF})$

$R^2(\text{Prediction, Truth})$



$\delta^{18}\text{O}_p = \text{FNO}(\text{SF})$

$R^2(\text{Prediction, Truth})$



SF (stratiform fraction) appears to be more informative than OLR (representing convective intensity) over ocean.

Preliminary Results

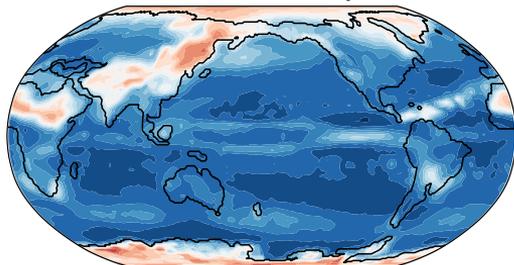
ID Exps.

Train: 1.5xCO₂; Test: 1.5xCO₂



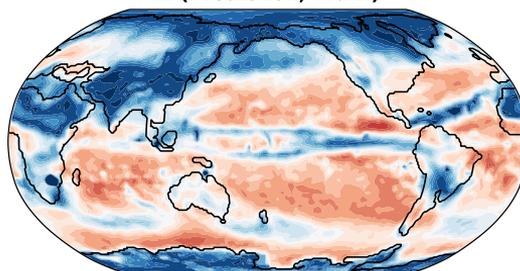
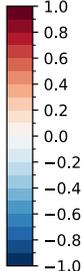
Diagnostics: local correlations

Corr(PRECL, d18Op)



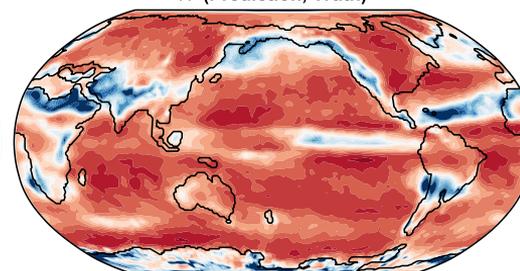
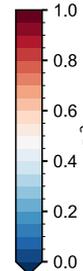
$\delta^{18}\text{O}_p = \text{LinearReg}(\text{PRECL})$

$R^2(\text{Prediction, Truth})$

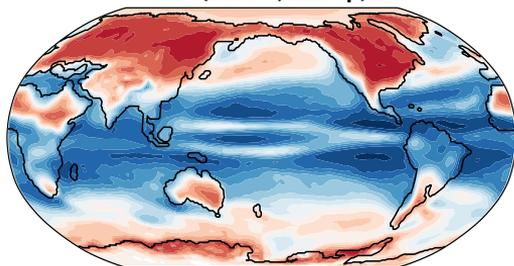


$\delta^{18}\text{O}_p = \text{FNO}(\text{PRECL})$

$R^2(\text{Prediction, Truth})$

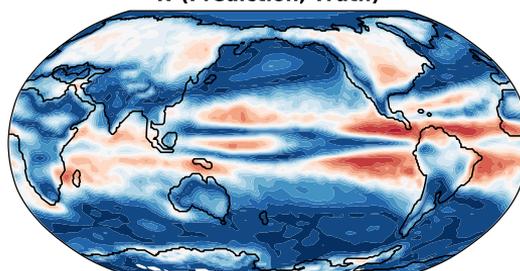
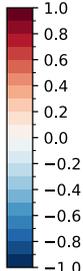


Corr(PRECC, d18Op)



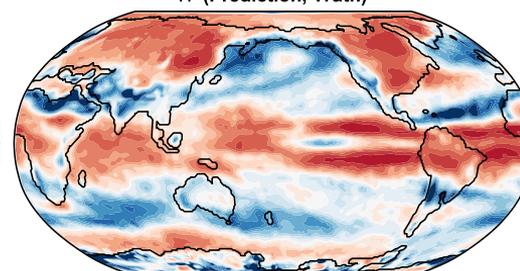
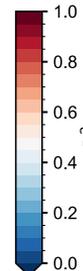
$\delta^{18}\text{O}_p = \text{LinearReg}(\text{PRECC})$

$R^2(\text{Prediction, Truth})$



$\delta^{18}\text{O}_p = \text{FNO}(\text{PRECC})$

$R^2(\text{Prediction, Truth})$



PRECL (stratiform precipitation) appears to be informative using FNO -- "Stratiform Amount Effect".

Preliminary Results

ID Exps.

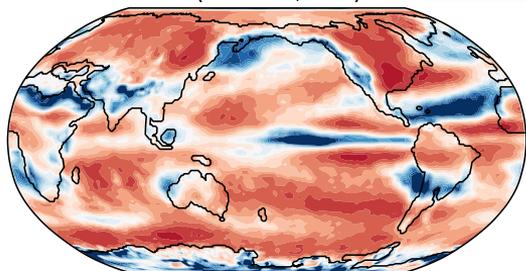
Train: 1.5xCO₂; Test: 1.5xCO₂



$\delta^{18}\text{O}_p = \text{FNO}(\text{SF})$

$R^2(\text{Prediction, Truth})$

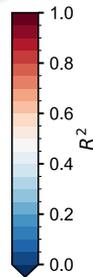
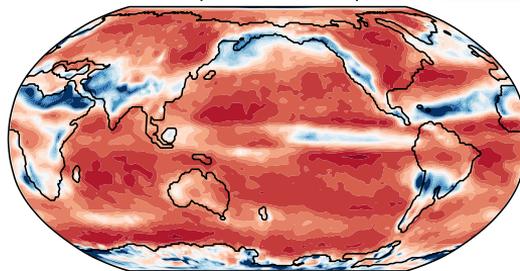
GM: 0.56



$\delta^{18}\text{O}_p = \text{FNO}(\text{PRECL})$

$R^2(\text{Prediction, Truth})$

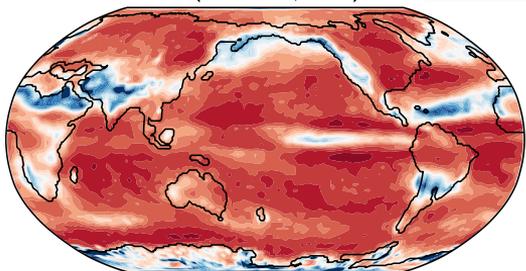
GM: 0.66



$\delta^{18}\text{O}_p = \text{FNO}(\text{pr, PRECL})$

$R^2(\text{Prediction, Truth})$

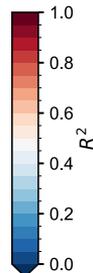
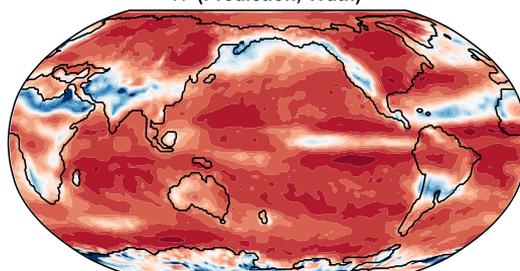
GM: 0.71



$\delta^{18}\text{O}_p = \text{FNO}(\text{tas, pr, PRECL})$

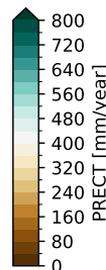
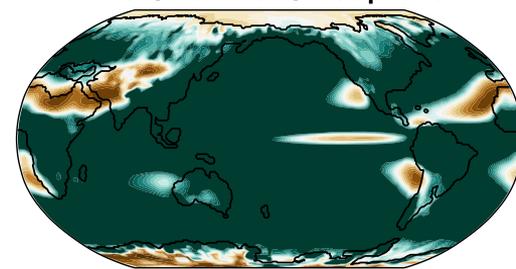
$R^2(\text{Prediction, Truth})$

GM: 0.72



A plausible cause of the weaker performance in specific regions: persistent drought conditions.

Annual Mean Total Precipitation



A mixture of the Temperature Effect, Amount Effect, and SF theory yields the best skill so far.

Preliminary Results

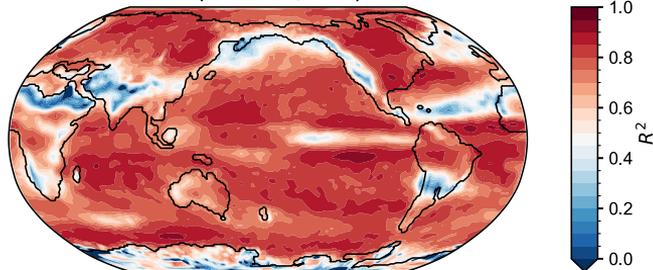
ID Exps.

Train: 1.5xCO₂; Test: 1.5xCO₂



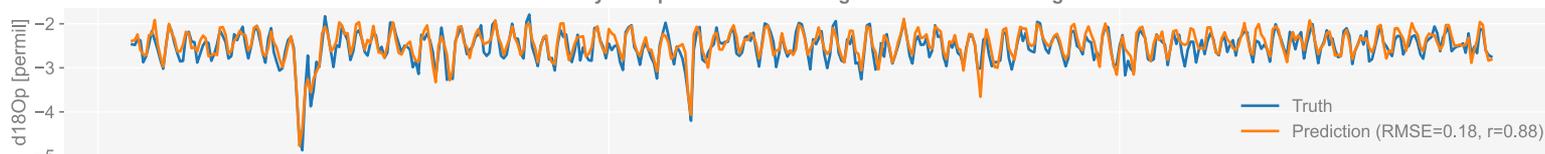
$$\delta^{18}\text{O}_p = \text{FNO}(\text{tas}, \text{pr}, \text{PRECL})$$

$R^2(\text{Prediction}, \text{Truth})$

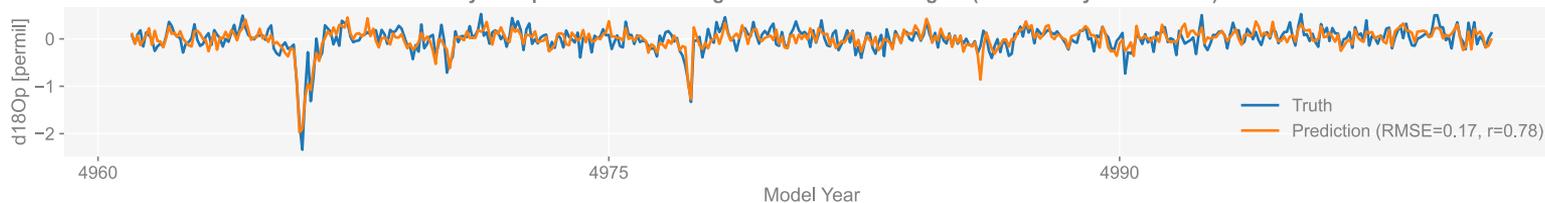


Good performance in internal variability predictions over the NINO3.4 region.

Monthly Precipitation d18O Average over the NINO3.4 Region



Monthly Precipitation d18O Average over the NINO3.4 Region (Seasonal Cycle Removed)



Preliminary Results

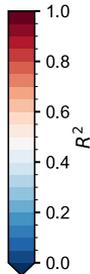
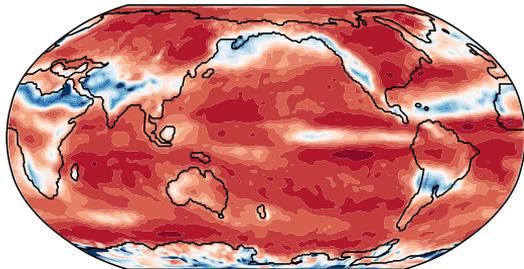
ID Exps.

Train: 1.5xCO₂; Test: 1.5xCO₂

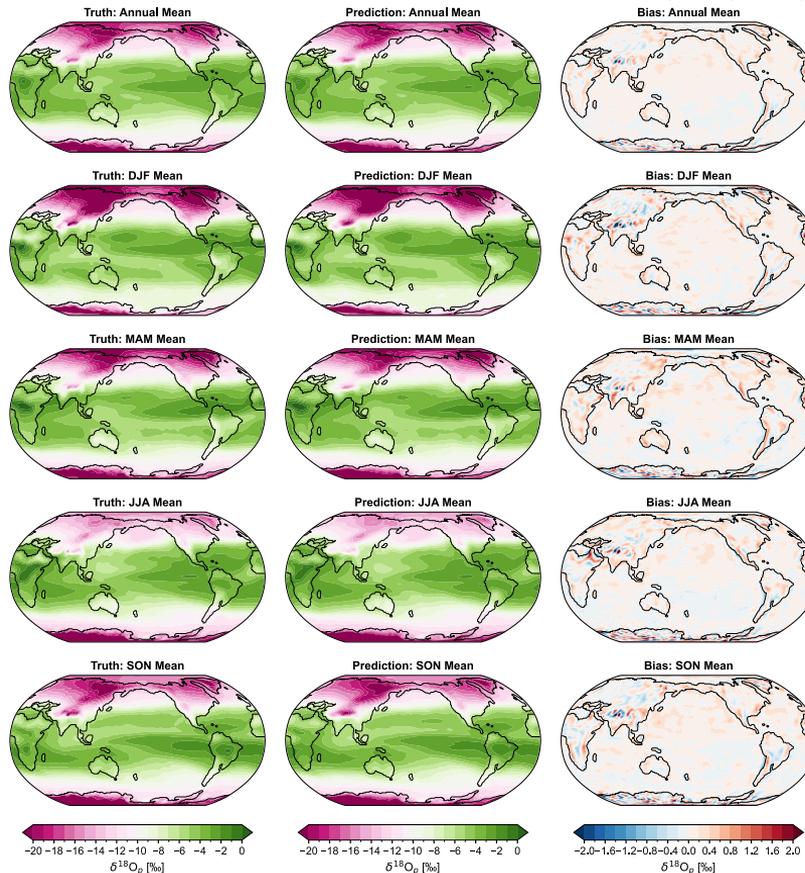


$$\delta^{18}\text{O}_p = \text{FNO}(\text{tas}, \text{pr}, \text{PRECL})$$

$R^2(\text{Prediction}, \text{Truth})$



Good performance in both annual and seasonal mean climate predictions.



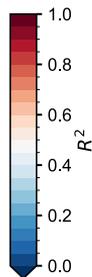
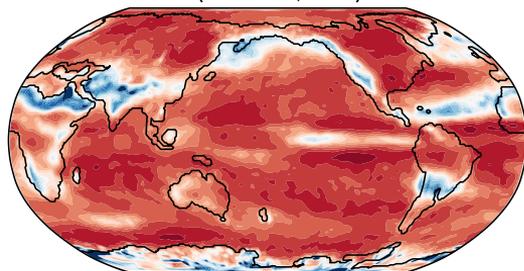
Preliminary Results

OOD Exps.
Train: 1.5xCO₂; Test: 3xCO₂



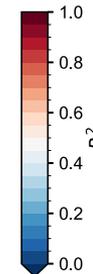
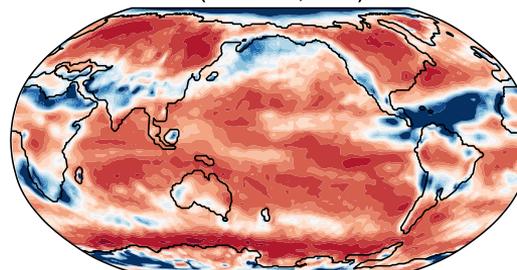
$\delta^{18}\text{O}_p = \text{FNO}(\text{tas}, \text{pr}, \text{PRECL})$ ID Test

$R^2(\text{Prediction, Truth})$



$\delta^{18}\text{O}_p = \text{FNO}(\text{tas}, \text{pr}, \text{PRECL})$ OOD Test

$R^2(\text{Prediction, Truth})$



The essential challenge of an OOD test:

- given the different distributions of the variables across climate regimes,
- normalizing the Test set using statistics from the Train set could be problematic.

Conclusions

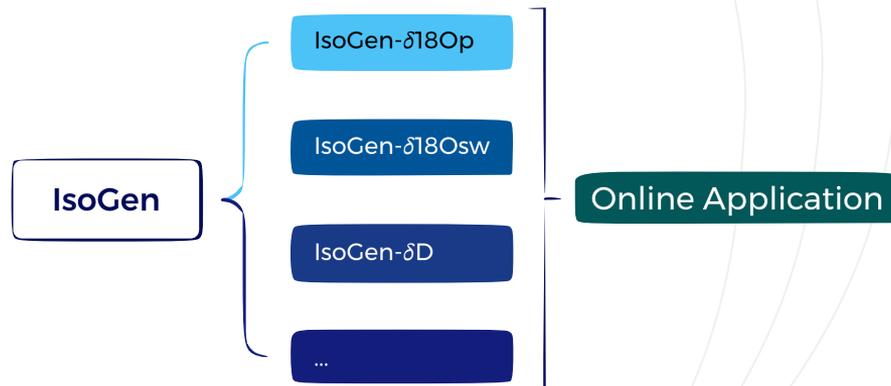


- It is **feasible** to predict $\delta^{18}\text{O}_p$ variability using **a machine learning based emulator** of the climate-isotope mapping and **apply it to different climatologies**.
- By testing different combinations of input variables, we gain **scientific insights** into the **leading drivers of $\delta^{18}\text{O}_p$ variability**.
- **Taking nonlinearity and nonlocality into account appears to be effective**, confirming the previous studies.
- The emulator $\delta^{18}\text{O}_p = \text{FNO}(\text{tas}, \text{pr}, \text{PRECL})$ mixing the **Temperature Effect, Amount Effect**, and **Stratiform-Fraction theory** yields the best skill so far.
- The weaker performance in specific regions (e.g., over the tropical Atlantic) is likely due to **persistent drought conditions**, leading to ill-defined $\delta^{18}\text{O}_p$ variability.

Future Research



- **Scientific interpretations [Q1]** via modeling, obs, and ML techniques on
 - the **nonlinearity** and **nonlocality** nature of the isotopic controls
 - the "**Stratiform Amount Effect**"
- **Improvements** on the OOD tests **across different climatologies [Q2]**
- **OOD tests across different ESMs [Q3]**
 - WisoMIP ([Bong et al., 2026](#)): iCAM5, iCAM6, ECHAM6-wiso, GISS-E2.1, IsoGSM3, LDMZ6, MIROC5-iso, NICAM-WISO
 - iHadCM3 ([Tindall et al., 2009](#))
- Emulating **other water isotopic variables**





CGD Laboratory



Thank You!

Questions and comments?

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