Optimizing Objective Model Calibration approaches using Single Column Models

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Outlines

1. **Parameter uncertainty:** What it is, why it exists, and why it limits model skill
2. **Motivation:** The role of *parametric uncertainty*, alongside structural uncertainty, in climate models
3. **Unique Part of Our Effort:** SCAM-based perfect-model framework for systematic, probabilistic calibration
4. **Key results:** Identifiability, equifinality, and robustness of Bayesian calibration
5. **Summary:** Implications for efficient and reliable GCM tuning

GCM Parametrization

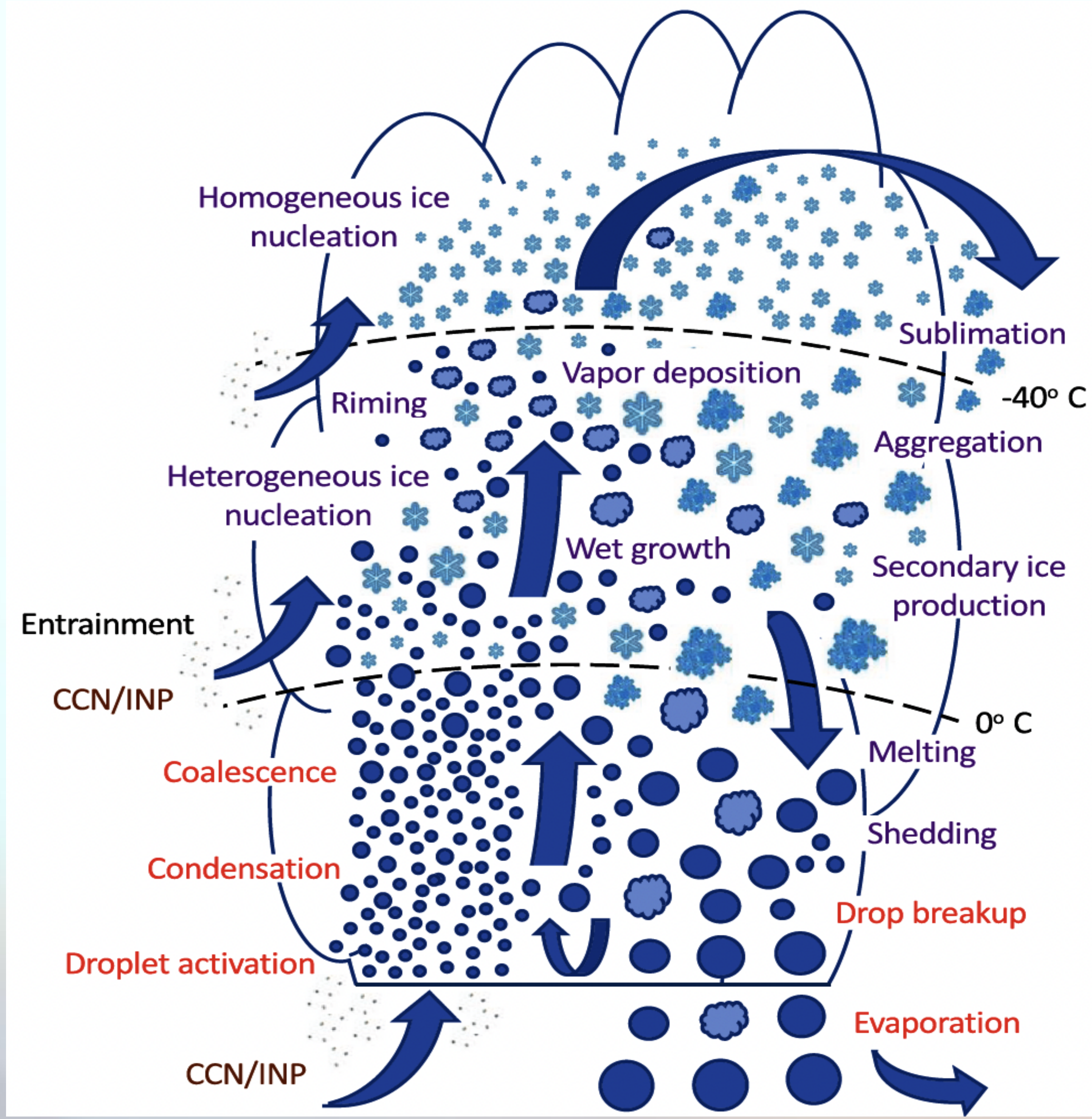


Figure: Microphysics

Represent through parameterizations:

1. Microphysics
2. Turbulence

• Computational Constraints

3. Convection
4. Aerosols

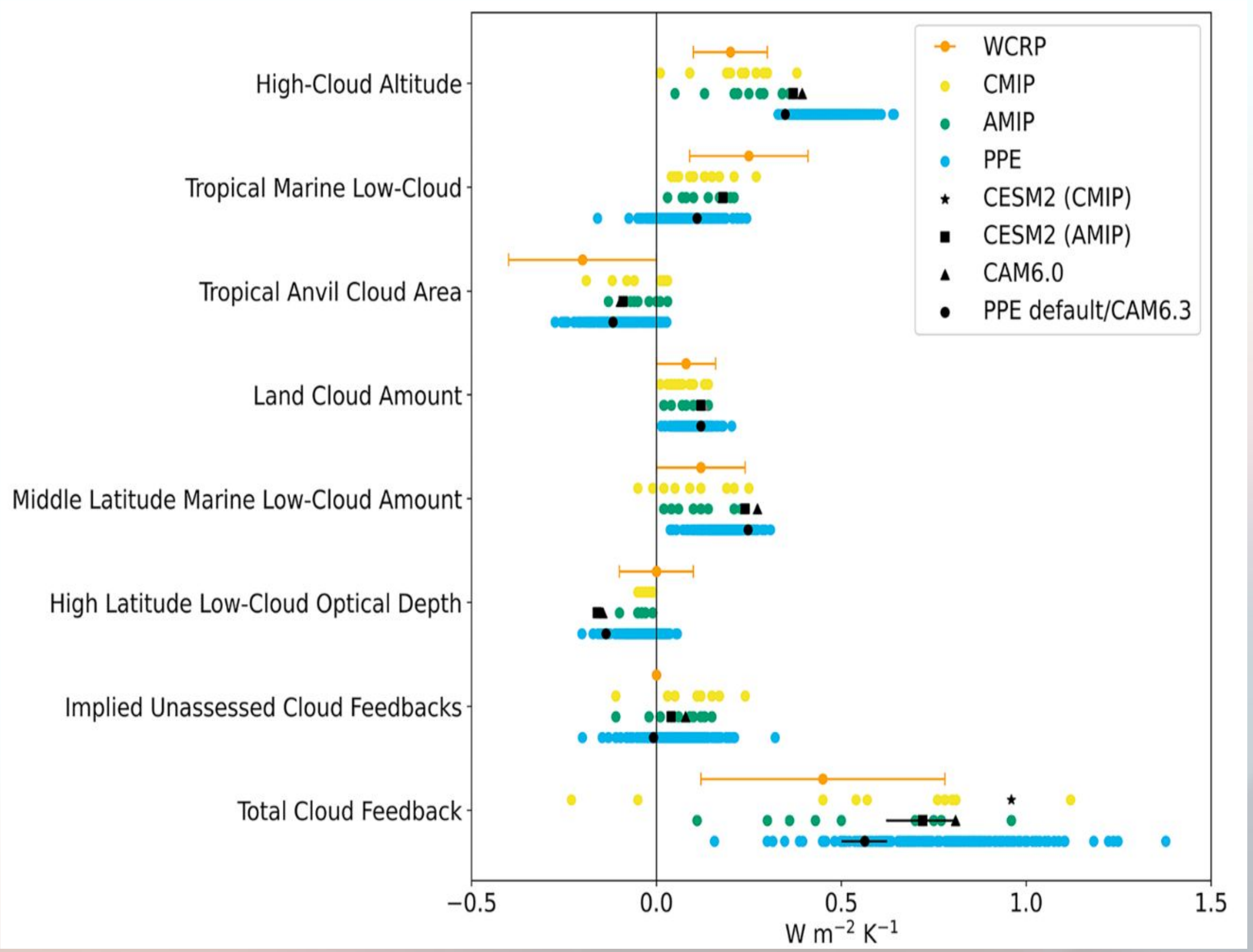
Morrison, H., van Lier-Walqui, M., Fridlind, A. M., Grabowski, W. W., Harrington, J. Y., Hoose, C., ... & Xue, L. (2020). Confronting the challenge of modeling cloud and precipitation microphysics. *Journ*
of advances in modeling earth systems, *12*(8), e2019MS001689.

Parameterization Uncertainty

Type 1: Structural
Different parameterization schemes yield different representations of sub-scale processes

Type 2: Parametric
Uncertainty in the values assigned to the model parameters

Cloud Feedbacks



*M. L. Duffy, B. Medeiros, A. Gettelman, and T. Eidhammer, “Perturbing Parameters to Understand Cloud Contributions to Climtae Change,” *J. Clim.*, vol. 37, no. 1, pp. 213–227, Dec. 2023, doi: 10.1175/JCLI-D-23-0250.1

Recent Calibration Efforts

https://doi.org/10.5194/gmd-17-7835-2024

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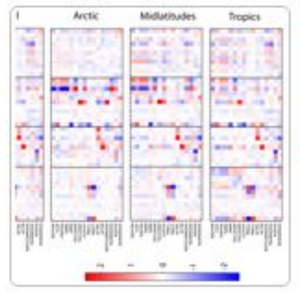
An extensible perturbed parameter ensemble for the Community Atmosphere Model version 6



Trude Eidhammer, Andrew Gettelman, Katherine Thayer-Calder, Duncan Watson-Parris, Gregory Elsaesser, Hugh Morrison, Marcus van Lier-Walqui, Ci Song, and Daniel McCoy

Abstract

This paper documents the methodology and preliminary results from a perturbed parameter ensemble (PPE) technique, where multiple parameters are varied simultaneously and the parameter values are determined with Latin hypercube sampling. This is done with the Community Atmosphere Model version 6 (CAM6), the atmospheric component of the Community Earth System Model version 2 (CESM2). We apply the PPE method to CESM2–CAM6 to understand climate sensitivity to atmospheric physics parameters. The initial simulations vary 45 parameters in the microphysics, convection, turbulence and aerosol schemes with 263

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Short summary
We describe a dataset where 45 parameters related to cloud processes in the Community Earth...
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Gregory S. Elsaesser, Marcus van Lier-Walqui, Qingyuan Yang, Maxwell Kelley, Andrew S. Ackerman, Ann M. Fridlind, Gregory V. Cesana, Gavin A. Schmidt, Jingbo Wu, Ali Behrangi ... See all authors

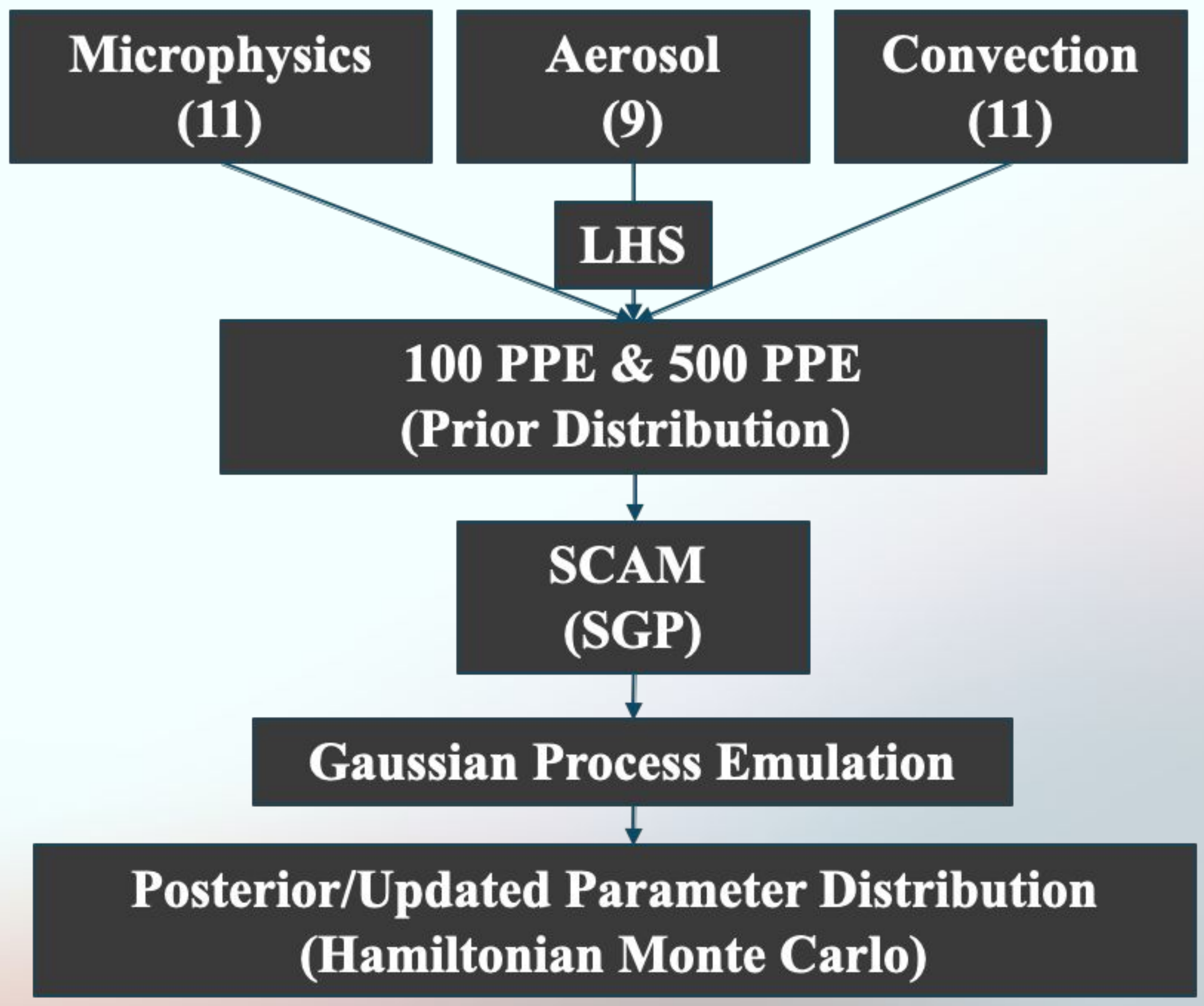
First published: 11 April 2025 | https://doi.org/10.1029/2024MS004713 | Citations: 1

Unique Part of Our Effort

1. Use of Single Column Atmospheric Model (SCAM)
   - Column of CAM6

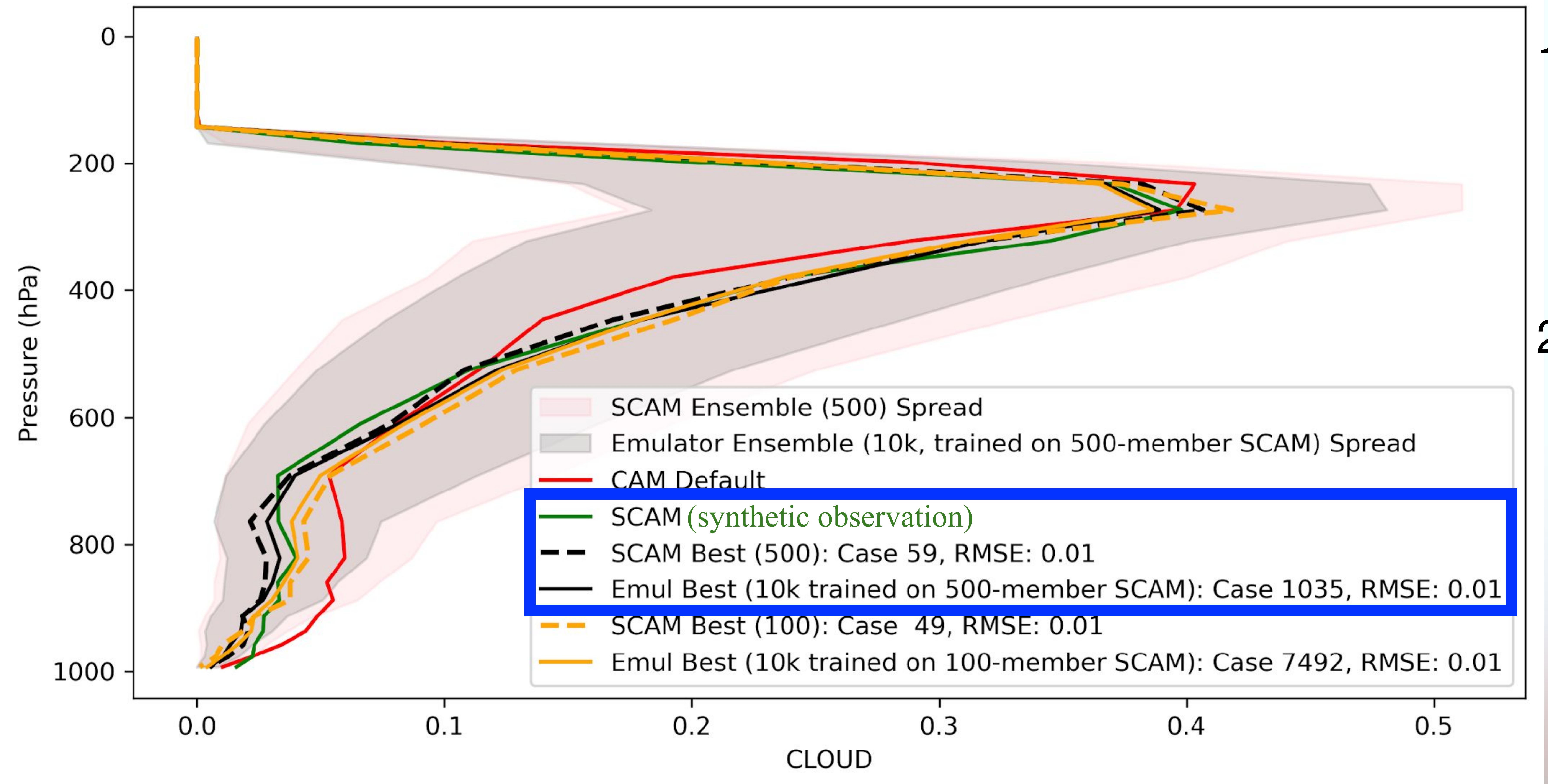
2. Perfect model framework
   - SCAM generated Intensive Observation Period (IOP) - '*synthetic*' (e.g., cloud profile)

3. Traditional Calibration vs Probabilistic Calibration
   - RMSE based observation fitting
   - Gaussian Process (GP) enabled Hamiltonian Monte Carlo (HMC) parameter calibration.



*Watson-Parris, D., Williams, A., Deaconu, L., & Stier, P. (2021). Model calibration using ESEm v1. 1.0–an open, scalable Earth system emulator. Geoscientific Model Development, 14(12), 7659-7672.

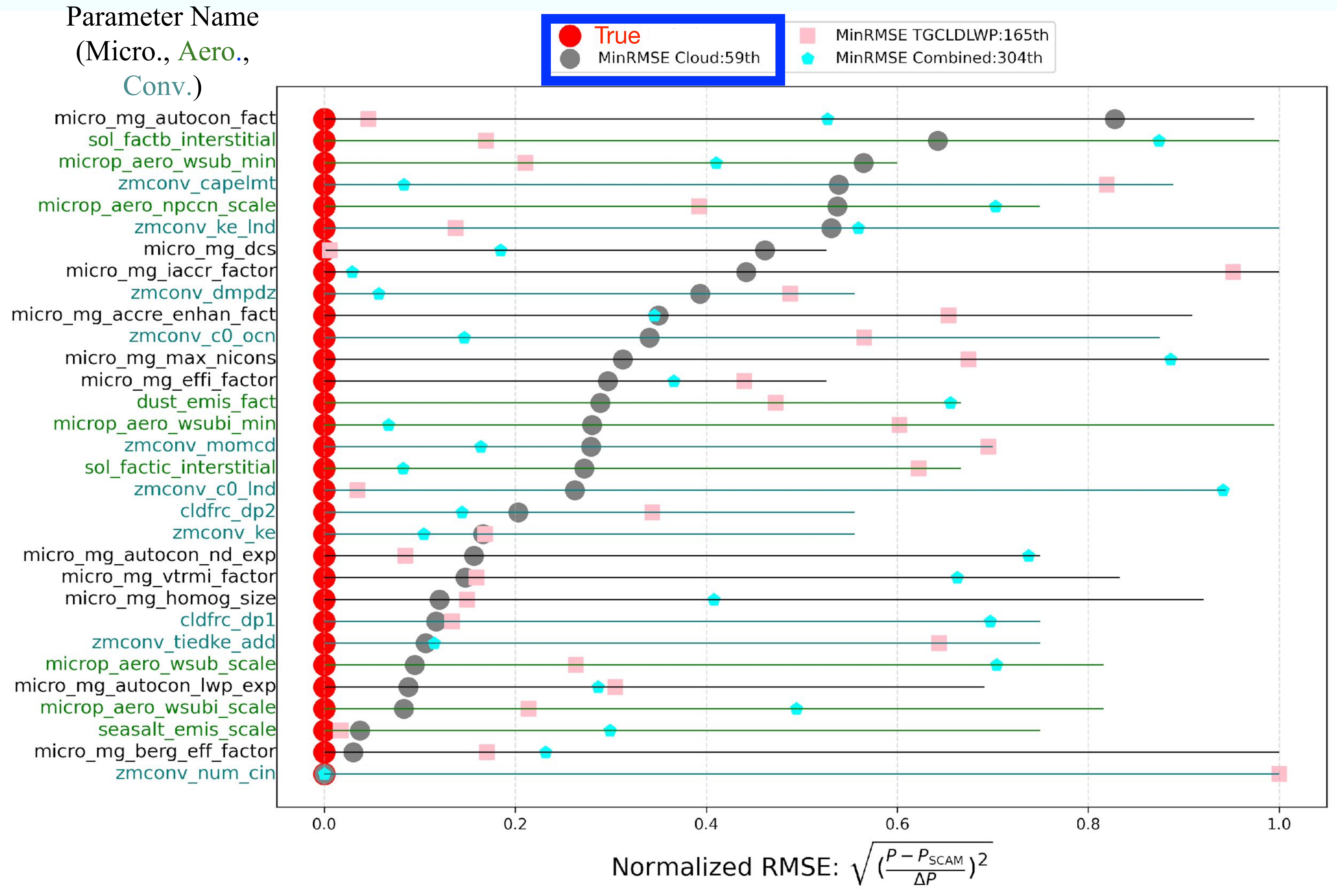
Traditional Calibration: Vertical Cloud Fraction



1. The best Case and synthetic observation Closely align (RMSE: 0.01)

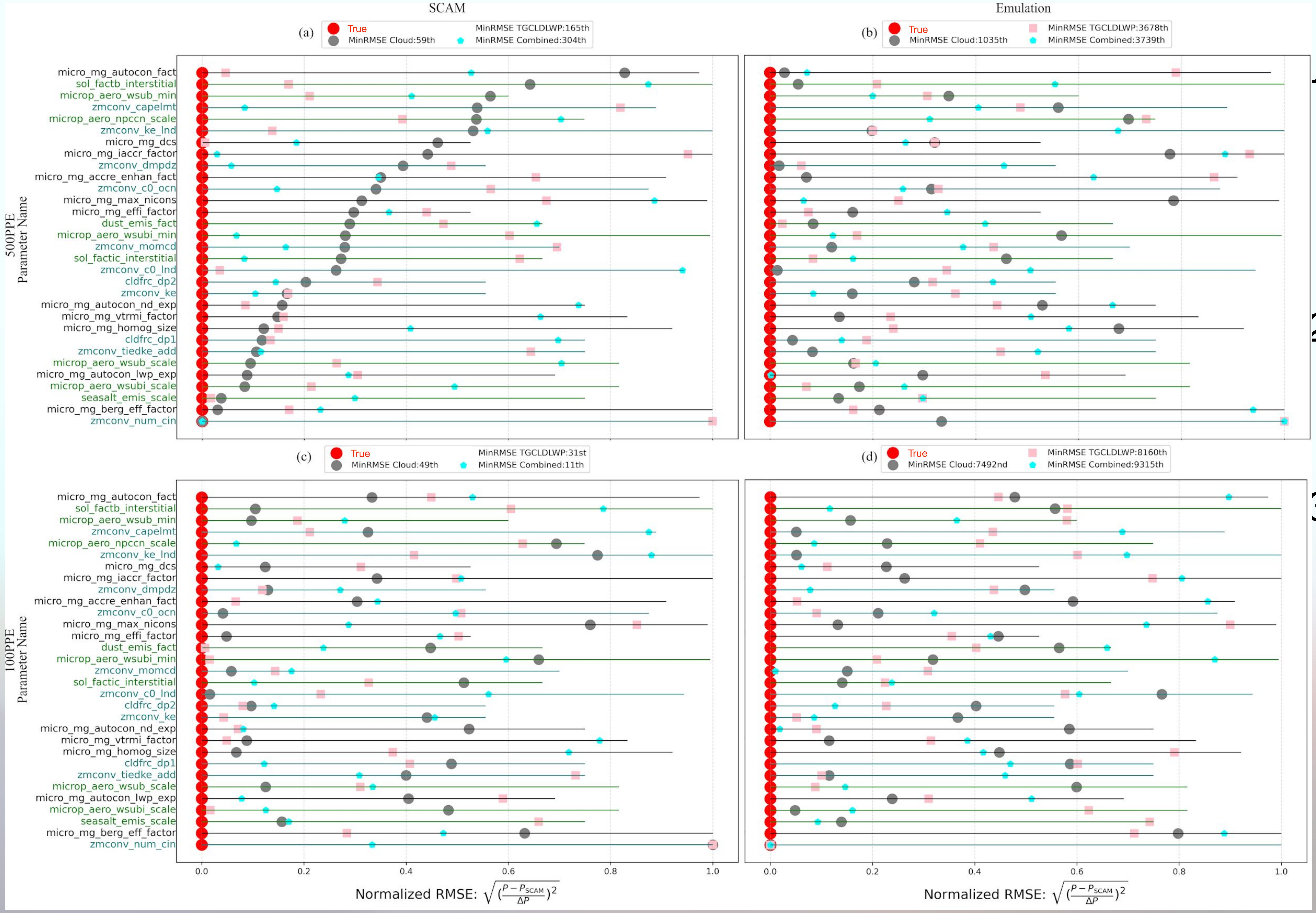
2. Therefore, the parameter values involved in these best cases should be close to the parameter value of synthetic observation?

Traditional Calibration: Normalized Parameter Error



1. The parameter set values associated with these best-match profiles differ substantially

Traditional Calibration: Normalized Parameter Error

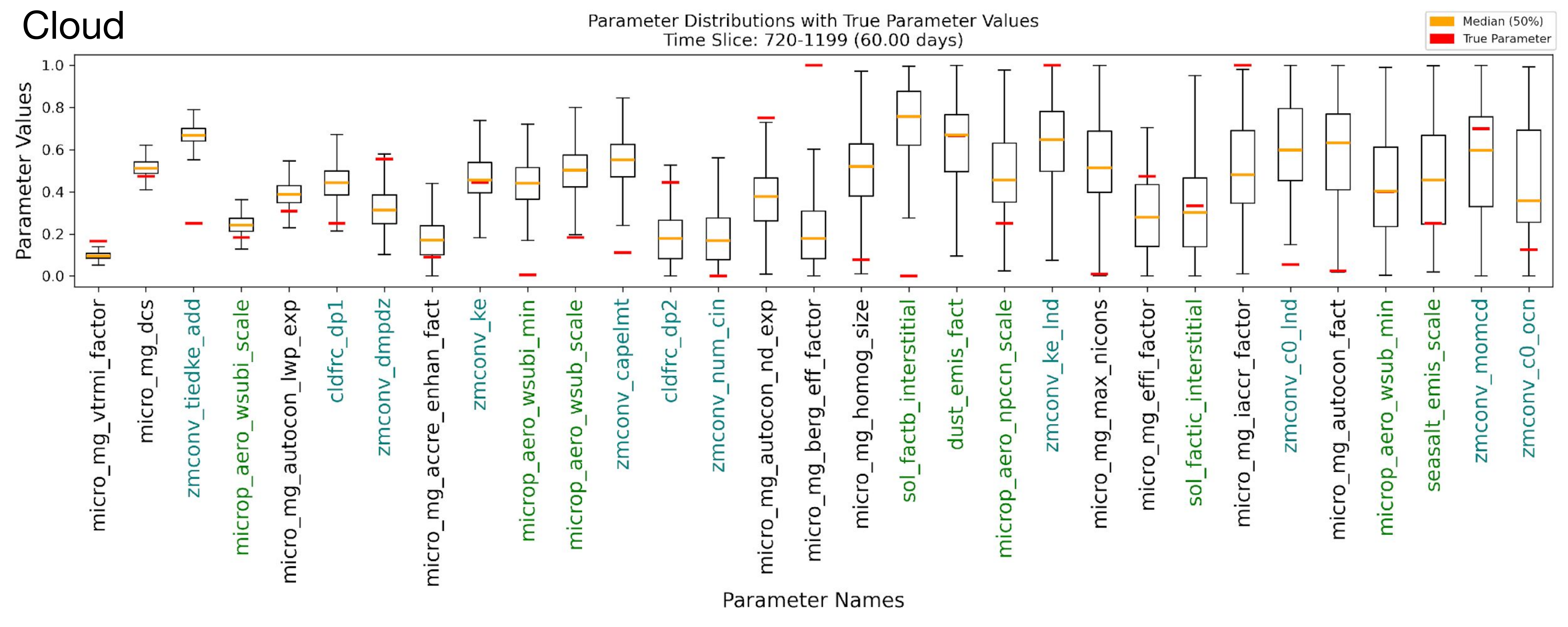


1. The parameter set values associated with these best-match profiles differ substantially

2. In each case Random parameters are retrieved (**equifinality**).

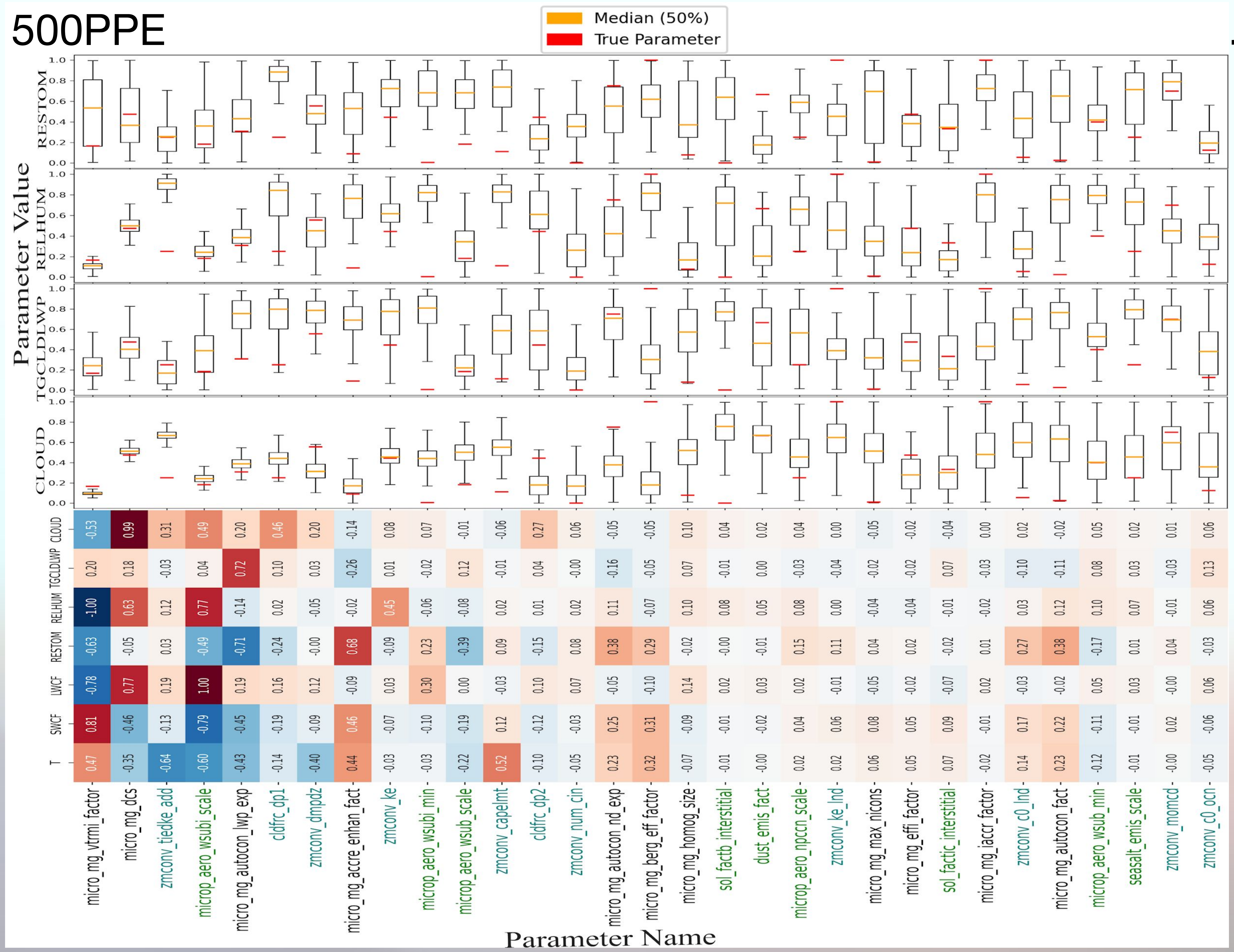
3. This result highlights the ill-posed nature of the inverse problem and suggests that additional constraints, process-aware metrics, or probabilistic approach may be required to improve parameter identifiability.

HMC Probabilistic Calibration: Normalized Posterior Distribution



1. **HMC constrains key parameters:** Posterior distributions identify a small subset of parameters.

HMC Probabilistic Calibration: Normalized Posterior Distribution



1. **HMC constrains key parameters:** Posterior distributions identify a small subset of parameters.
2. **Consistency across variables:** Same parameters are constrained for LWP (TGCLDLWP), relative humidity (RELHUM), and residual energy balance (RESTOM).
3. **Reason: sensitivity matters:** Constrained parameters are the most sensitive; insensitive parameters remain unconstrained, as expected.
4. **Robust across ensembles (100 & 500 PPE)** unlike typical RMSE-based calibration which often selects random parameters.

Summary

1. **Traditional observation matching fails to retrieve 'true' parameters:** Even in a perfect-model (synthetic observation) setup, best-match or RMSE-based tuning cannot reliably recover true parameter values due to equifinality and compensating errors.

2. **Probabilistic calibration is robust and informative:** A Bayesian GP–HMC framework successfully identifies sensitive parameters and quantifies uncertainty through posterior distributions, providing physically meaningful constraints rather than arbitrary point estimates.

3. **Consistency across variables and ensemble sizes:** GP–HMC consistently recovers the same subset of identifiable parameters for all variables using both 500-member and 100-member PPEs, in contrast to observation matching, which selects different parameters in each realization.

SCAM as an efficient training tool for GCMs

SCAM enables computationally efficient parameter identification and uncertainty quantification, serving as a powerful pre-conditioning step for full 3D climate model tuning and reducing expensive trial-and-error simulations.

Interested in collaboration?
Please feel free to reach out: **pappup2@illinois.edu**

Thank You

Motivation: Recent Calibration Efforts

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About

Learning the Earth with Artificial Intelligence and Physics (LEAP) is an NSF Science Technology Center (STC) launched in 2021.

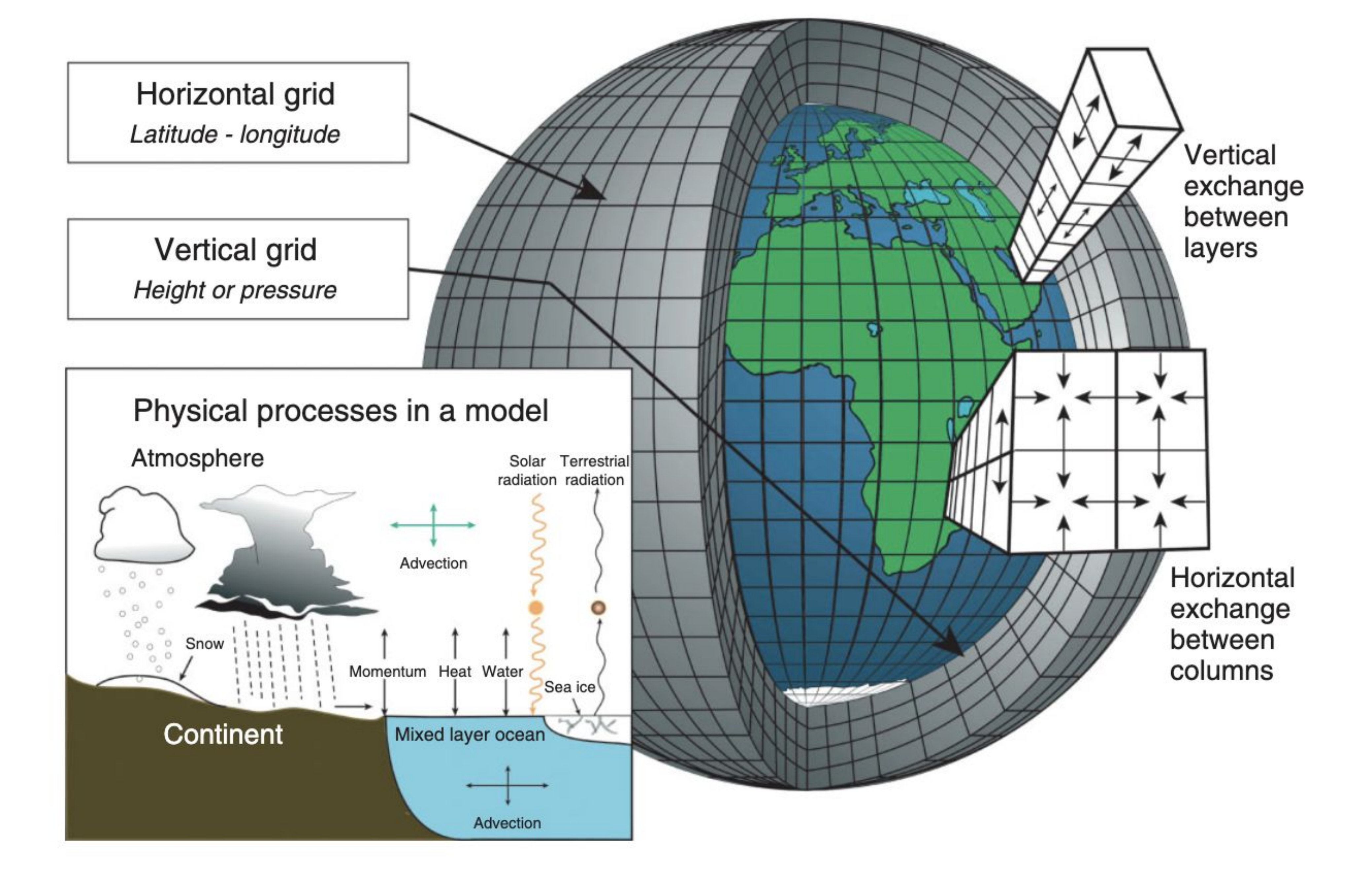
Research Focus

LEAP will focus on hybridizing ML by integrating physical knowledge for implementation with the open-source Community Earth System Model (CESM) by:

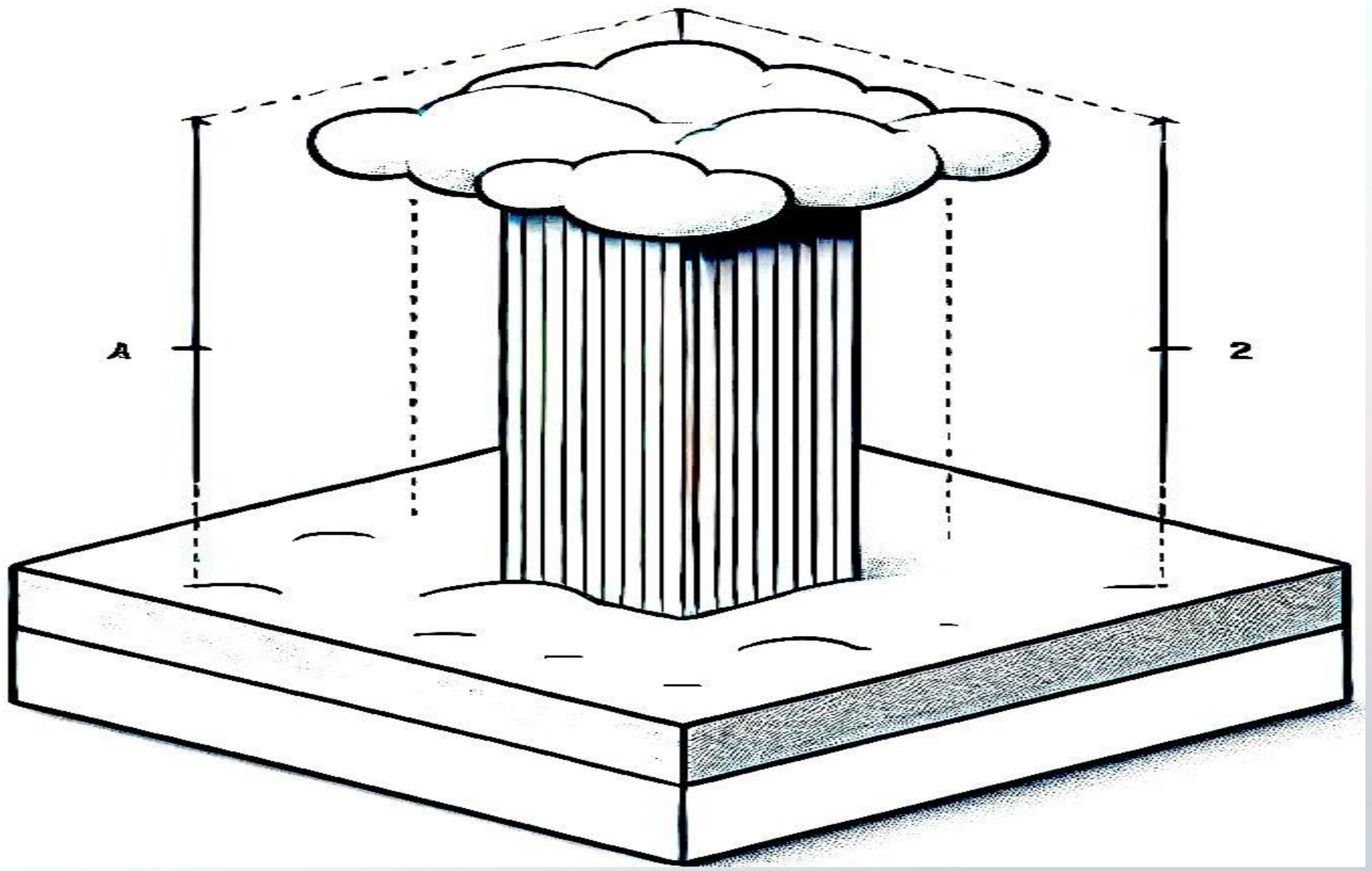
1. Reducing the existing model structural errors related to the lack of comprehension of the process at play (e.g., clouds + microphysics);
2. Optimally estimating the model parameters using a Bayesian approach; and
3. Developing new observational products which will be used to evaluate the CESM skill.

*https://leap.columbia.edu/research-home/

Single Column Model (SCM)



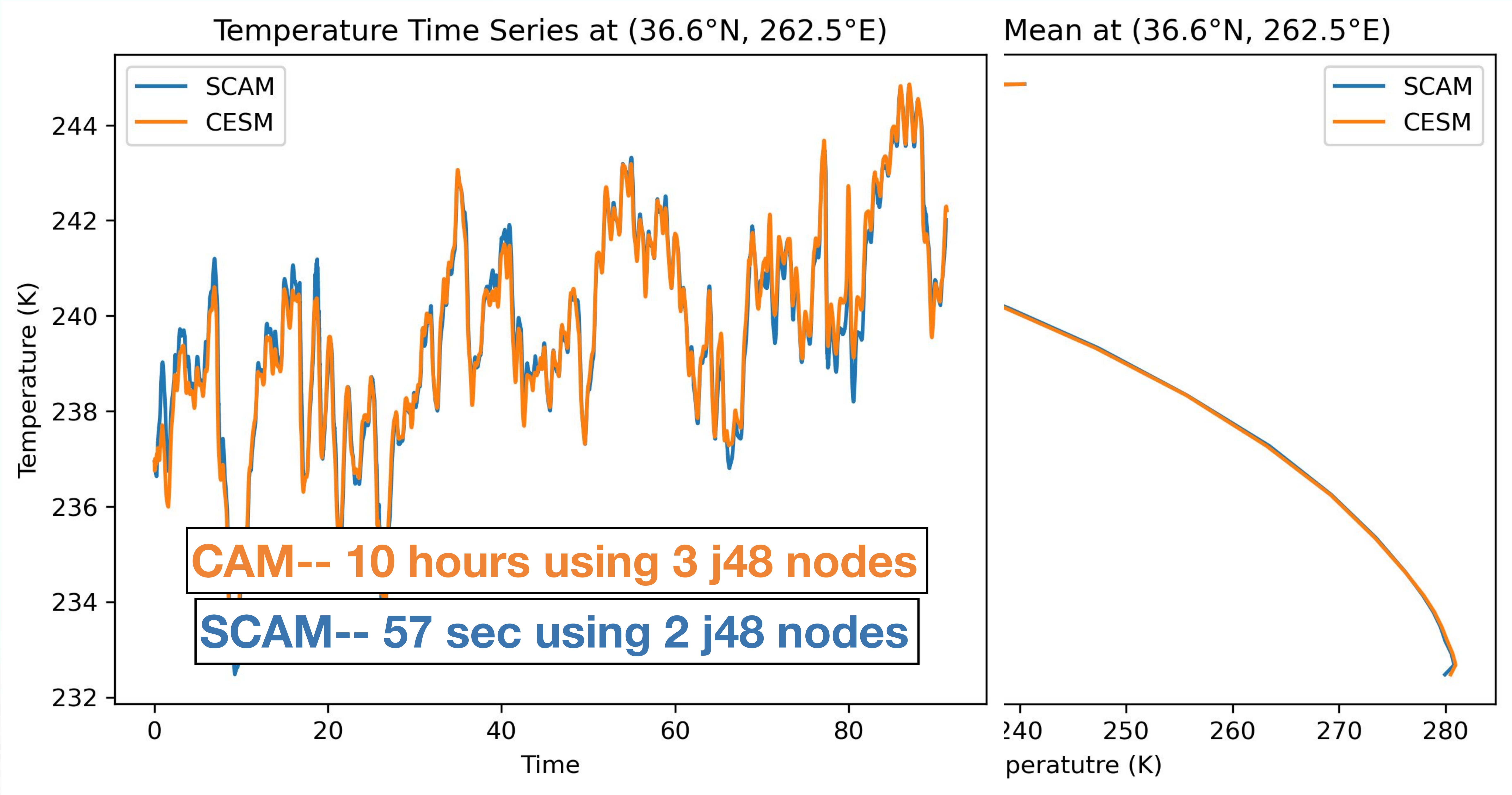
Structure of a GCM



Structure of a SCM

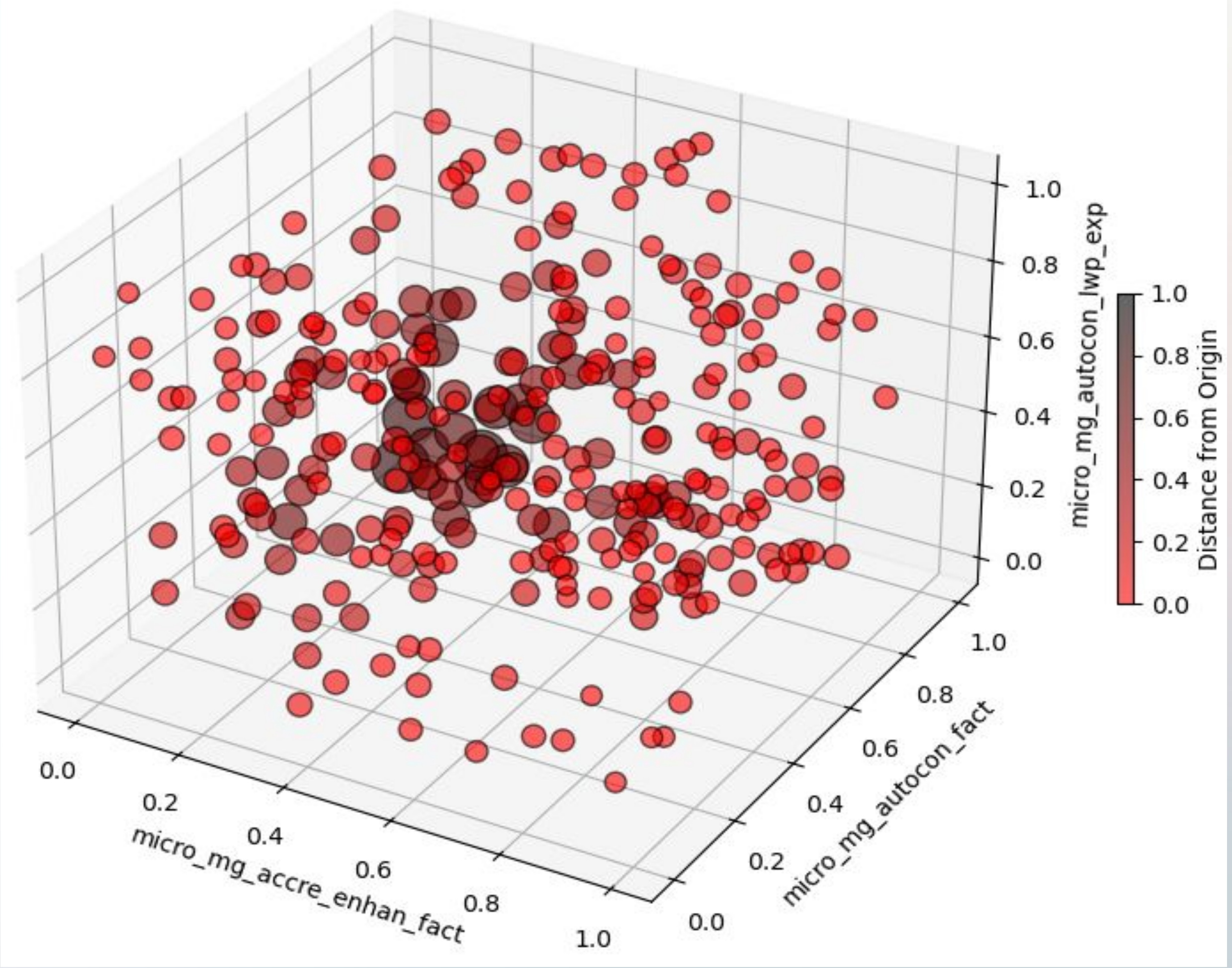
Edwards, P. N. (2011). History of climate modeling. *Wiley Interdisciplinary Reviews: Climate Change*, *2*(1), 128-139.

Why SCAM?


Temperature Time Series at (36.6°N, 262.5°E)
SCAM
CESM
Temperature (K)
Time
CAM-- 10 hours using 3 j48 nodes
SCAM-- 57 sec using 2 j48 nodes
Mean at (36.6°N, 262.5°E)
SCAM
CESM
peratutre (K)

Physics Scheme	Parameter Name	Description	Default	Max	Min	Unit
Microphysics (11)	micro_mg_accre_enhan_fact	Accretion enhancing factor	1.0	10.0	0.1	
	micro_mg_autocon_fact	Autoconversion factor	0.01	0.2	0.005	
	micro_mg_autocon_lwp_exp	LWP exponent	2.47	3.30	2.1	
	micro_mg_autocon_nd_exp	Autoconversion exponent	-1.1	-0.8	-2.0	
	micro_mg_berg_eff_factor	Bergeron efficiency factor	1.0	1.0	0.1	
	micro_mg_dcs	Autoconversion size threshold ice–snow	500e-6	1000e-6	50e-6	m
	micro_mg_effi_factor	Scale effective radius for optics calculation	1.0	2.0	0.1	
	micro_mg_homog_size	Homogeneous freezing ice particle size	25e-6	200e-6	10e-6	m
	micro_mg_iaccr_factor	Scaling ice and snow accretion	1.0	1.0	0.2	
	micro_mg_max_nicons	Maximum allowed ice number concentration	100e6	10000e6	1e5	kg^{-1}
	micro_mg_vtrmi_factor	Ice fall speed scaling	1.0	5.0	0.2	ms^{-1}
Aerosol (9)	microp_aero_npccn_scale	Scale activated liquid number	1.0	3.0	0.33	
	microp_aero_wsub_min	Min subgrid velocity for liquid activation	0.2	0.5	0	ms^{-1}
	microp_aero_wsub_scale	Subgrid velocity for liquid activation scaling	1.0	5.0	0.1	
	microp_aero_wsubi_min	Min subgrid velocity for ice activation	0.001	0.2	0	ms^{-1}
	microp_aero_wsubi_scale	Subgrid velocity for ice activation scaling	1.0	5.0	0.1	
	dust_emis_fact	Dust emission scaling factor	0.7	1.0	0.1	
	seasalt_emis_scale	Sea salt emission scaling factor	1.0	2.5	0.5	
	sol_factb_interstitial	Below-cloud scavenging of interstitial modal aerosols	0.1	1.0	0.1	
	sol_factic_interstitial	In-cloud scavenging of interstitial modal aerosols	0.4	1.0	0.1	
Convection (11)	cldfrc_dp1	Parameter for deep convection cloud fraction	0.1	0.25	0.05	
	cldfrc_dp2	Parameter for deep convection cloud fraction	500	1000	100.0	
	zmconv_c0_lnd	Convective autoconversion over land	0.0075	0.1	0.002	m^{-1}
	zmconv_c0_ocn	Convective autoconversion over ocean	0.3	0.1	0.02	m^{-1}
	zmconv_capelmt	Triggering threshold for ZM convection	70	350	35.0	Jkg^{-1}
	zmconv_dmpdz	Entrainment parameter	-1.0e-3	-2.0e-4	-2e-3	m^{-1}
	zmconv_ke	Convective evaporation efficiency	5.0e-6	1.0e-5	1.0e-6	$(kgm^{-2}s^{-1})^{0.5}s^{-1}$
	zmconv_ke_lnd	Convective evaporation efficiency over land	1.0e-6	1.0e-5	1.0e-5	$(kgm^{-2}s^{-1})^{0.5}s^{-1}$
	zmconv_momcd	Efficiency of pressure term in ZM downdraft CMT	0.7	1.0	0	
	zmconv_num_cin	Allowed number of negative buoyancy crossings	1.0	5.0	1.0	
	zmconv_tiedke_add	Convective parcel temperature perturbation	0.5	2.0	0	K

LHS



SCM Variables & Observation Sources

Variables Name (Unit)	ARM IOPs	Observation Sources
Temperature (K)	SGP, TWP, NSA, etc	MODIS, MERRA-2
Relative Humidity (-)	SGP, TWP, NSA, etc	MERRA-2
Cloud Fraction (-)	SGP, TWP, NSA, etc	MODIS, CALIPSO, CERES
Cloud Liquid (g/kg)	SGP, TWP, NSA, etc	MODIS, CALIPSO, CloudSat, GPM
Cloud Ice (g/kg)	-	MODIS, CALIPSO, CloudSat
Liquid Water Path (g/kg)	SGP, TWP, NSA, etc	MODIS, CloudSat
Precipitable Water (mm)	SGP, TWP, NSA, etc	MODIS, CERES, CloudSat, GPM
Short Wave Cloud Radiative Effect (W/m2)	SGP, TWP, NSA, etc	MODIS, CERES
Long Wave Cloud Radiative Effect (W/m2)	SGP, TWP, NSA, etc	MODIS, CERES
Surface Latent Heat Flux (W/m2)	SGP, TWP, NSA, etc	CERES, MERRA-2
Deep Convection Mass Flux (kg/kg/s)	-	CERES, GPM, MERRA-2

Gaussian Process Emulator

A **Gaussian Process** is a **non-parametric** method that defines a distribution over functions. In the context of emulation, we model a function $f(\theta)$ using a GP:

$$f(\theta) = GP(m(\theta), k(\theta, \ldots$$

$$K(\theta, \theta') = \sigma' exp(-\frac{1}{2}(\theta - \theta')^T L(\theta \ldots$$

Prediction, $E[f(\theta)] = \mu' = K'(K + \sigma^2 I \ldots$

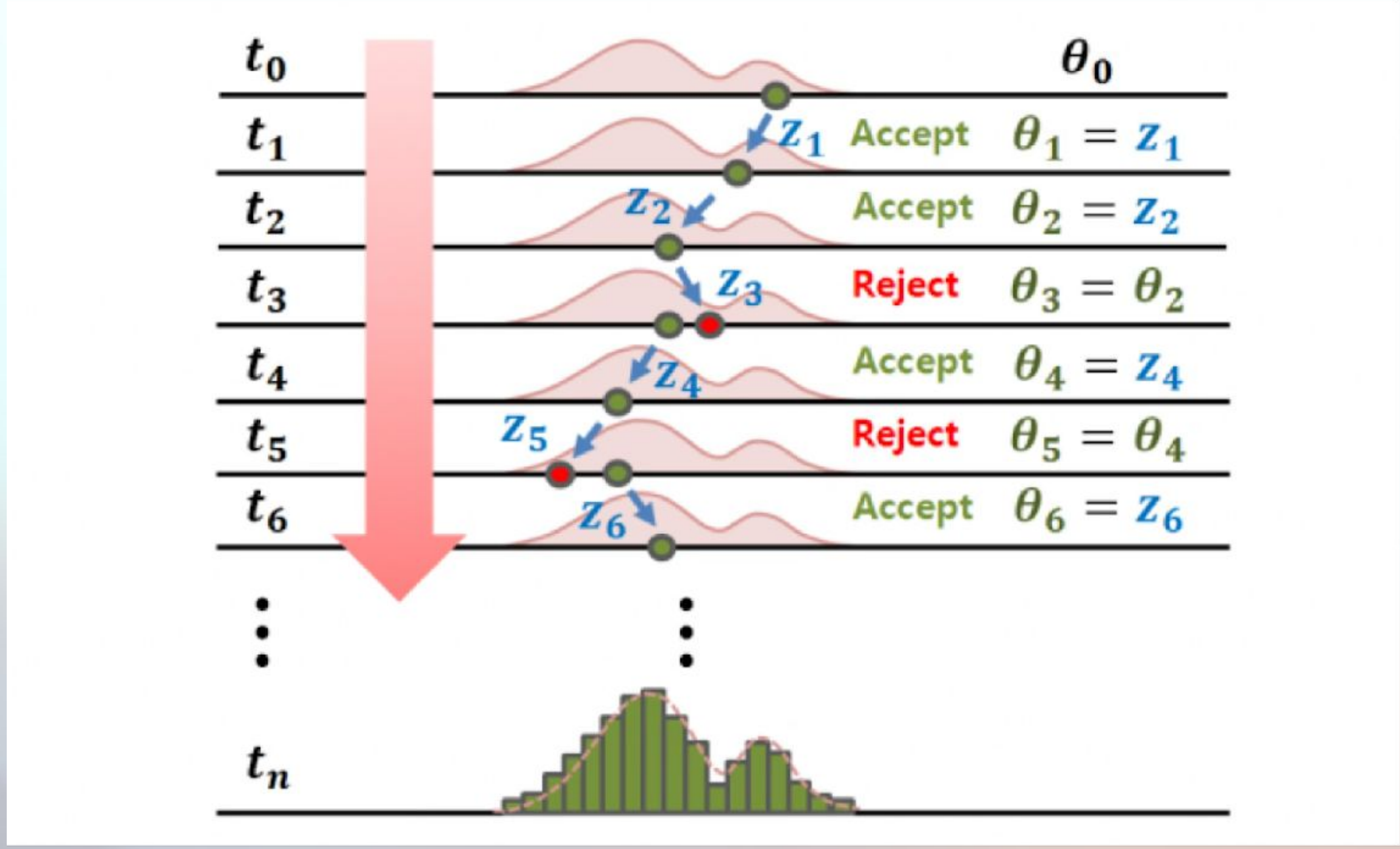
Here, θ is the input parameter vector represents microphysics, convection parameters and aerosol parameters..

$m(\theta)$ is the mean function

$K(\theta, \theta')$ is the covariant function or kernel and K' is the covariance between training and test points and K is the covariance between training points only.

Markov Chain Monte Carlo

$$\log \mathscr{L}(\boldsymbol{\theta}) = -\frac{1}{2}\sum_{i=1}^{n}\left(\frac{y_i^{\text{obs}} - \hat{y}_i(\boldsymbol{\theta})}{\sigma}\right)^2$$



Hamiltonian Monte-Carlo (HMC)

Given the joint probability distribution described by Eq. 2 and an initial choice of parameters θ' and (emulated) output Y', the acceptance probability r of a new set of parameters (θ) is given by:

$$r = \frac{p\left(Y^0|Y'\right)p\left(\theta'|\theta\right)p(\theta')}{p\left(Y^0|Y\right)p\left(\theta|\theta'\right)p(\theta)} \tag{4}$$

The `esem.sampler.MCMCSampler` class uses the TensorFlow-probability implementation of Hamiltonian Monte-Carlo (HMC) which uses the gradient information automatically calculated by TensorFlow to inform the proposed new parameters θ. For simplicity, we assume that the proposal distribution is symmetric: $p\left(\theta'|\theta\right) = p\left(\theta|\theta'\right)$, which is implemented as a zero log-acceptance correction in the initialisation of the TensorFlow target distribution. The target log probability provided to the TensorFlow HMC algorithm is then:

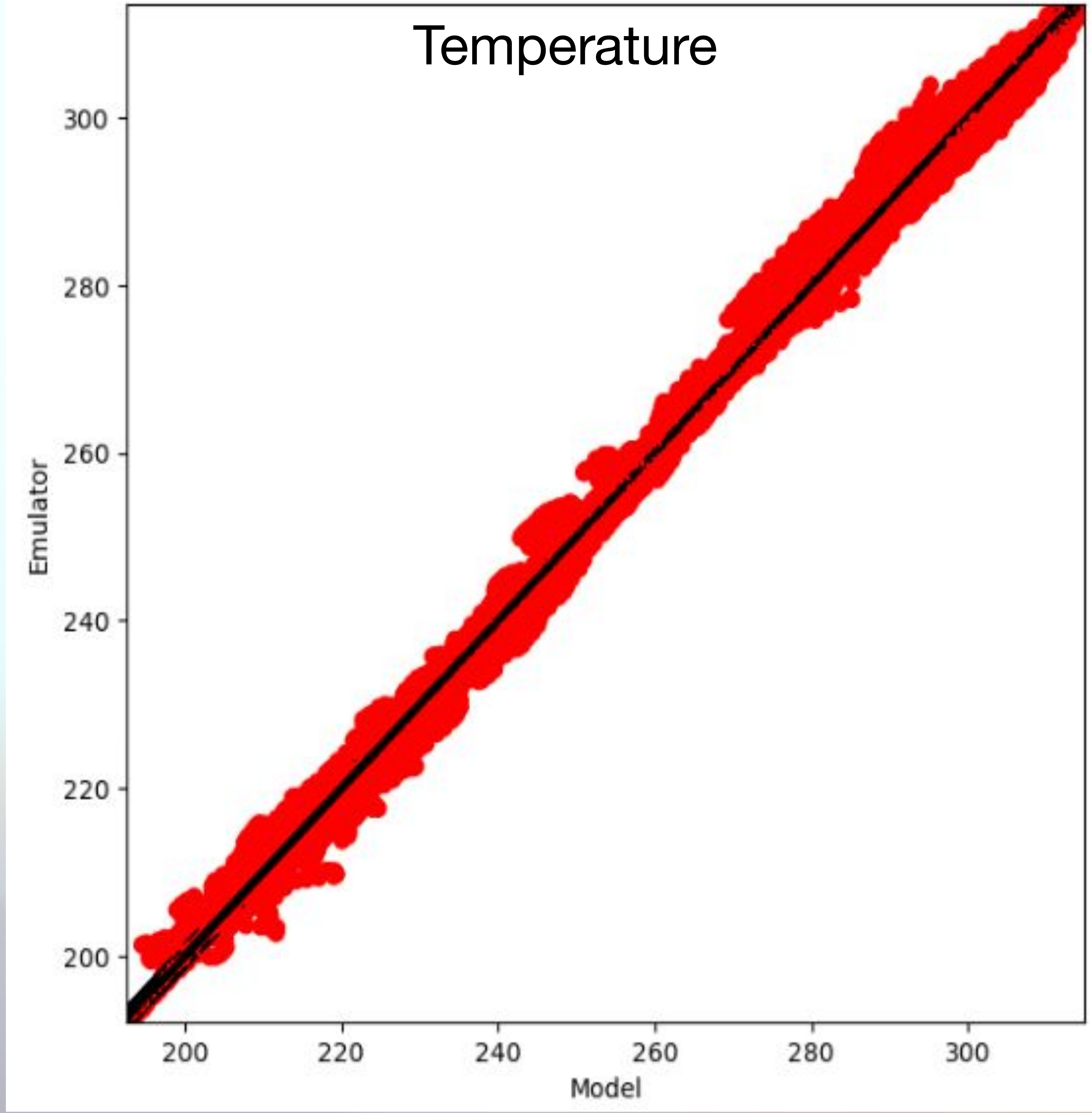
$$log(r) = log(p\left(Y^0|Y'\right)) + log(p(\theta')) - log(p\left(Y^0|Y\right)) - log(p(\theta)) \tag{5}$$

Note, that for this implementation the distance metric ρ must be cast as a probability distribution with values [0, 1]. We therefore assume that this discrepancy can be approximated as a normal distribution centred about zero, with standard deviation equal to the sum of the squares of the variances as described in Eq. 3:

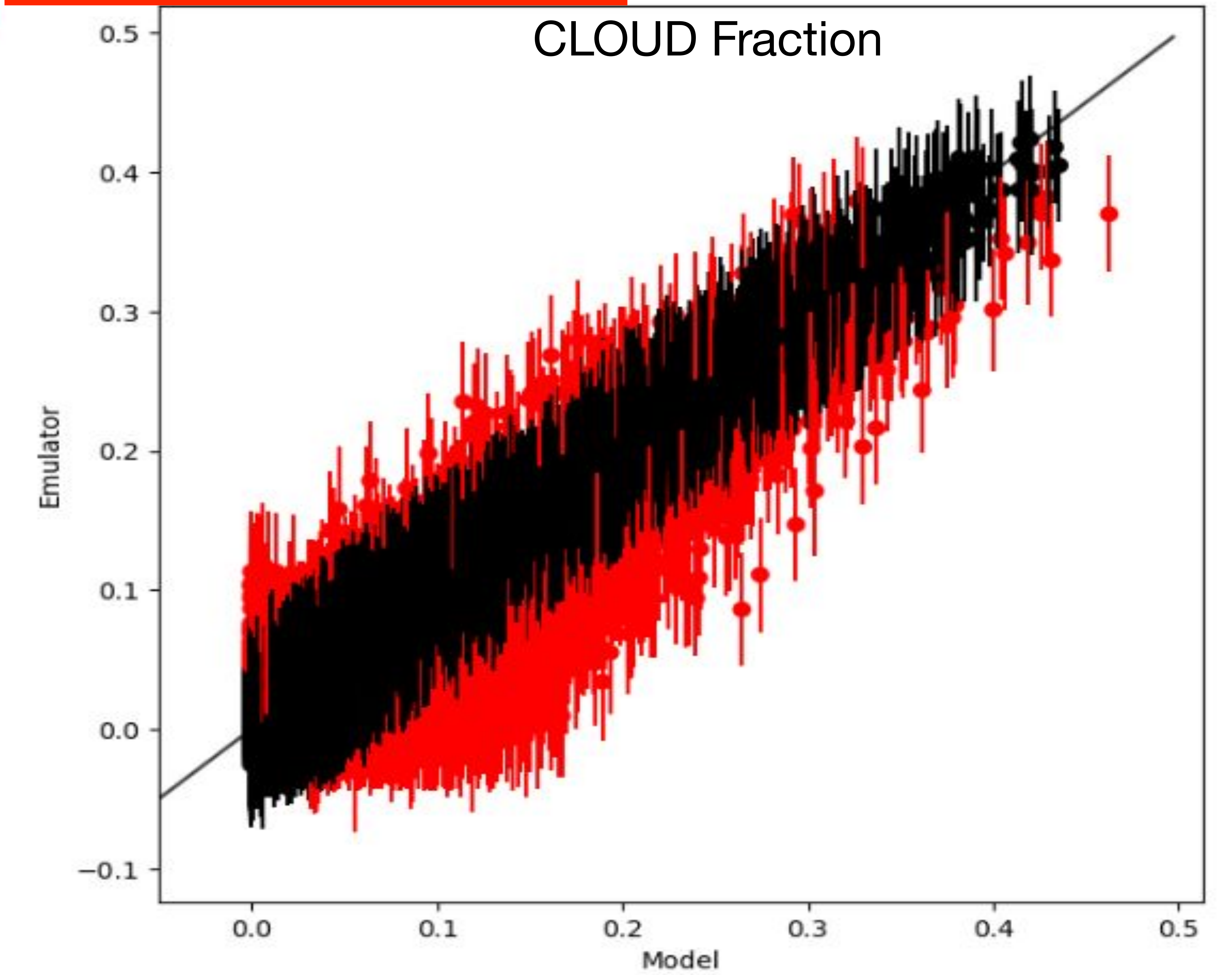
$$p\left(Y^0|Y\right) \approx \frac{1}{\sigma_t\sqrt{2\pi}}e^{-\frac{1}{2}\left(\frac{Y^0-Y}{\sigma_t}\right)^2}, \quad \sigma_t = \sqrt{\sigma_E^2 + \sigma_Y^2 + \sigma_R^2 + \sigma_S^2} \tag{6}$$

Results: Validation of GP

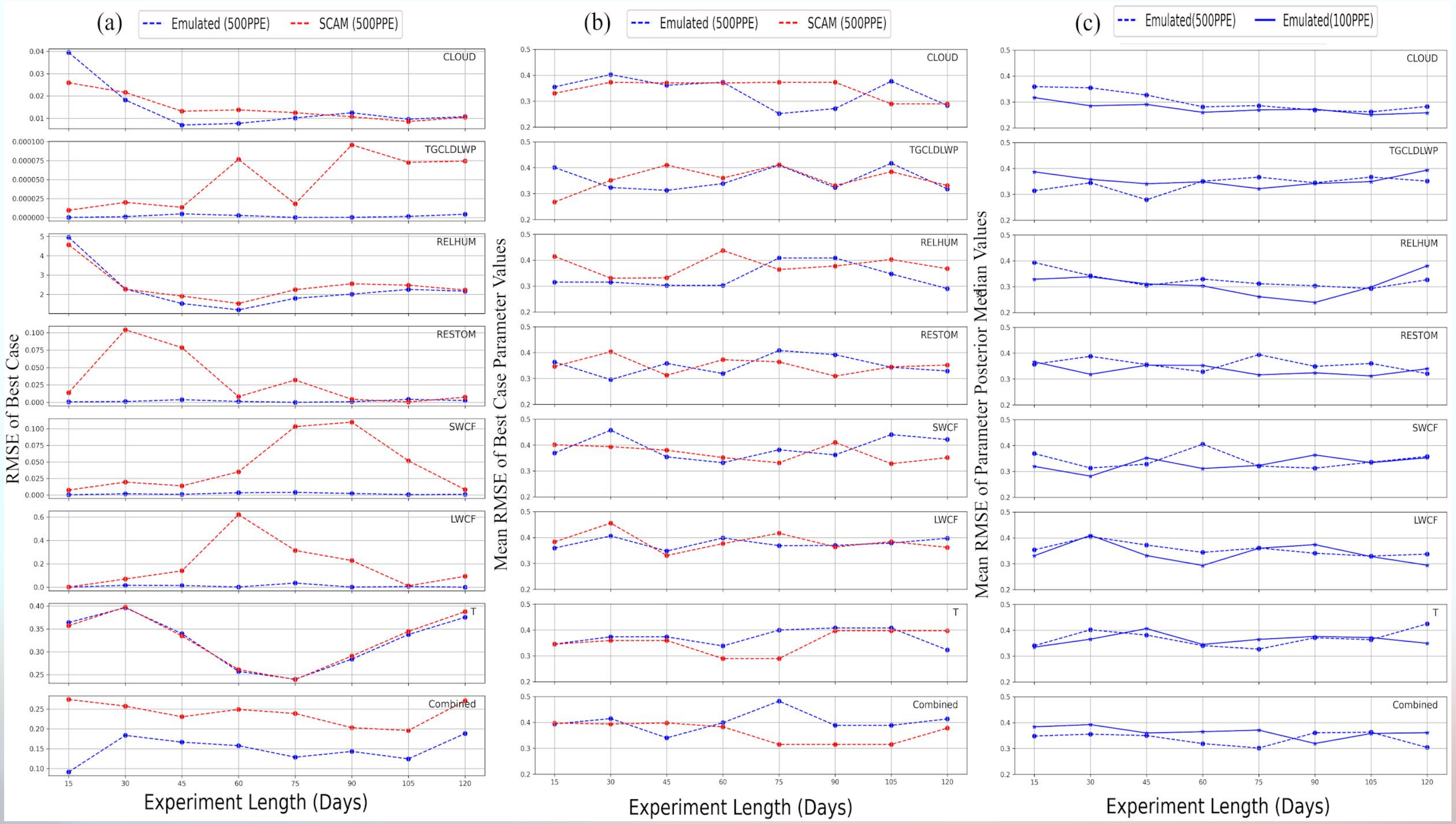
Proportion of 'Bad' estimates : 7.45%



Proportion of 'Bad' estimates : 9.11%

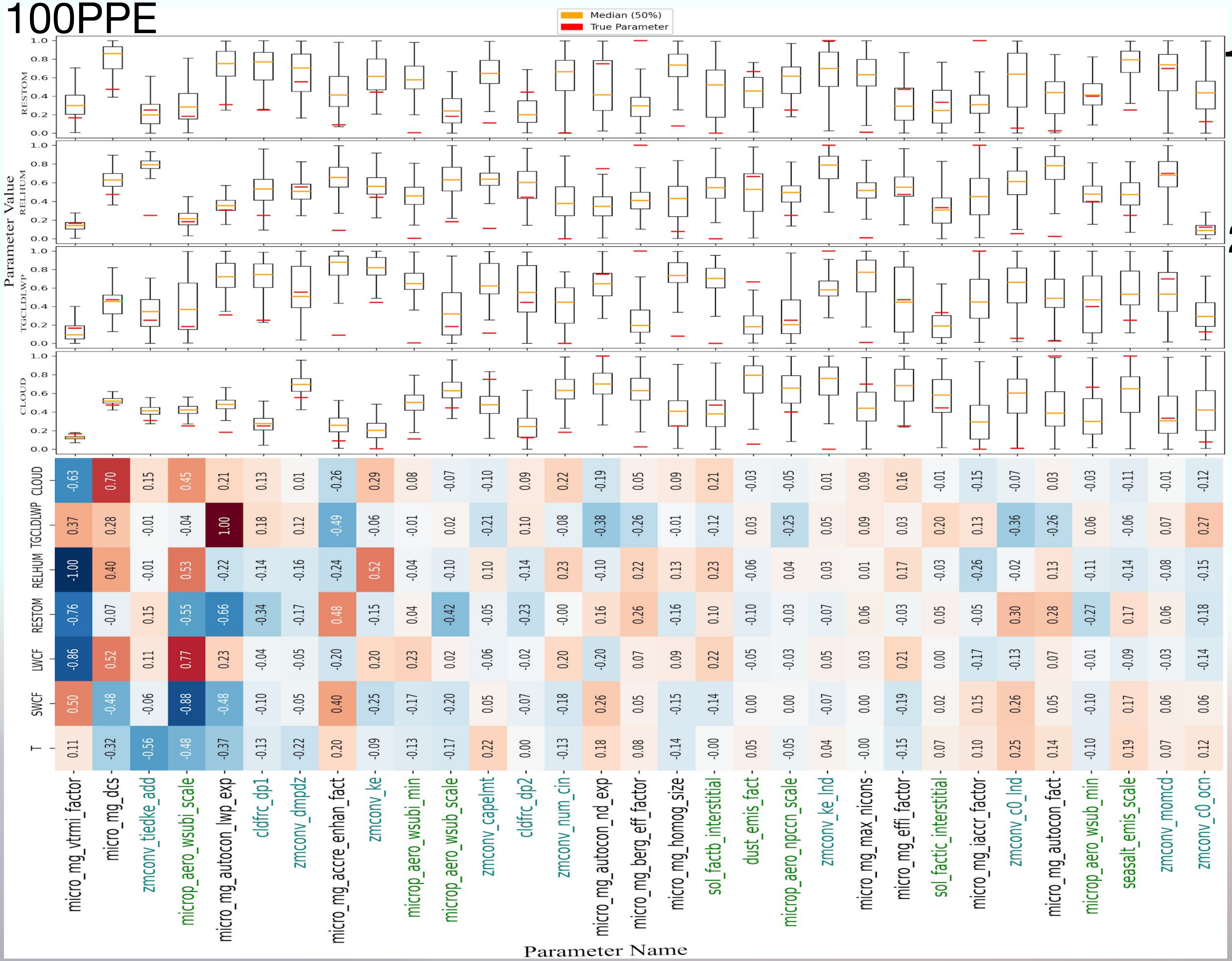


Results: Observation Requirement



Probabilistic Calibration: Normalized Posterior Distribution

100PPE



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