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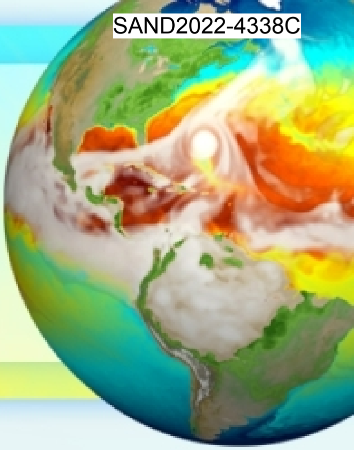

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E3SM Atmosphere surrogate construction and calibration using machine learning and reduced order modeling

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E3SM Energy Exascale Earth System Model

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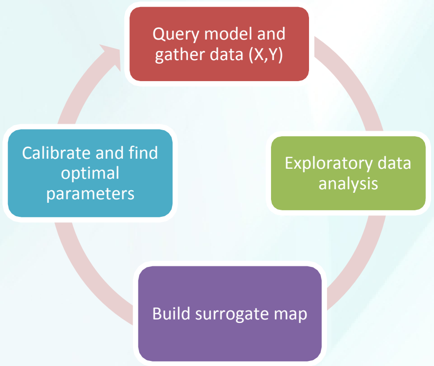
Motivation: Tuning is arbitrary, expensive, and time consuming

Expert manual tuning	Automated tuning (goal)
Time-consuming (6-12 months)	Less than 6-12 months
Deterministic: one set of “tuned” parameters per model release	Probabilistic: a distribution of parameters per model release OR observational target
Non-reproducible	Reproducible
Computationally expensive	Computationally expensive (upfront only)

Motivation and setup

- To expedite and formalize E3SM tuning *in parallel with model development* we want:
  - A method to identify
    - an optimal parameter set
    - a distribution of likely parameter sets
  - A practical number (10's-100's) of E3SM forward simulations, as short in duration as possible
- For intuition into how E3SM parameters affect climate, and for personalization of cost functions by the user we want:
  - A surrogate model for spatial fields
- In our first pass at balancing these competing goals we chose **5** uncertain E3SM parameters and performed **250 10-year** E3SM simulations

E3SMv2 simulations



Ensemble	Res.	Config.	# Simulations	Yrs.	Nodes per bundle	Sims. per bundle	SYPD per bundle
Ultra-low resolution (ULR)*	~7.5°	F2010	500	10	100	50	5100
Low resolution (LR)	~1°	F2010	250	10	100	10	95

*E3SM ULR is not tuned or scientifically validated

E3SMv2 sampled atm. parameters and observational targets

E3SM Parameters

Parameter	Description	Low-Default-High [1]
clubb_c1	Constant for dissipation of variance of mean(w'²)	1.0__**1.335**__5.0
clubb_gamma_coef	Constant of the width of PDF in w coordinate	0.1__**0.32**__0.5
zmconv_tau	Time scale for consumption rate deep CAPE	1800__**3600**__14400
zmconv_dmpdz	Parcel fractional mass entrainment rate	-2.0e-3__**-0.7e-3**__-0.1e-3
micro_mg_ai	Fall speed parameter for cloud ice	350__**500**__1400

[1] Qian et al., 2018

Target Fields

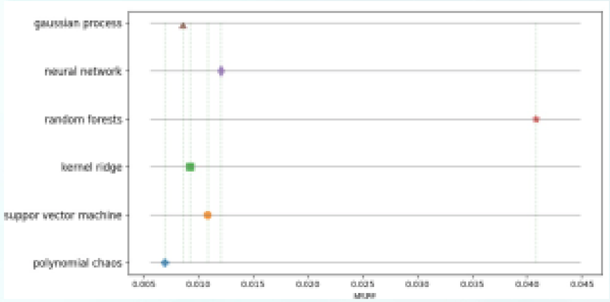
Field	Coordinates	Size ULR	Size LR
TREFHT	lat x lon	24x48	24x48, 180x360
PRECT	lat x lon	24x48	24x48, 180x360
SWCF	lat x lon	24x48	24x48, 180x360
LWCF	lat x lon	24x48	24x48, 180x360
PSL	lat x lon	24x48	24x48, 180x360
FLNT	lat x lon	24x48	24x48, 180x360
FSNT	lat x lon	24x48	24x48, 180x360
Z500	lat x lon	24x48	24x48, 180x360
U200	lat x lon	24x48	24x48, 180x360
U850	lat x lon	24x48	24x48, 180x360
RELHUM	**lat x lev**	**24x37**	**24x37, 180x37**
T	**lat x lev**	**24x37**	**24x37, 180x37**
U	**lat x lev**	**24x37**	**24x37, 180x37**

Surrogate construction

- Sample EAM parameters (Latin hypercube, Dakota)
  - Compute 5yr and 10yr climatologies for 13 spatial fields, i.e. the "target space"

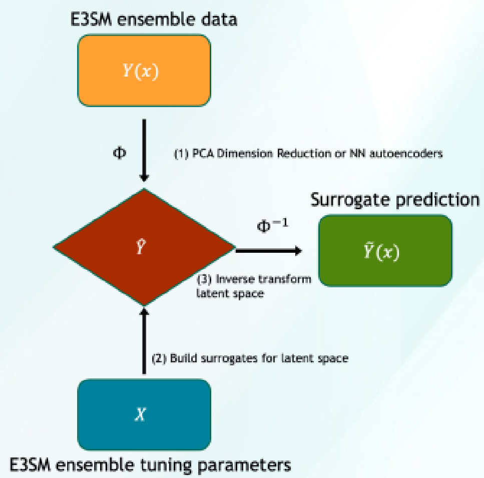
Weeks on HPC

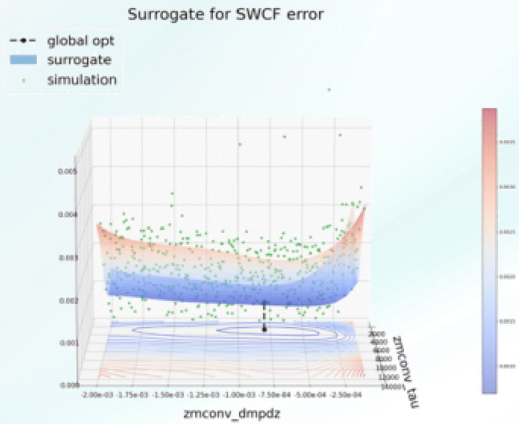
- Dimension reduction (PCA) on the target spaces
  - PCA all fields together (top 16 components)
- Fit reduced space using ML method



- Inverse transform latent space to surrogate prediction for each field

Minutes on laptop





Calibration

$$\mathrm{MSE}_{\mathrm{scaled}}(\boldsymbol{x}) = \frac{\sum_{i,j=1}^{N,M} (Y_{ij}^{\mathrm{sur}}(\boldsymbol{x}) - Y_{ij}^{\mathrm{obs}})^2}{\sum_{i,j=1}^{N,M} (Y_{ij}^{\mathrm{obs}} - \bar{Y}^{\mathrm{obs}})^2}$$

N=lat; *M*=lon

Spatial variance of the observed field [1]

$$\mathrm{BMSE}_{\mathrm{scaled}}^{k}(\boldsymbol{x}, \sigma_k) \propto \frac{1}{2\sigma_k^2} \frac{\sum_{i,j=1}^{N,M} (Y_{ijk}^{\mathrm{sur}}(\boldsymbol{x}) - Y_{ijk}^{\mathrm{obs}})^2}{\sum_{i,j=1}^{N,M} (Y_{ijk}^{\mathrm{obs}} - \bar{Y}_k^{\mathrm{obs}})^2} + \mathrm{penalty}(\sigma_k)$$

Noise (between surrogate and obs.) = $N(0, \sigma_k^2)$

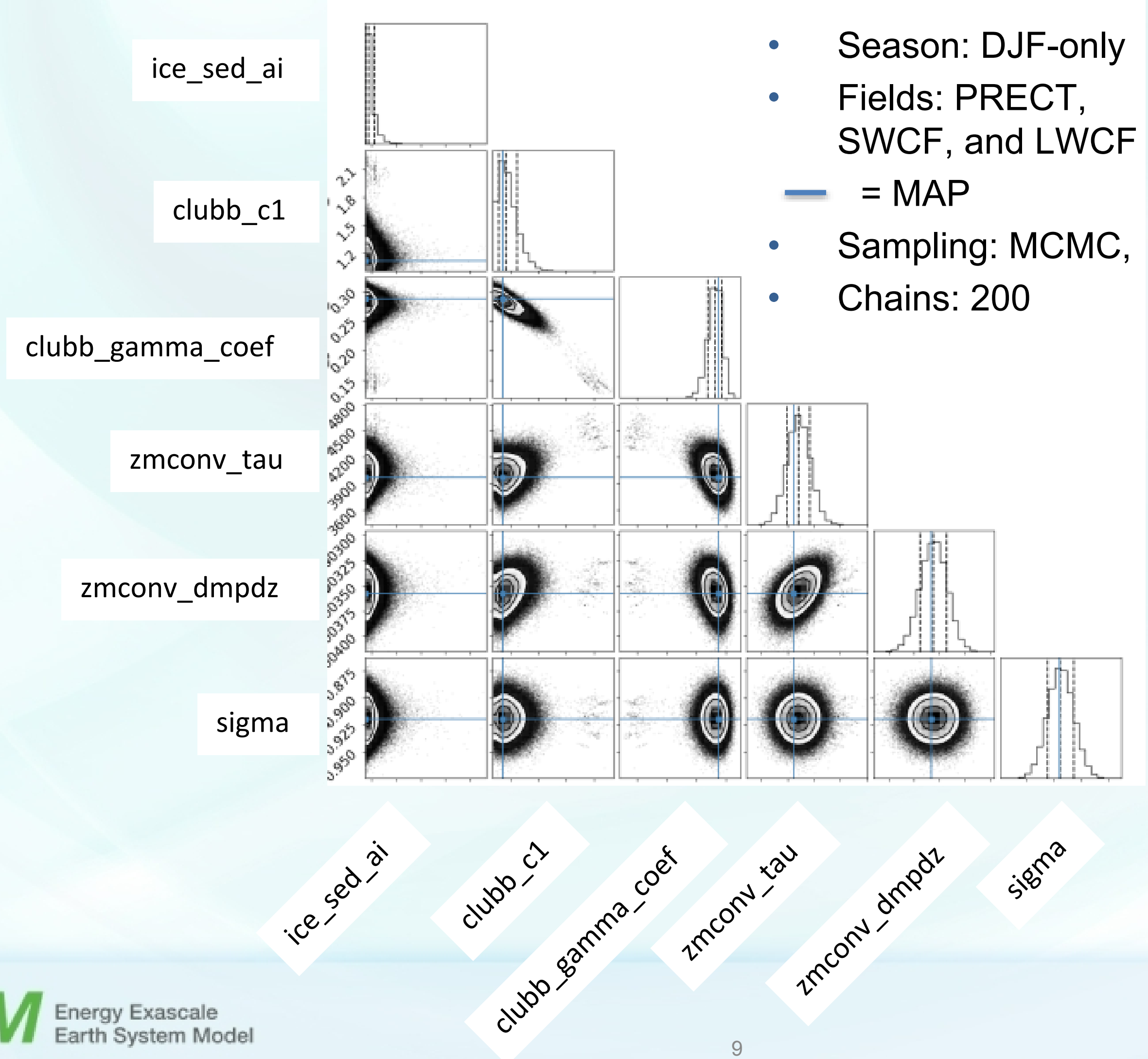
MAP (deterministic): Quasi-Newton gradient-based solver with different starting points.

$$\boldsymbol{x}_{\mathrm{multi}}^{*} = \mathrm{argmin}_{\boldsymbol{x}, \sigma_1, \ldots, \sigma_K} \sum_{k=1}^{K} \mathrm{BMSE}_{\mathrm{scaled}}^{k}(\boldsymbol{x}; \sigma_k)$$

1. Pierce et al., 2009; Fletcher et al., 2021

Calibration

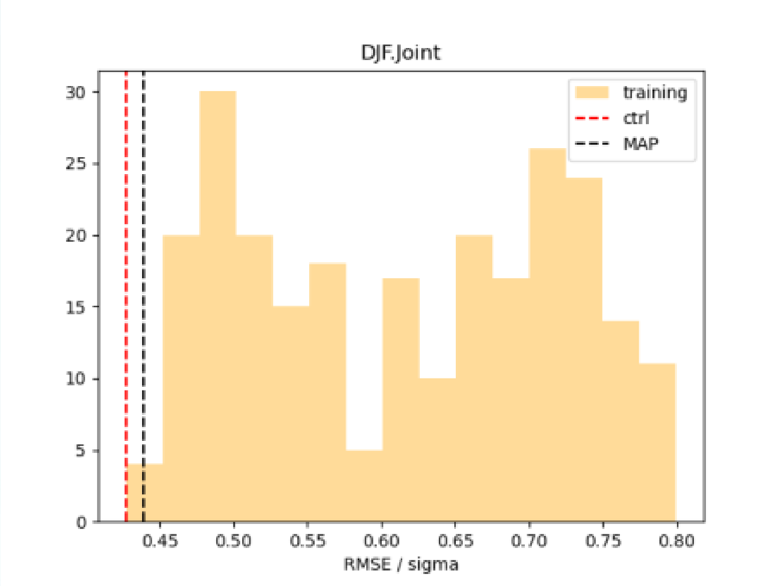
$$x^*_{\mathrm{MMAP}} = \mathrm{argmin}_{x,\sigma_1,\ldots,\sigma_K} \sum_{k=1}^{K} \mathrm{BMSE}^k_{\mathrm{scaled}}(x;\sigma_k)$$



- Season: DJF-only
- Fields: PRECT, SWCF, and LWCF
- — = MAP
- Sampling: MCMC,
- Chains: 200

How important are surrogate errors?

- Surrogate errors are large enough to significantly affect the MAP estimate for the 24x48 surrogate.
  - Parameter sets that are predicted to outperform the default often do not.
- For 250 samples and 10-year simulations, the zonal-mean surrogates show more potential.



An E3SM simulation using the surrogate-predicted MAP parameters (black line) for DJF LWCF, SWCF, and PRECIP unexpectedly fails to beat the default tuning (red line).

Surrogate fit to 250 E3SM simulations (training data)

	Zonal mean	24x48 lat x lon
5-yr E3SM climo.	R^2=0.817	R^2=0.502
10-yr E3SM climo.	R^2=0.874	R^2=0.624

Zonal mean surrogates for 5-year climatologies are even more accurate than full-field surrogates for 10-year climatologies.

Validating alternative parameter sets

- Alternative parameter sets cause small changes to persistent biases
  - Structural bias AND insufficient # of perturbed parameters.
- DJF-tuned multi-target parameter sets actually show degradation in DJF precip.

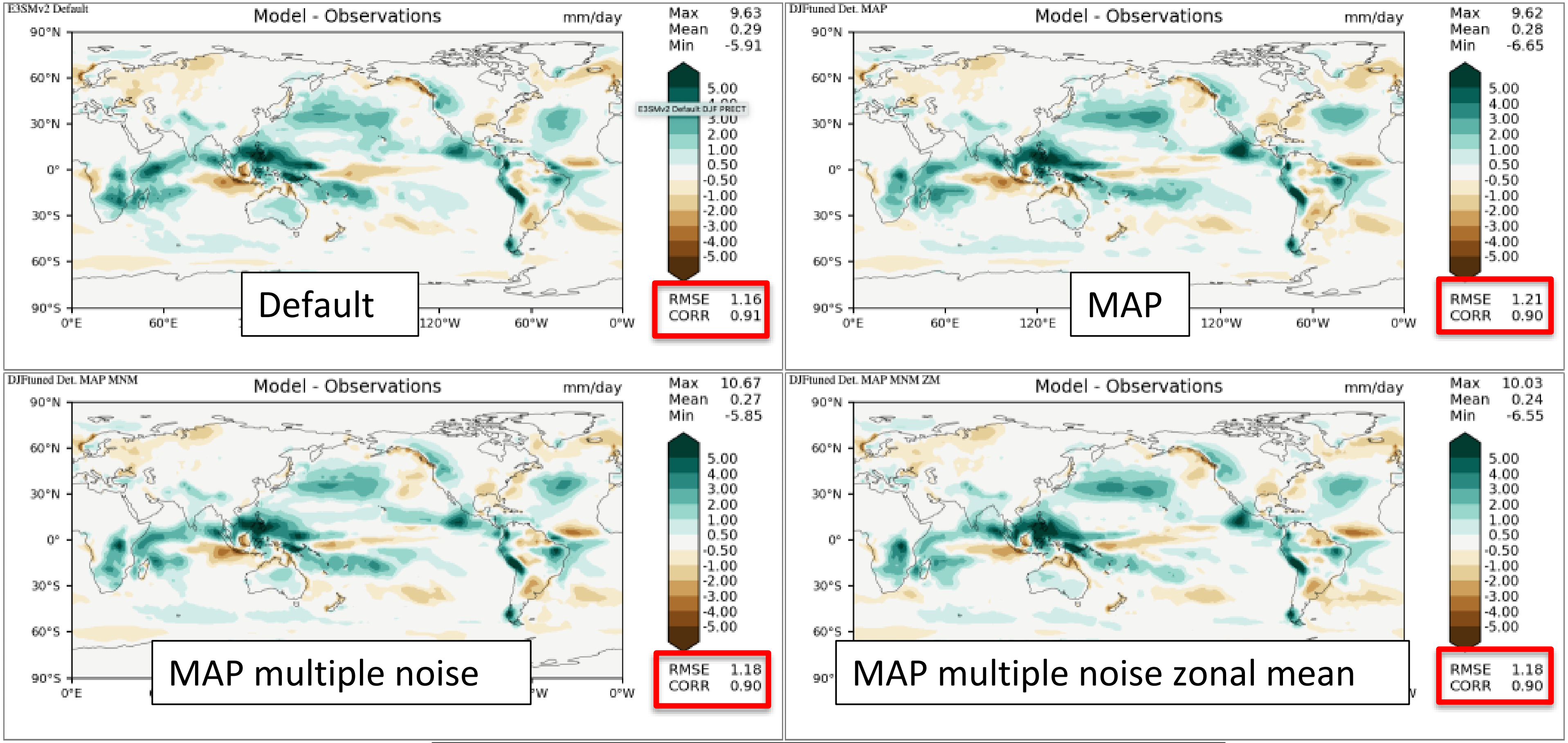


Fig. DJF precip. minus observations

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Validating alternative parameter sets

- Encouraging: **DJF**-tuned multi-target parameter sets show robust improvement in annual-mean precipitation, driven by a much better **JJA** precipitation field.

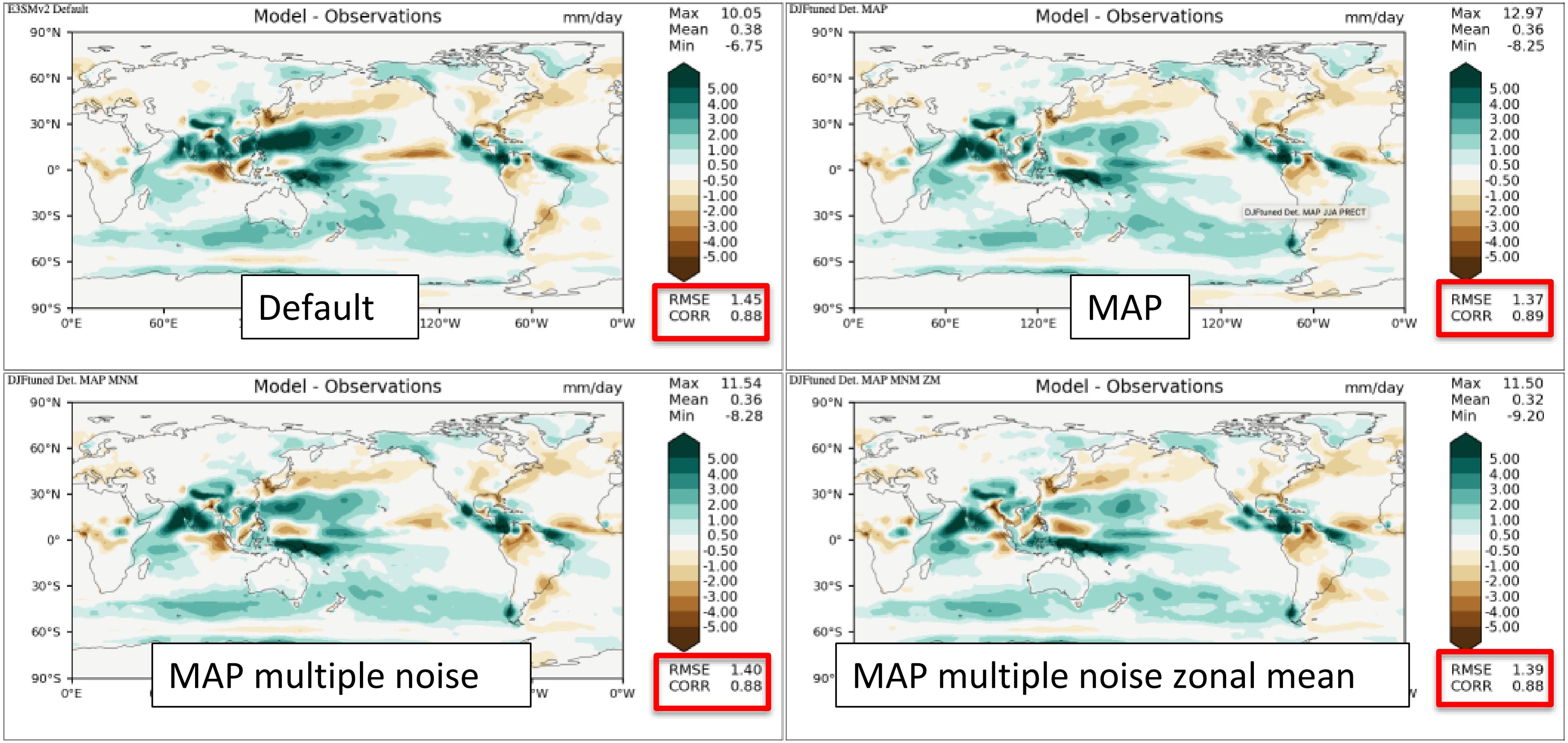

Fig. JJA precip. minus observations

Conclusions and Discussion

- Given 5 uncertain parameters, 250 simulations, and 10-year climatologies:
  - We can reliably predict high-performing models, but not an “optimal” model using 24x48 lat x lon surrogates
  - Zonal-mean surrogates better predict the training data
    - Preliminary results show that their full-field realizations in E3SM also perform well
  - Future work focuses on zonal mean, or even emulating the global mean RMSE
  - Fast surrogate creation (Kenny Chowdhary) may facilitate creating surrogates for any cost function, decreasing the incentive to make surrogates for model fields
- > 5 uncertain parameters may be needed to significantly improve on the default simulation

Next steps

- Combine seasons and n=13 target fields
- Deal with effective sample size
  - Affects posterior distributions of E3SM parameters
- Software development for end-to-end automated tuning with optional expert customization of cost function

References and Acknowledgements

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Surrogate construction using Kenny Chowdhary's "tesuract" software: https://github.com/kennychowdhary/tesuract

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Extra slides