



PennState

Experimenting with machine learning hindcast emulators to help tune CAM (a.k.a wherein I attempt "scikit-learn for dummies")

Colin Zarzycki (@weatherczar) 
+ others!





[MomentumCPT]

- Two primary core code-level improvements...
 - Directly prognosing momentum flux evolution in CLUBB

$$\frac{\partial \overline{u'_h w'}}{\partial t} = \underbrace{-\overline{w} \frac{\partial \overline{u'_h w'}}{\partial z}}_{ma} - \underbrace{\frac{1}{\rho_s} \frac{\partial \rho_s \overline{w'^2 u'_h}}{\partial z}}_{ta} - \underbrace{\overline{w'^2} \frac{\partial \overline{u_h}}{\partial z}}_{tp} - \underbrace{\overline{u'_h w'} \frac{\partial \overline{w}}{\partial z}}_{ac} + \underbrace{\frac{g}{\theta_{vs}} \overline{u'_h \theta'_v}}_{bp} \\ - \underbrace{\frac{C_6}{\tau} \overline{u'_h w'}}_{pr1} + \underbrace{C_7 \overline{u'_h w'} \frac{\partial \overline{w}}{\partial z}}_{pr2} - \underbrace{C_7 \frac{g}{\theta_{vs}} \overline{u'_h \theta'_v}}_{pr3} + \underbrace{C_7 \overline{w'^2} \frac{\partial \overline{u_h}}{\partial z}}_{pr4} \\ + \underbrace{\frac{\partial}{\partial z} \left[(K_{w6} + \nu_6) \frac{\partial \overline{u'_h w'}}{\partial z} \right]}_{dp1}$$

Larson (2020), Guo et al., (2021), Nardi et al., (2022)

- Defining a “regime-specific” eddy timescale formulation

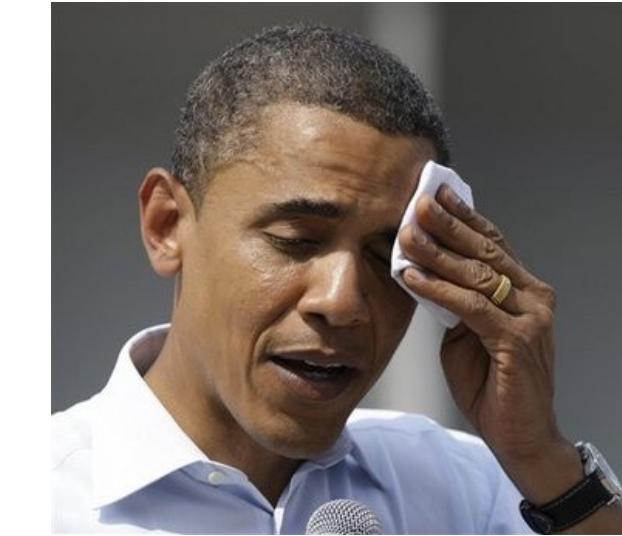
$$L_{scale} = \tau \sqrt{TKE}$$

$$\frac{1}{\tau} = \underbrace{\frac{C_{\tau,back}}{\tau_{ref}}}_{1} + \underbrace{C_{\tau,sfc} \left(\frac{u^*}{K} \right) \left(\frac{1}{z - z_s + z_{dis}} \right)}_{2} + \underbrace{C_{\tau,shear} \left(\left(\frac{\partial u}{\partial z} \right)^2 + \left(\frac{\partial v}{\partial z} \right)^2 \right)^{\frac{1}{2}}}_{3} + \underbrace{C_{\tau,N} \sqrt{\max(N^2, 0)}}_{4}$$



[MomentumCPT]

Parameter	EAM-def	EAM-taus
C1 = C1b	1.335	–
C14	1	–
C2rt = C2thl	1.75	–
C2rtthl	2.275	–
C6rt = C6thl	4	–
C6rtb = C6thlb	6	–
C6rtc = C6thlc	1	–
C6rt_Lscale0	14	–
C6thl_Lscale0	14	–
wpxp_L_thresh	60	–
C8	4.3	0.5
C11	0.8	0.5
C11b	0.35	0.5
C11c	0.5	–
gamma_coef	0.32	0.3
gamma_coeffb	0.32	0.3
beta	1	2
C_{itsfc}	–	0.3
$C_{itshear}$	–	0.15
C_{itbknd}	–	1.5
C_{itN}	–	0.65
$C_{itN,clr}$	–	2.0
z_s	–	300 m
$C_{irwpxpRi}$	–	3
$C_{lxpx2Ri}$	–	1
$z_{displace}$	–	10 m
N_{thresh}^2	–	3.3E-4



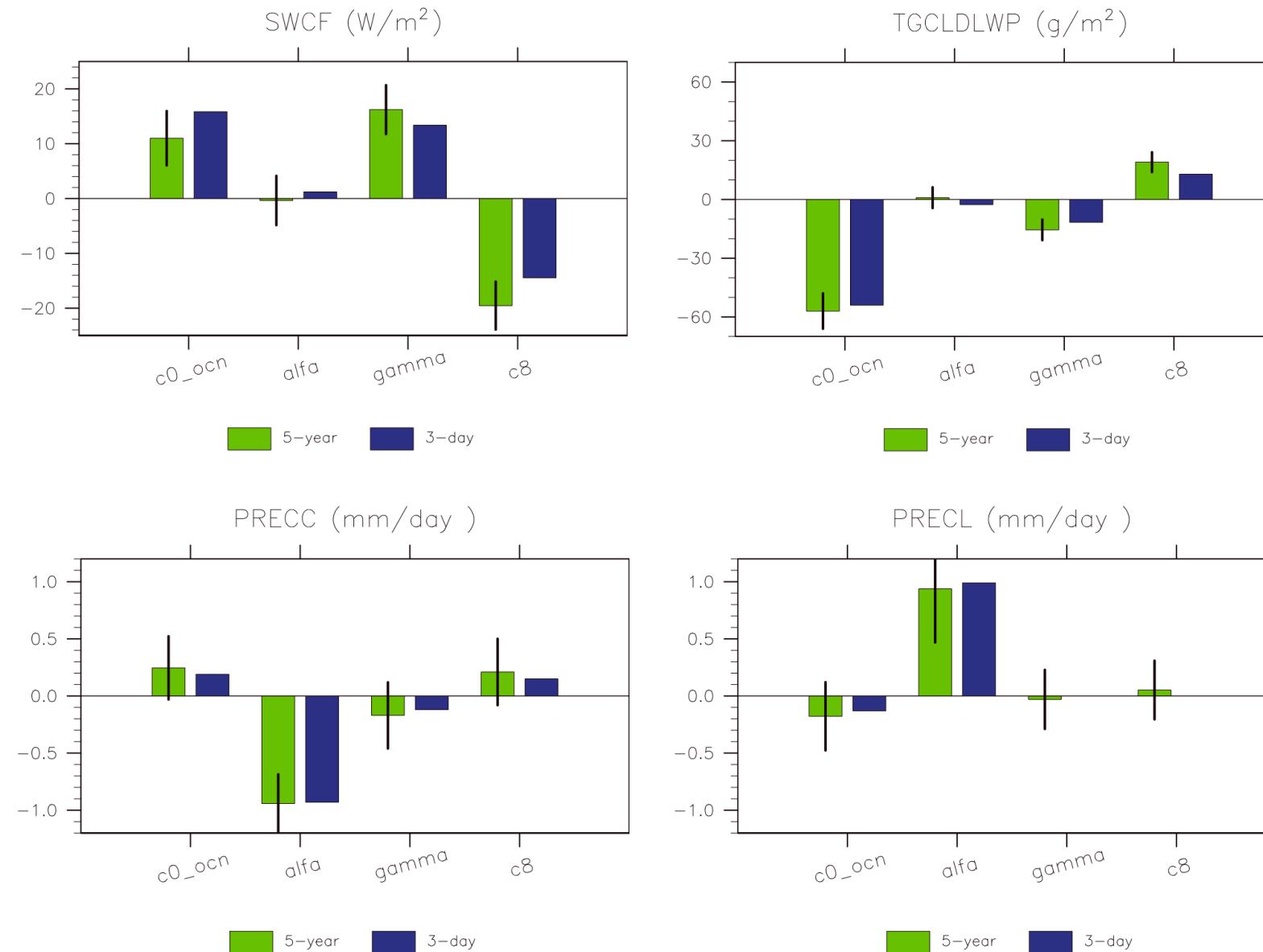
Trade ~10 parameters, **no added DoFs to CLUBB's tunable parameter set**

More “control” over momentum fluxes -> more **interpretable** from a process-oriented standpoint



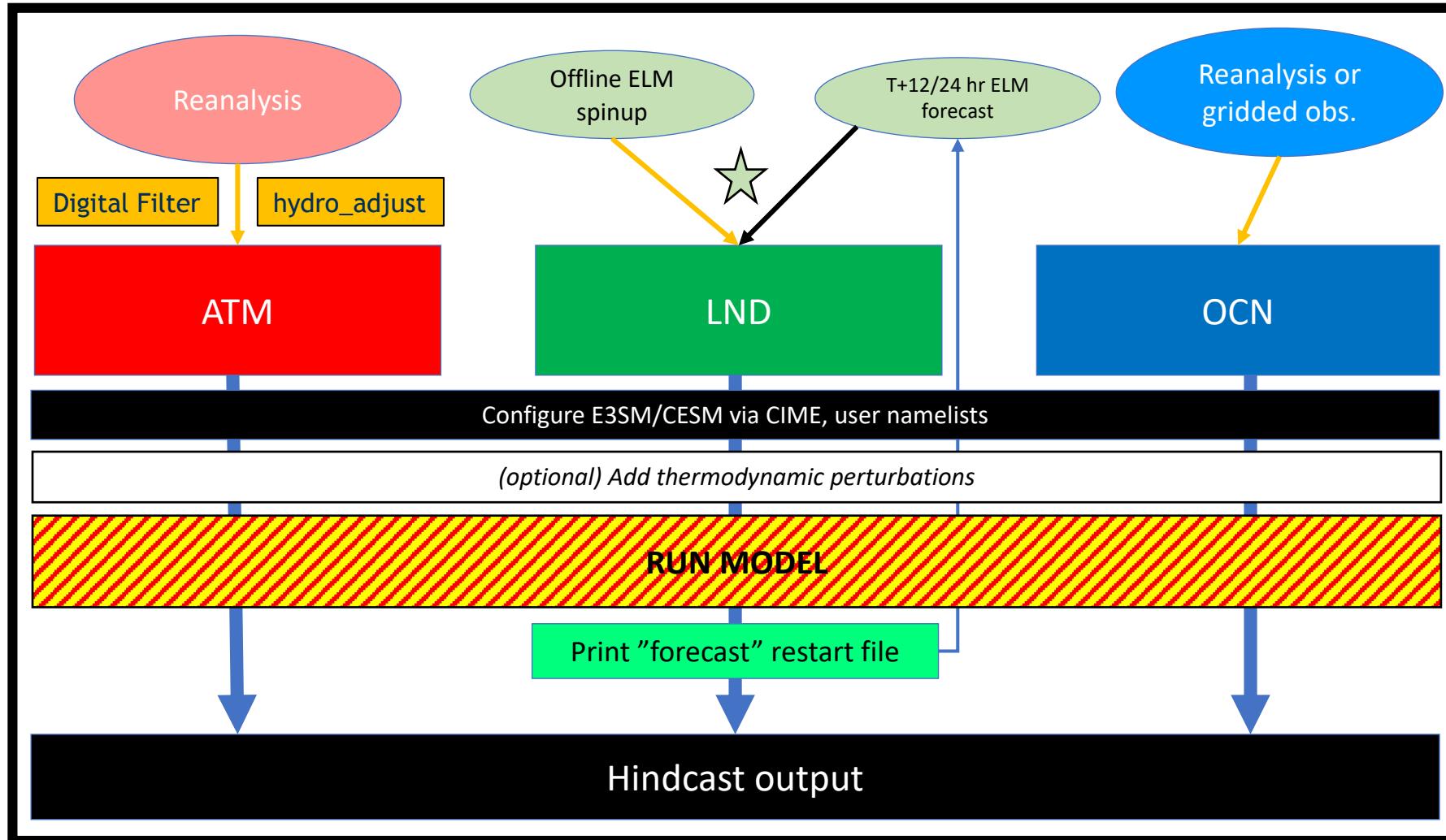
Using short-term simulations to predict long-term response

3-day run
5-year run



Betacast: hindcast support for CESM

<https://github.com/zarzycki/betacast>





The process?

Generate set (P) of parameter inputs and ranges

```

lubb_C_invs_tau_bkgnd,0.1,5.0
clubb_C_invs_tau_sfc,0.01,2.0
clubb_C_invs_tau_shear,0.01,2.0
clubb_C_invs_tau_N2,0.005,1.0
clubb_gamma_coef,0.1,0.9
clubb_gamma_coeffb,0.1,0.9
clubb_c11,0.1,0.9
clubb_c11b,0.1,0.9
clubb_c8,2,8
clubb_beta,1.0,3.0
clubb_c_uu_shr,0,1
clubb_c_uu_buoy,0,1
clubb_c_invs_tau_n2_clear_wp3,
clubb_c_invs_tau_n2_wp2,0,1.2
clubb_c_invs_tau_n2_xp2,0,0.7
clubb_c_invs_tau_n2_wpxp,0,0.05
clubb_c_invs_tau_wpxp_ri,0,1.0
clubb_altitude_threshold,25.0,1000.0
clubb_up2_sfc_coef,0,10
zmconv_tau,1800.,14400.
zmconv_ke,0.5e-6,10.0e-6
zmconv_c0_ocn,0.001,0.008
se_nu,0.20e15,1.0e15

```

P = 23

Generate LHS sample of size Z

```

# Do LHS calculations
sampler = qmc.LatinHypercube(d=num_vars)
#optimization="random-cd" added in 1.8.0
#sampler = qmc.LatinHypercube(d=num_vars, optimization="random-cd")
sample = sampler.random(n=num_samples)
scaled_sample = qmc.scale(sample, l_bounds, u_bounds)

```

Z = 1200

Resulting set of combinations (P lines, N columns)

```

2.235948e+00,1.554339e-02,1.952923e-01,9.122890e-01,2.279078e-01,5.576333
+02,4.783025e+00,5.193065e+03,4.999672e-06,4.165975e-03,3.956101e+14
3.534685e+00,1.608991e+00,5.220681e-01,9.069053e-01,4.120342e-01,3.70315
+02,5.741669e+00,3.907741e+03,7.819348e-06,5.576695e-03,9.961181e+14
1.705845e+00,3.213369e-01,1.386629e+00,4.559371e-01,8.768336e-01,4.25828
+02,5.133134e+00,1.380007e+04,9.195500e-06,7.161500e-03,7.955536e+14
2.072631e-01,1.503143e+00,2.491256e-02,4.590301e-01,1.559282e-01,2.09377
+02,2.995484e-01,2.404167e+03,2.502762e-06,5.110206e-03,7.337338e+14
1.130345e+00,9.305662e-01,1.616388e+00,9.387361e-02,2.904719e-01,7.20795
+02,1.640975e+00,5.032015e+03,7.666990e-06,7.470773e-03,7.911111e+14
1.679859e+00,1.175868e+00,9.201679e-01,9.885945e-01,8.134322e-01,8.04374
+02,5.218515e+00,1.051964e+04,8.461415e-06,3.343271e-03,6.808574e+14
9.343254e-01,4.103287e-01,8.032468e-01,1.136831e-01,4.711610e-01,6.30015
+02,9.459529e+00,3.936652e+03,6.452451e-06,6.152243e-03,7.255034e+14
2.281685e+00,1.522456e+00,5.030232e-02,8.805720e-01,7.752457e-01,2.15028
+02,4.948609e+00,3.441481e+03,9.873246e-06,7.043738e-03,4.584735e+14
@
"param_values.csv" 1200L, 358800B

```

Each line is a single set of parameters to pass in via user_nl_cam



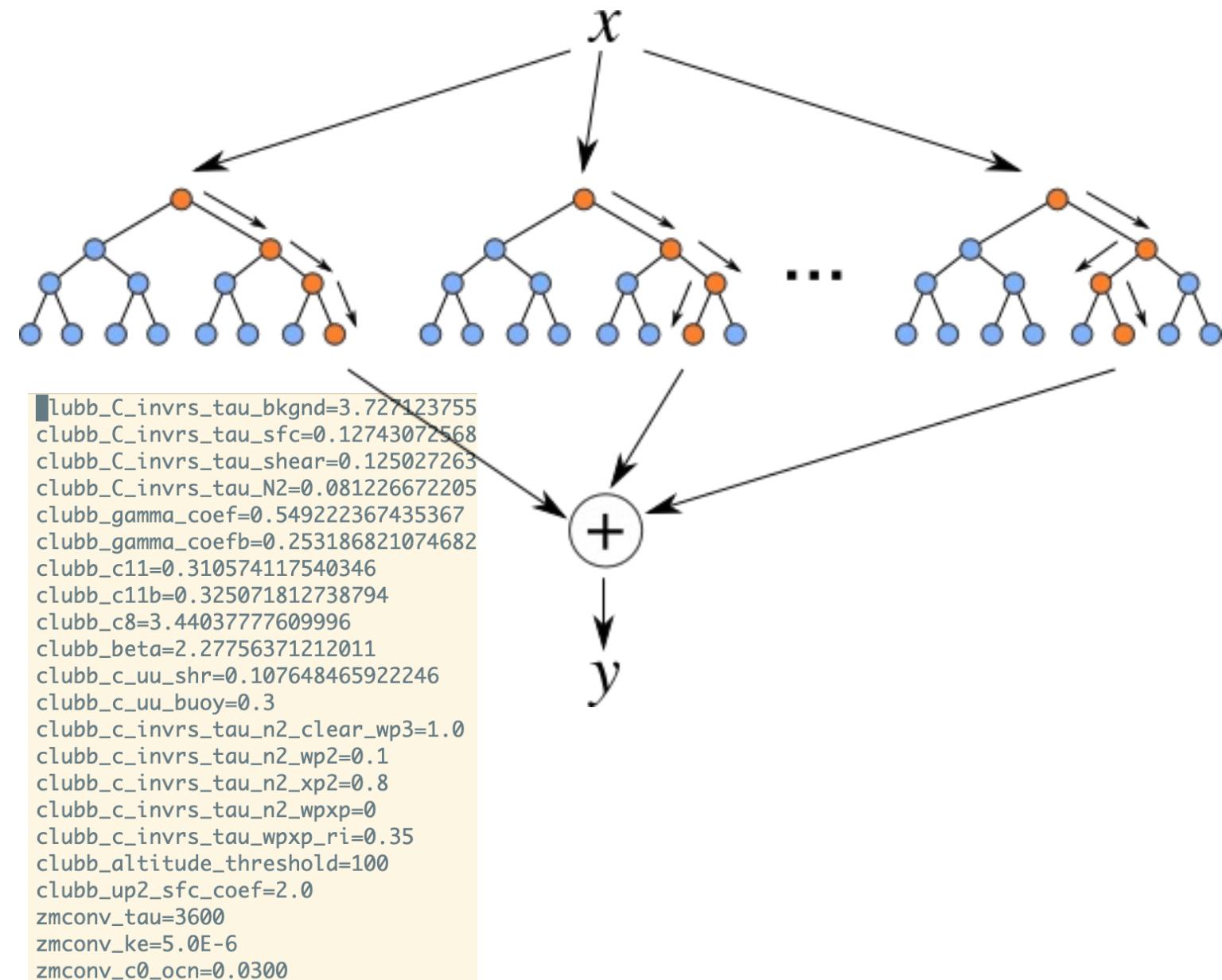
The mechanics?

- Pick N_inits (6, JMMJSON) that each run for D (3) days
- So we have $Z * N_{\text{inits}} = 7,200$ simulations to run
- Parallelize on Cheyenne, not so bad! ~3-4 "real" days if spread out across 20 jobs
- Average output fields +24-36 hours for climate metrics, compute anomaly relative to reference (i.e., benchmark)
 - Currently aggregating to 5x5 grid boxes, although more of a practicality
 - Results in 1200 "outputs" which are $n_{\text{lat}} \times n_{\text{lon}}$ array for each CAM variable ($1200 \times 2263 = 2.7\text{M}$ points)



The tool?

- Train output "vectors" (flattened 2-D arrays) using *random forest regressor*
- Model can be run with user editing a `user_nl_cam` (i.e., x vector)
- Model predicts *anomaly* vector relative to *reference*
- Reshape back to 2-D array for analysis!



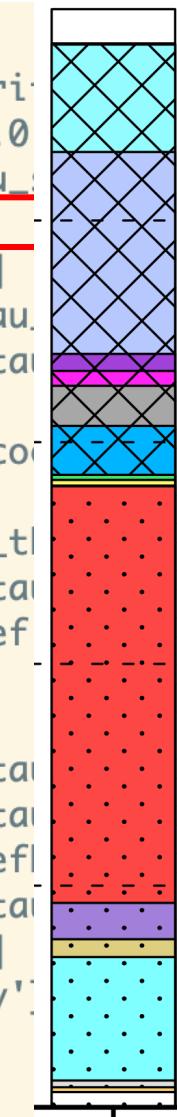


Interpretable: what is important in making a prediction?

Qian et al., 2018

CLDLOW	RF	PRECT
{'bootstrap': True, 'max_depth': 0.0, 'criterion': 'squared_error', 'min_impurity_decrease': 0.0, 'min_weight_fraction_leaf': 0.0, 'n_estimators': 200, 'random_state': 0.21145597135218605}	['clubb_C_invs_tau_shear']	
0.12463443474785157	['clubb_c8']	
0.12342257234142996	['clubb_c_uu_shr']	
0.07391954146511641	['clubb_gamma_coef']	
0.06919068386443027	['clubb_c_invs_tau_n2_xp2']	
0.0577467637024121	['clubb_c_invs_tau_n2_wp2']	
0.05464471274454084	['clubb_up2_sfc_coef']	
0.049369764776027704	['clubb_c11b']	
0.030048289208605573	['clubb_c11']	
0.02360788463659788	['clubb_C_invs_tau_N2']	
0.022327059578247193	['clubb_C_invs_tau_sfc']	
0.018762494092775136	['clubb_gamma_coeff']	
0.018036163351335226	['clubb_C_invs_tau_bkgnd']	
0.016158214378506144	['clubb_c_invs_tau_wpxp_ri']	
0.015510901361020353	['zmconv_tau']	
0.014994598952002312	['zmconv_c0_ocn']	
0.012494952361274148	['clubb_altitude_threshold']	
0.01215		
0.01075		
0.01035		
0.01030		
0.01012		
0.009995213743247003	['clubb_c_uu_buoy']	
MAE is 0.023259240956448914		

- Benefit of RF, training provides ranking of sensitivity
- See Kyle Nardi's talk later today



RF

RF	PRECT
{'bootstrap': True, 'max_depth': 0.0, 'criterion': 'squared_error', 'min_impurity_decrease': 0.0, 'min_weight_fraction_leaf': 0.0, 'n_estimators': 200, 'random_state': 0.3660887501511995}	['clubb_C_invs_tau']
0.23207146949825044	['zmconv_tau']
0.10274271767942769	['clubb_c_uu_shr']
0.03815391055362532	['clubb_C_invs_tau']
0.031082624577777974	['clubb_C_invs_tau']
0.019294462641779916	['zmconv_ke']
0.018479361177184808	['clubb_up2_sfc_coef']
0.017884228805207063	['clubb_c8']
0.014472660114623509	['clubb_altitude_tl']
0.013667826436264269	['clubb_C_invs_tau']
0.013630740292987121	['clubb_gamma_coef']
0.012188004150956996	['se_nu']
0.01162726859095599	['clubb_c11b']
0.011555666832940022	['clubb_c_invs_tau']
0.011453657677168197	['clubb_c_invs_tau']
0.011386226102659524	['clubb_gamma_coef']
0.011260959725820783	['clubb_c_invs_tau']
0.009707215903686292	['clubb_c_invs_tau']
MAE is 0.2078194178048861	PRECT



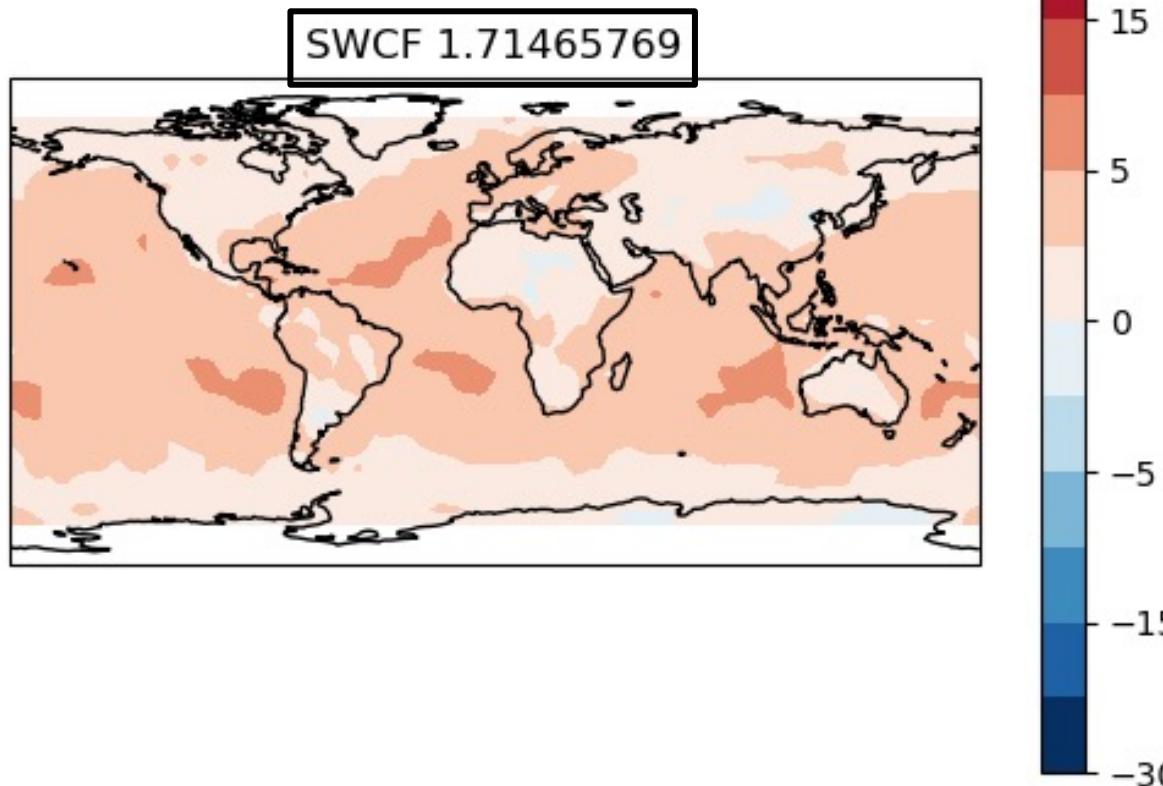
Reference -> perturbation

- Let's try changing a few things...
 - clubb_C_invs_tau_shear=0.1 (from 0.12)
 - clubb_gamma_coef=0.5 (from 0.55)
 - clubb_c8=2.8 (from 3.4)
 - clubb_c_uu_shr=0.5 (from 0.1)
 - clubb_c_invs_tau_n2_wp2=0.05 (from 0.1)
 - clubb_c_invs_tau_n2_xp2=2.0 (from 0.8)
 - clubb_altitude_threshold=20 (from 100)



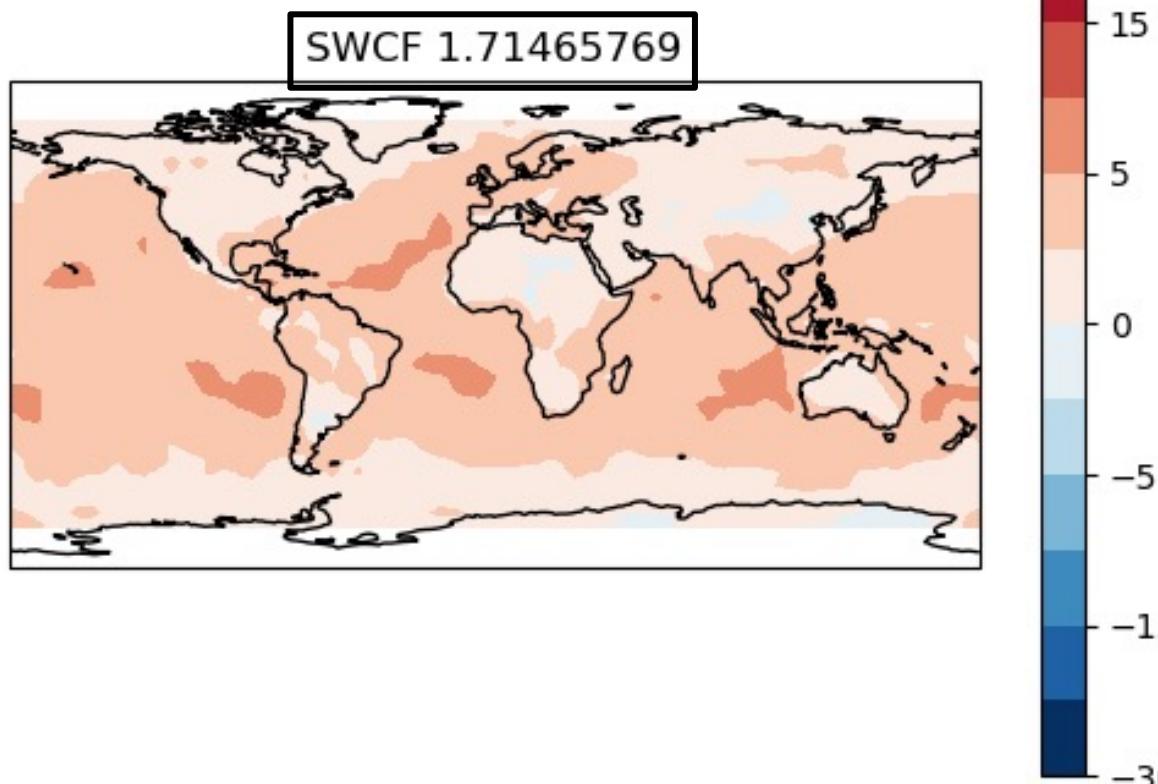
SWCF prediction

- Emulator predicts...

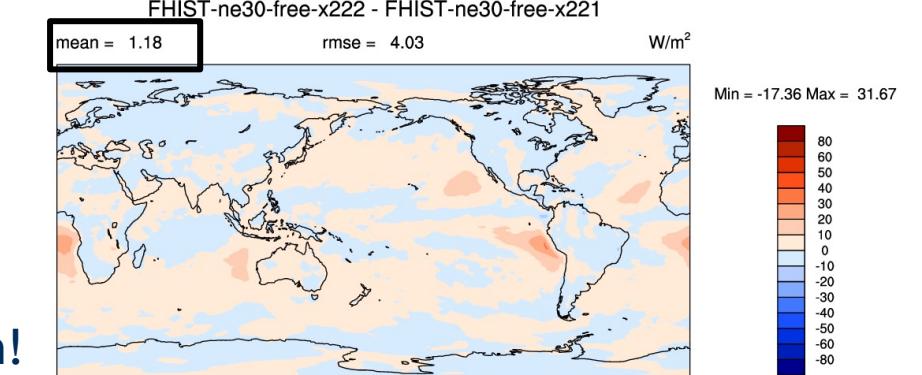
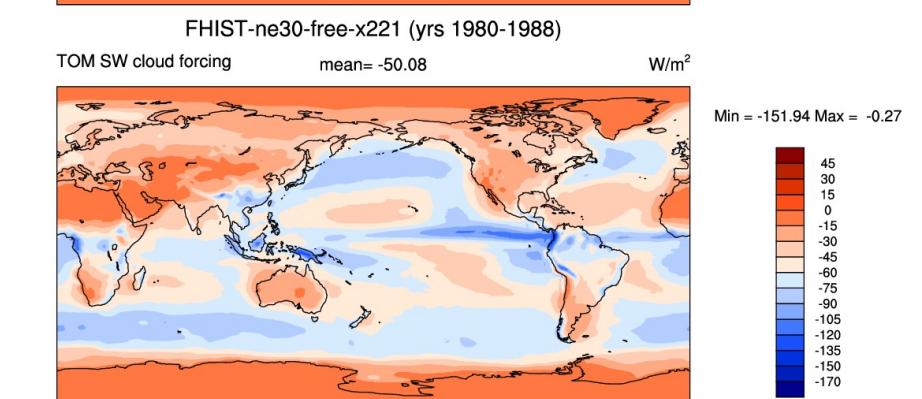
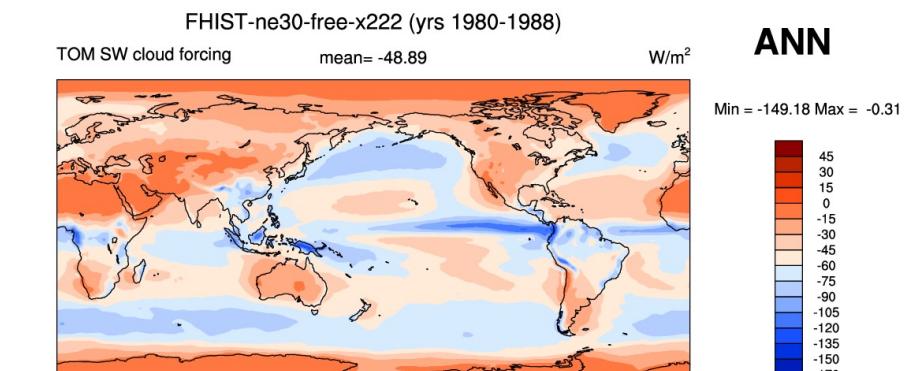


SWCF prediction

- Emulator predicts...

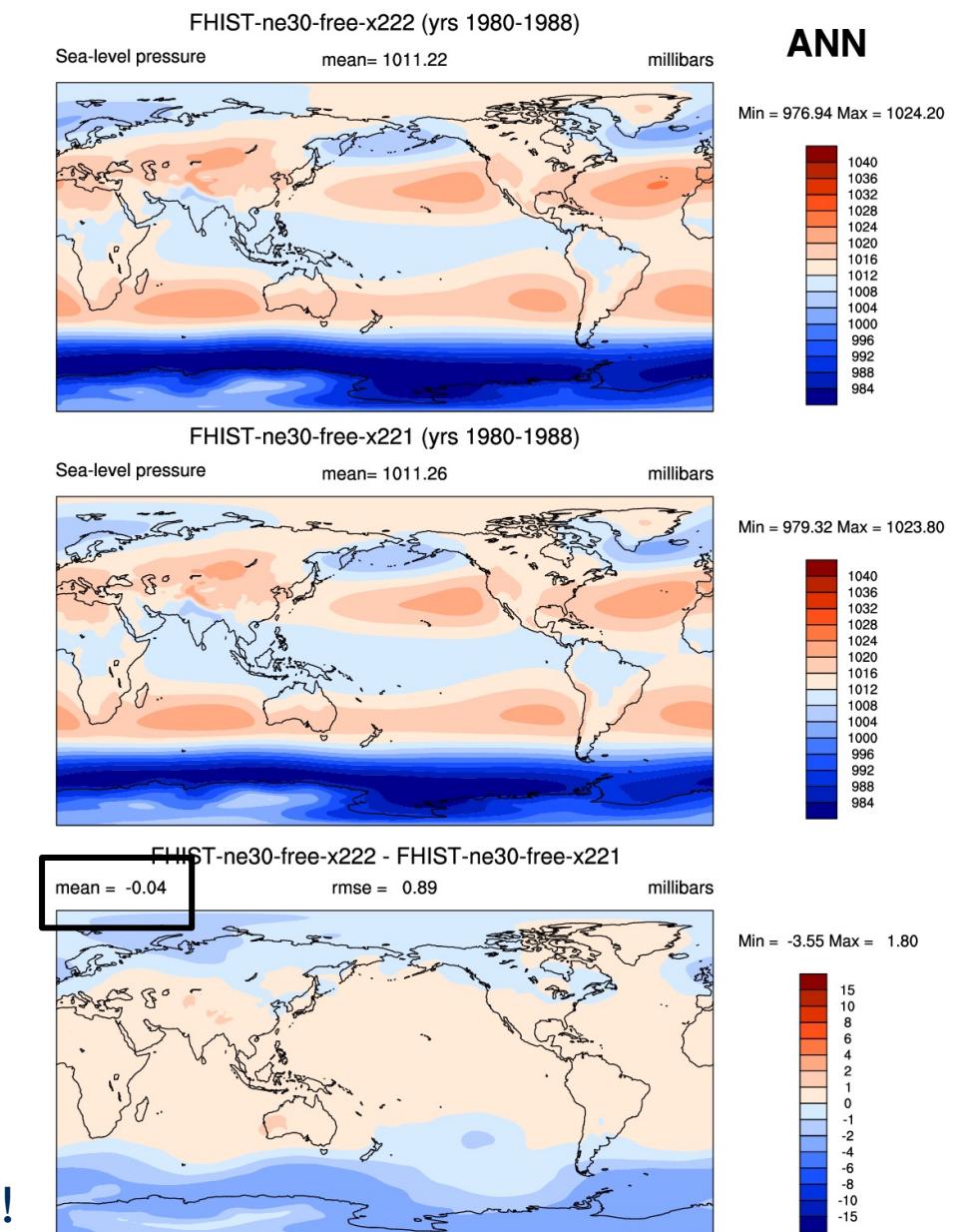
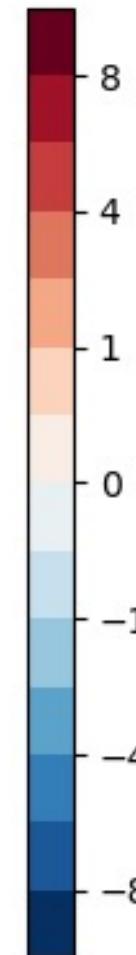
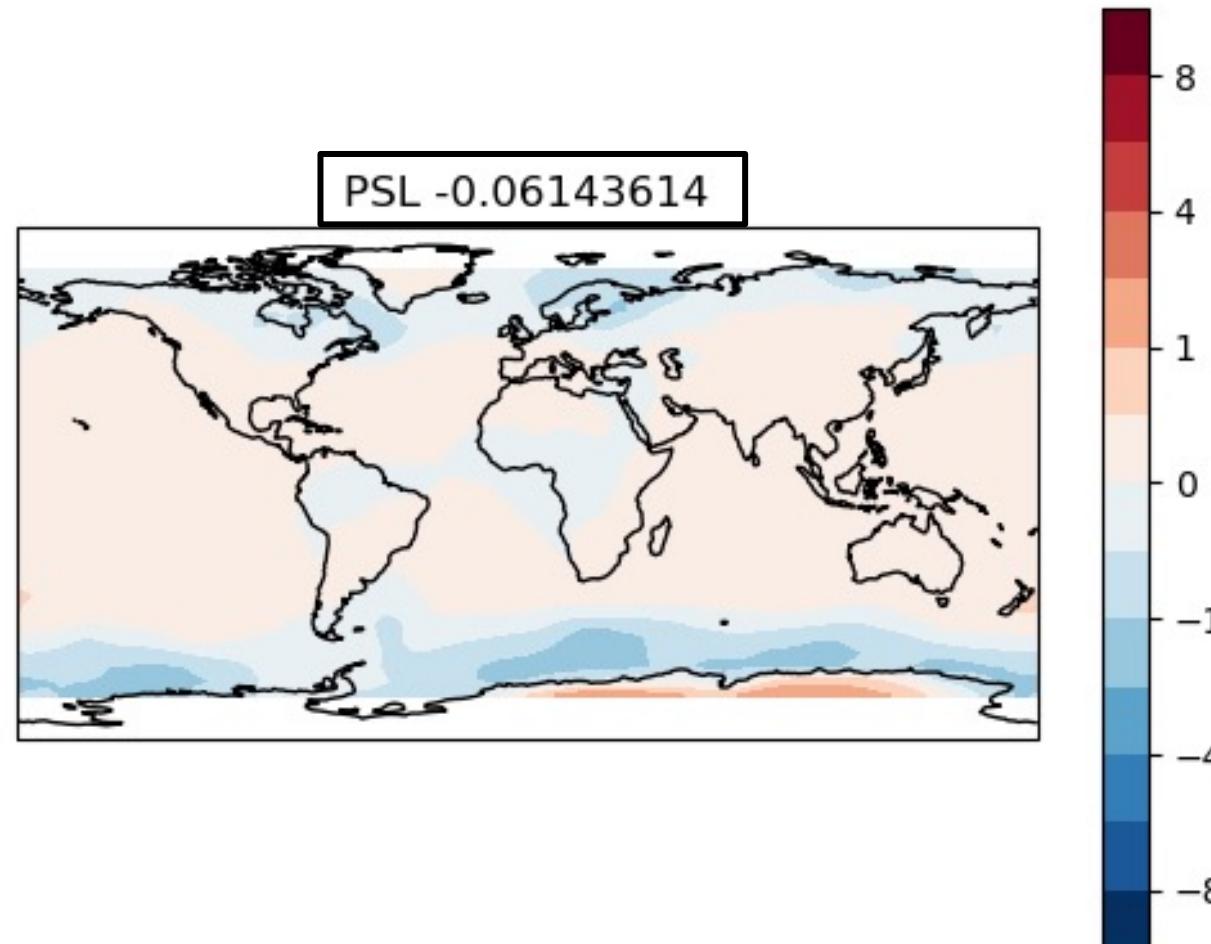


Note, color bars don't match!





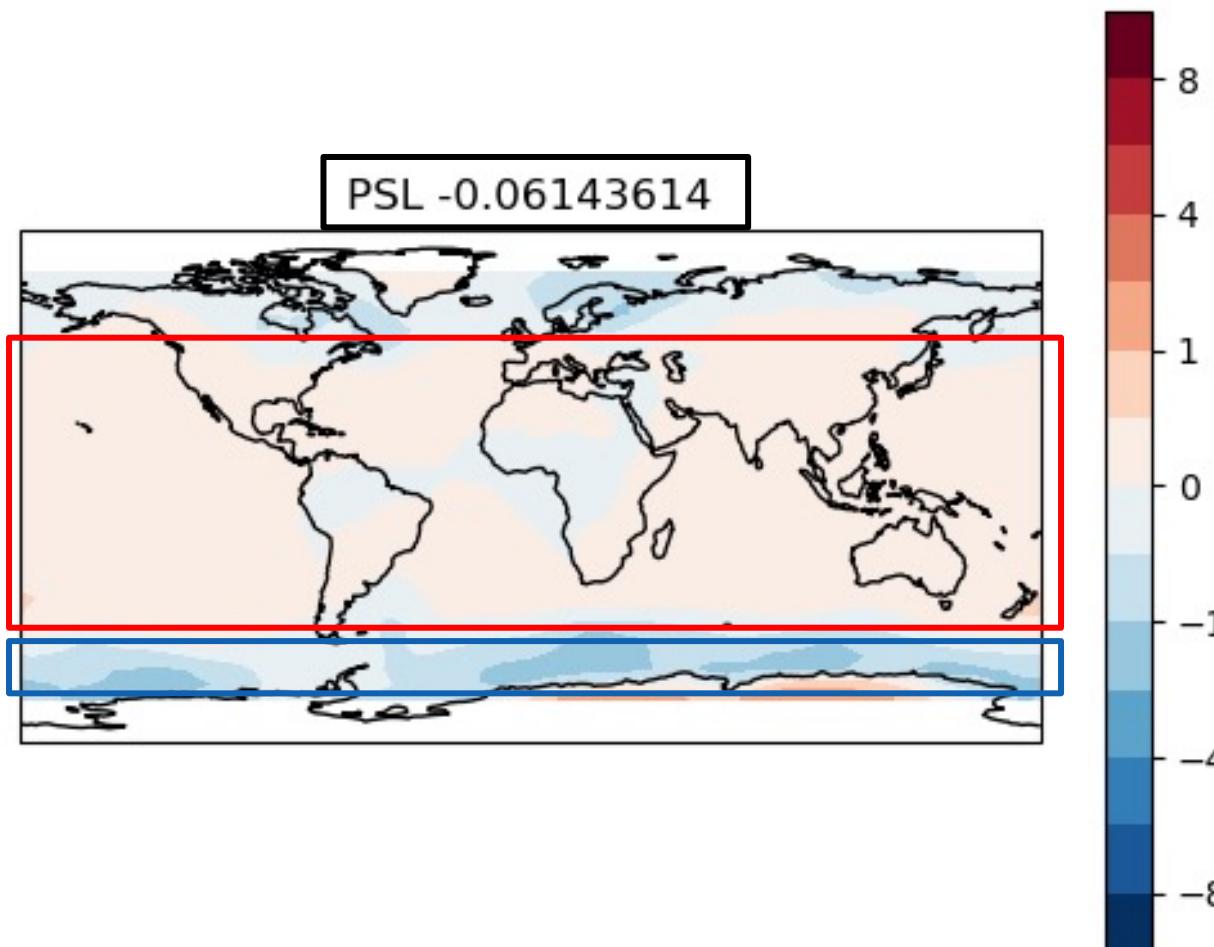
PSL prediction



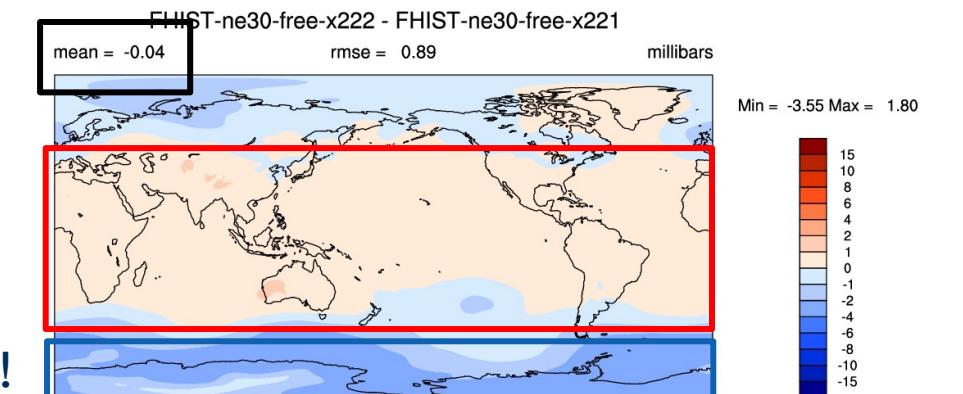
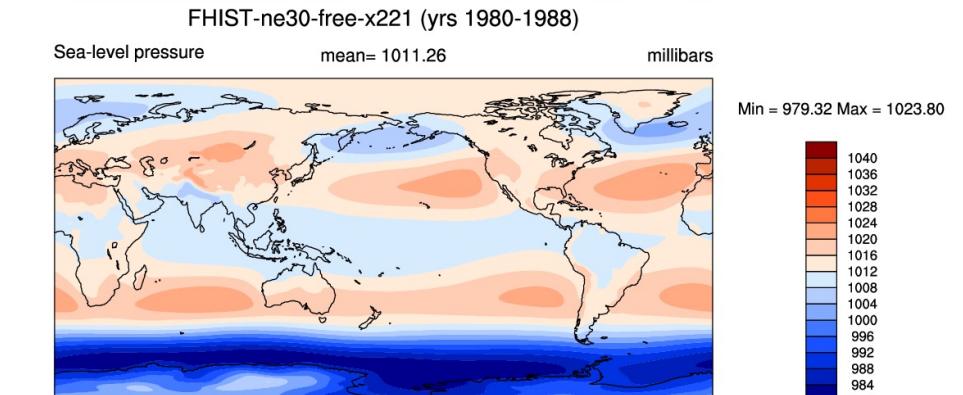
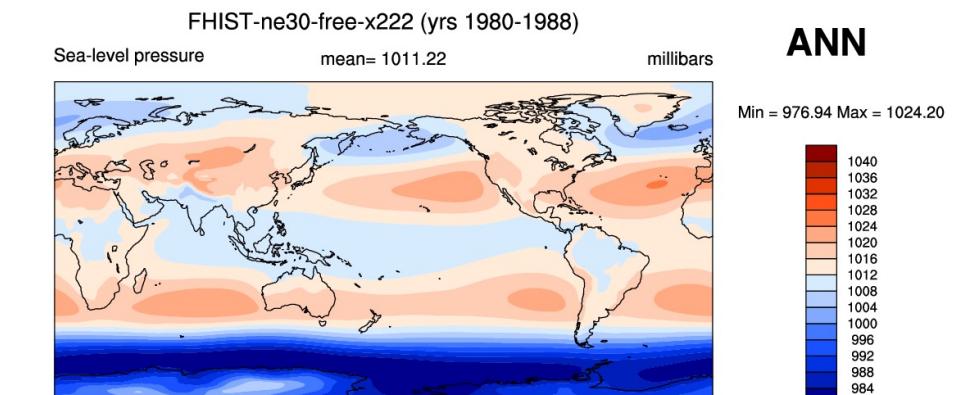
Note, color bars don't match!



PSL prediction



Note, color bars don't match!





Cost?

- Cost: we have $Z * N_{\text{inits}} * D$ days we have to integrate CAM for
 - Here, 21,600 days =~60 year single member
 - Runs are small, help fill "economy" backfill!
- Outputs distilled into climatology files from CAM output $O(1\text{GB})$
- Training for each var ~15 seconds on Macbook Pro (longer for XGBoost and NNs, but not otherworldly) → can be "pickled"
- Each "model" var takes ~8 seconds to run



Summary

- First blush?
 - Excellent for global mean *directional signal*!
 - Not bad for global mean *magnitude* (?)
 - Hint of regional information, but unclear (???)
 - Fast!
- Next steps:
 - Code cleanup / organization
 - Automatic optimization
 - Incorporate information about CLUBB booleans
 - New deck with expanded LHS using 6_3_091
- AMWG questions?
 - How to better leverage short runs for development + tuning?
 - Can this provide alternative pathways for physical interpretability?