Climate Reproducibility: Updates

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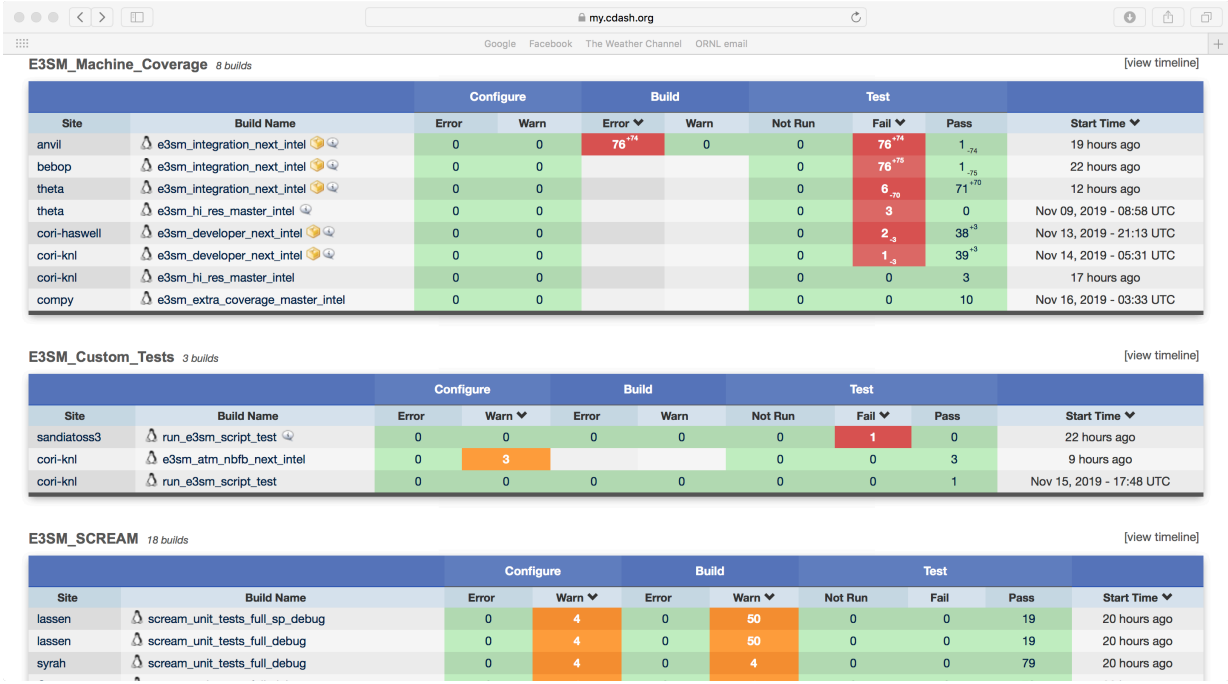
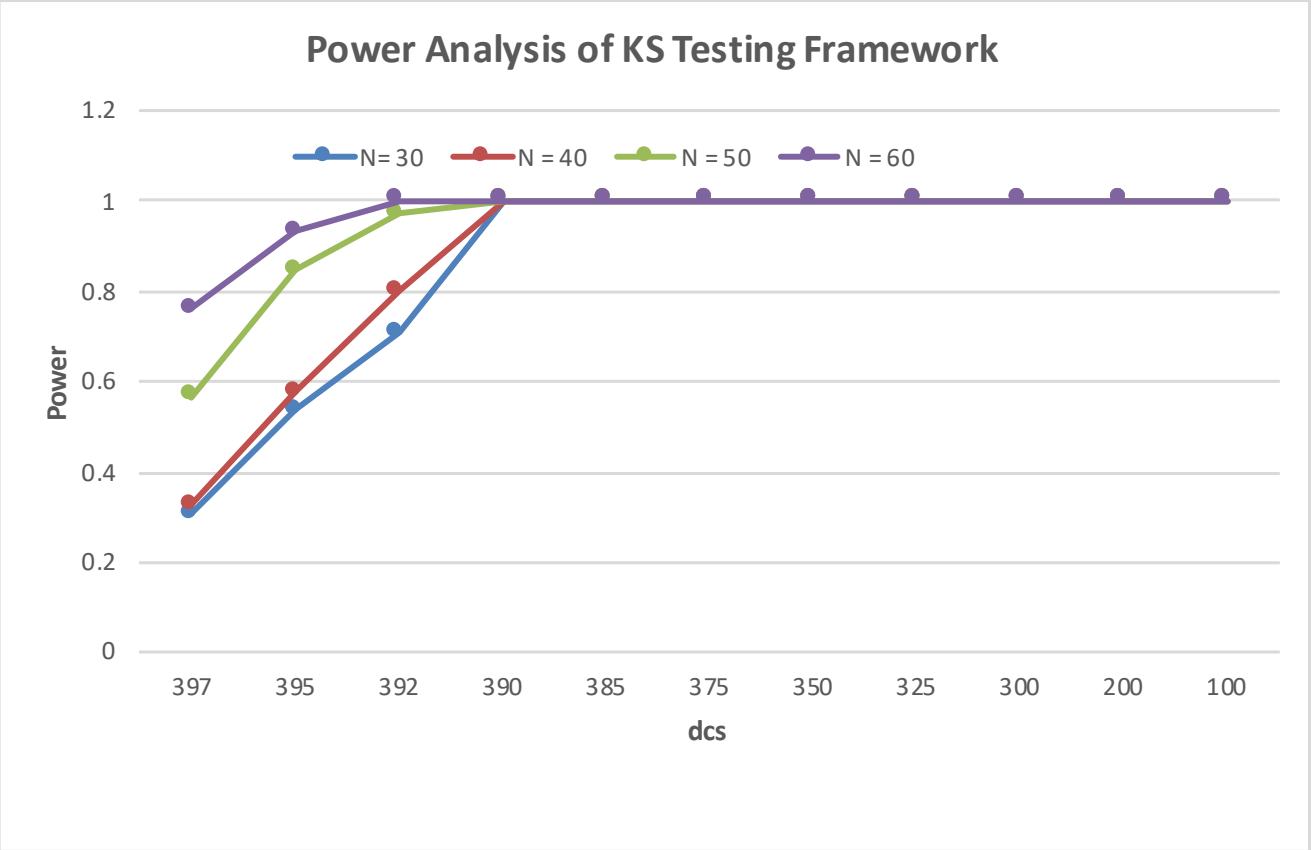
CMDV-SM Reproducibility Tests (EAM) on Master

- Nightly tests run on Cori
  - Time step convergence test
  - Perturbation growth test
  - KS testing framework
- Departures: Joe Kennedy
- Arrivals: Michael Kelleher
- On CDASH under E3SM_Customs_Tests
  - https://my.cdash.org/index.php?project=ACME_Climate
- All runs archived:
  - Large ne4 1yr F1850C5 ensemble available (>1000)



Power Analysis: Atmosphere tests

- Expand on Power Analysis:
  - More tuning parameters
    - ice_sed_ai
    - sol_factb_interstitial
    - sol_factic_interstitial
    - cldfrc_dp1
    - zm_conv_lnd
    - dcs
    - zm_conv_ocn
    - zm_conv_dmpdz
- KS testing framework most powerful:
  - detects changes of smaller magnitudes confidently
  - compared to Kernel and Energy test.

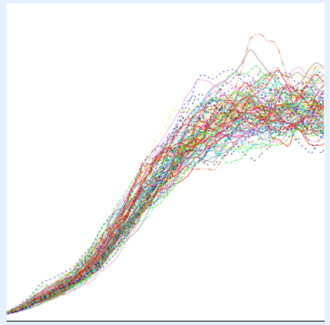


Example of Power Analysis. *Probability of correctly rejecting a false null hypothesis (Power)* of the test in detecting changes to a EAM tuning parameter from a control case (*dcs = 400*) for different short simulation (*1yr*) ensemble sizes (*N*).

Cori vs. Edison

Evaluate if E3SMv1 DECK simulations on Edison can be reproduced on Cori

- Conducted short simulation (1yr) ensembles on both Edison and Cori:
  - F1850C5-CMIP6 compset
  - ne4 (100 ensemble members)
  - ne30 (30 ensemble members)
- All three - TSC (Hui), perturbation growth (Balwinder), and KS - climate reproducibility tests passed.
- Implications: Cori can be confidently used for remaining DECK simulations



Can We Switch Computers?

Will the difference between simulated past and future climates be due to greenhouse gases or due to a change of DOE supercomputers? Thanks to a software modernization project, E3SM developers can answer this question and more. Read more.

EVV: Extended Verification & Validation for Earth System Models

Kolmogorov-Smirnov test

F1850C5-CMIP6.ne30_ne30_Edison_v_Cori

Perturbation growth test

F1850C5-CMIP6.ne30_ne30_Edison_v_Cori

Time step convergence test

F1850C5-CMIP6.ne30_ne30_Edison_v_Cori

Kolmogorov-Smirnov test

	Test status	Variables analyzed	Rejecting	Critical value	Ensembles
F1850C5-CMIP6.ne30_ne30_Edison_v_Cori	pass	118	4	13	statistically identical

Perturbation growth test

	Test status	Null hypothesis	T test (t, p)	Ensembles
F1850C5-CMIP6.ne30_ne30_Edison_v_Cori	pass	accept	(1.173e-05, 0.999991)	statistically identical

Time step convergence test

	Test status	Global	Land	Ocean	Ensembles
F1850C5-CMIP6.ne30_ne30_Edison_v_Cori	pass	pass	pass	pass	statistically identical

MPAS-O Reproducibility tests: Ensembles

- Testing approaches to generate ensembles
  1. Initial conditions from a long control run:
     - Conducted a 120 year long run CMPAS-O-NYF comp-set QU240 resolution
     - Still transient, non stationary: not useful as initial conditions for ensembles
     - Run longer?

  2. Multi-instance approach (work in progress):
     - Perturb initial condition to machine order precision:
       - Add perturbations to 3D temperature field initial condition
       - Save perturbed initial condition files
     - Use multi-instance (or create_clone) to generate ensembles:
       - each run reading a different perturbed initial condition file

  3. Pertlim capability for MPAS-O (near future):
     - Replicate capability within EAM to MPAS-O
     - Automatically perturb initial conditions
     - Generate ensembles by tweaking a namelist parameter.

Machine Precision Perturbations to T at each grid point, j

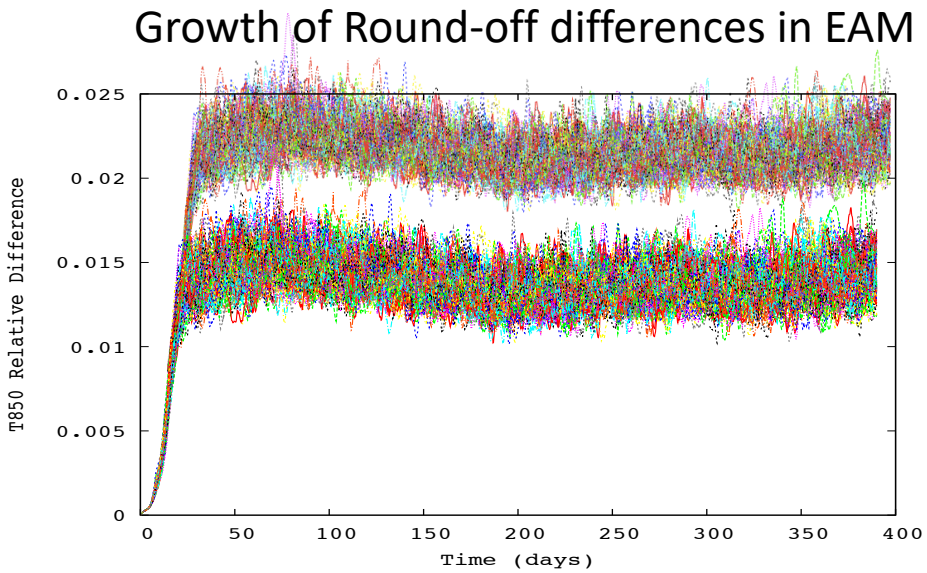
$$T'_j = (1+x')T_j$$

x' is a uniform random number transformed to range from $(-10^{-14}, 10^{-14})$

MPAS-O Reproducibility tests: Approach

Larger Null Hypothesis: Control and perturbed ensembles belong to the same population

- Generate control and perturbed ensembles at QU240 resolution
- Evaluate 5 prognostic variables (Baker et al. 2016)
  - SSH, T, U, V, Salinity
- Ocean variability is spatially very heterogenous (as compared to the atmosphere):
  - Evaluate at each grid point.
- Conduct fine-grained null hypothesis tests at each grid point:
  - Two sample KS test: Popular non-parametric test
  - Cucconi test: Better power, rank based non-parametric test.



MPAS-O Reproducibility Tests: Approach

Correct for simultaneous multiple null hypothesis tests (M grid points)

False Discovery Rate (FDR) approach (*Wilks et al. 2006, Ventura et al. 2004*):

- For single test, null hypothesis is rejected if:
  - Test statistic p-value (*p*) is less than a critical value, α (say 0.05): $p <= \alpha$
  - For *M* tests, αM would be rejected for true null hypotheses just by chance

- For multiple tests, FDR constrains critical value (α_{FDR}) for local hypothesis tests (H_0):

$$\alpha_{FDR} = \max_{j=1,2,\ldots,M} \{p_j : p_j \leq \alpha(j/M)\}$$

p_j are sorted p-values of *M* tests

- *Global Null Hypothesis Test (G_0): Reject if $p_j <= \alpha_{FDR}$ at any grid point.*

- Robust for correlated tests – e.g. spatial correlations (Wilks et a. 2006, Renard et al. 2008).
- Used in testing field significance

MPAS-O Reproducibility Tests: Preliminary Results

Known climate changing test cases:

- Segments of QU240 CMPASO-NYF 120 yr run (still transient)
- EAM runs as test cases

Examples:

Ensemble A	Ensemble B	Ens. size	Variable	α_{FDR} *for α=0.05 Cucconi Test*	Grid Points Rejecting H_0	Global Null Hypothesis Test
CMPAS-NYF Yrs 31-60	CMPAS-NYF Yrs 61-90	30	SSH	0.01	100%	Reject
CMPASO-NYF Yrs 31-60	CMPASO-NYF Yrs 41-70	30	SSH	0.011	100%	Reject
F1850C5 Ice_sed_ai = 705	F1850C5 Ice_sed_ai = 1000	100	FSNT	0.036	80%	Reject
F1850C5 zm_c0_ocn =0.007	F1850C5 zm_c0_ocn = 0.045	100	FSNT	0.042	85%	Reject

MPAS-O Reproducibility Tests: Preliminary Results

Known non-climate changing test cases

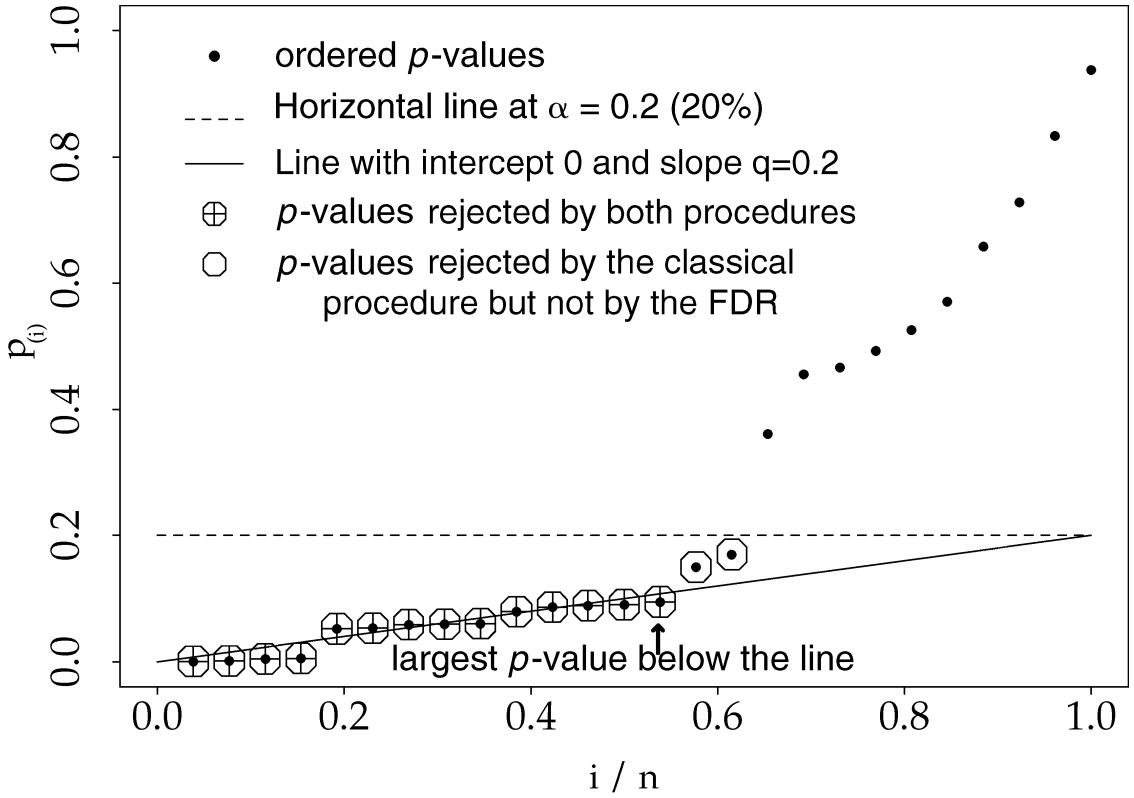
Examples:

Ensemble A	Ensemble B	Ens. size	Variable	α_{FDR} for α=0.05 Cucconi Test	Grid Points Rejecting H_0	Global Null Hypothesis Test
F1850C5 ne4 Ens. 1-30	F1850C5 ne4 Ens. 31-60	30	FSNT	0.00	0	Accept
F1850C5 ne4 Ens. 1-30	F1850C5 ne4 Ens. 61-90	30	FSNT	0.00	0	Accept
F1850C5 ne4 Ens. 31-60	F1850C5 ne4 Ens. 61-90	30	FSNT	0.00	0	Accept

Planned near future work

- Generate proper MPAS-O ensembles
  - Known climate-changing and non-climate-changing changes
- Power Analysis with controlled changes to tuning parameters
  - Determine length of short simulations
  - Determine no. of ensemble members needed
- Parallelize python code implementation
- Evaluate other approaches for multiple simultaneous tests - resampling, etc.
- Evaluate other univariate and multivariate tests – kernel test, energy test, Lepage test, etc.
- Identify software kernel in EAM to target for applying ensemble testing:
  - RRTMG? – stochasticity from sub-columns
  - CLUBB? – stochasticity from joint pdfs of sub-grid vertical velocity, T and Q
  - MG2? – stochasticity from pdfs of mass mixing ratio, number concentration of cloud droplets and ice
  - SCM? – stochasticity from full model physics, albeit at a single column

FDR Approach: Illustration



$$\alpha_{FDR} = \max_{j=1,2,\ldots,M} \{p_j : p_j \leq \alpha(j/M)\}$$

FIG. 2. Illustration of the traditional FPR and FDR procedures on a stylized example, with $q = \alpha = 20\%$. The ordered p-values, $p_{(i)}$, are plotted against i/n, $i = 1, \ldots, n$, and are circled and crossed to indicate that they are rejected by the FPR and FDR procedures, respectively.

Ventura et al. 2004

Cucconi Test

- Test Statistic:

$$\mathrm{CUC} = \frac{U^2 + V^2 - 2\rho UV}{2(1-\rho^2)}.$$

U: squared sum of ranks of samples in Ensemble A in the two sample pool of Ensembles A and B

V: squared sum of contrary-ranks of samples in Ensemble A in the pool.

ρ: Correlation coefficient between U and V

- Larger test-statistic indicates that Ensemble A and B come from different populations.
- Popular in other fields like hydrology, quality control, etc. (e.g. Mukherjee and Marozzi et al. 2014)