UQ study of parameter sensitivity in POP

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OMWG

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Outlines

- Introduction – LLNL UQ pipeline
- Climate Model Uncertainty Quantification @ LLNL
  - ➢ UQ studies across CESM components
- UQ sensitivity study of POP:
  - ➢ Methodology – learning from POP failures
  - ➢ Examples and applications
- Conclusions
- Future work

Climate Model Uncertainty Quantification @ LLNL

- Perturbed parameter ensembles of the Community Earth System Model (CESM)
- Constrain parameter PDFs with satellite observations
- Calculate PDF of climate sensitivity
- Climate change UQ using coupled models and LLNL's *UQ Pipeline*

Model input uncertainties

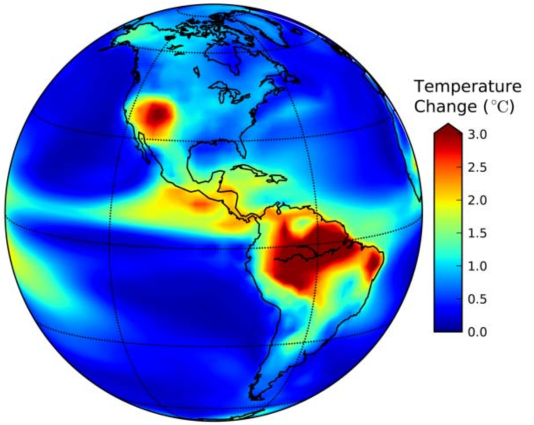
Parameter calibration

Output uncertainties

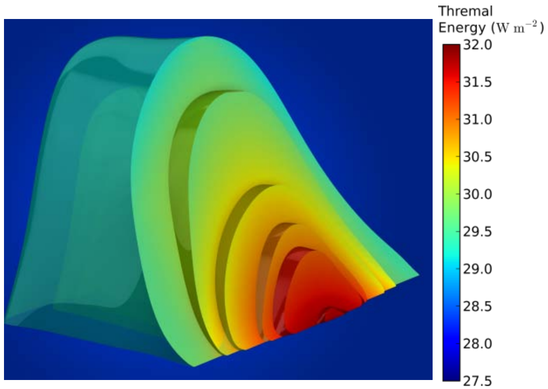
Sensitivities

Surrogate models

Ensembles & PDFs



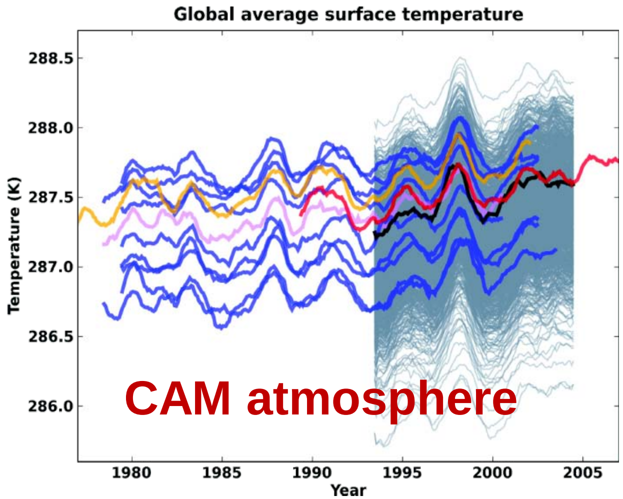
Example of a sensitivity map calculated using the Morris method on CAM3 in a high dimensional parameter space.



Example of a response surface generated using polynomial chaos expansions on CAM3 ensembles. (rendering by Kwei-Yu Chu)

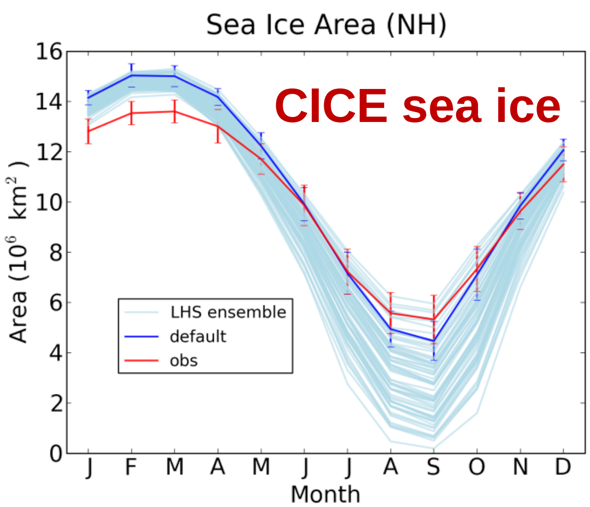
UQ simulations across *Community Earth System Model* (CESM) components

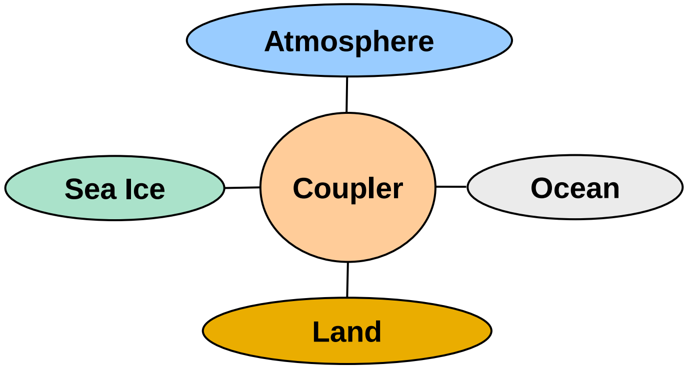
- **CESM is one of the most widely used "high end" climate models in the United States**
- **3-D models for the ocean, atmosphere and sea ice**

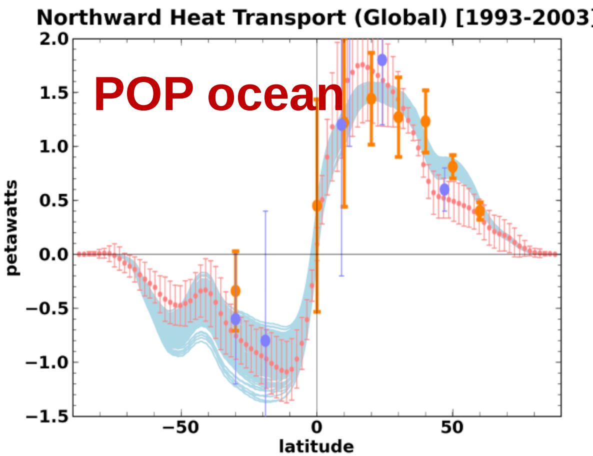


Our UQ ensembles

- **>5,700 simulations**
- **>92,000 climate model years**
- **54 parameters sampled**
- **>450 TB of monthly-avg data**







Community Earth System Model CESM

http://www.cesm.ucar.edu

UQ Simulations Across CESM Components

CESM Components	Purpose	# of Params	# of Sims	Sim-years	Archive
CAM	Parameter sensitivity, calibration of CAM	21-29	over 3,300	over 40,000	~50TB
CAM+CICE+ SOM	Parameter sensitivity, calibration of CICE	7	70	2,800	~5TB
CAM+CICE+ SOM	Climate sensitivity UQ	12-36	~600	~19,000	~35TB
POP+CICE +data Atm	Parameter sensitivity of POP	18-22	~540	~6,200	~105TB
CAM+CICE+ POP	UQ on fully-coupled system	up to 53	on-going	on-going	on-going

Computing resources for UQ ensembles provided through Livermore Computing

POP Set up

- Coupled CICE 4.0 + POP 2.0 runs with data Atm
- gx1v6, 60 vertical levels, 1h time step
- Normal year Large and Yeager climatology forcing
- 540 runs, 20-yr integration
- Anisotropic viscosity horizontal mixing (*Smith and McWilliams, 2003*),
- G&M isopycnal tracer horizontal mixing (*Gent and McWilliams, 1990*),
- KPP vertical mixing (*Large et al., 1994*),
- Sub-mesoscale and mixed layer eddies (*Fox-Kemper et al., 2008*)
- Abyssal tidal mixing (*Jayne, 2009*)
- Diffusion type of convective adjustment

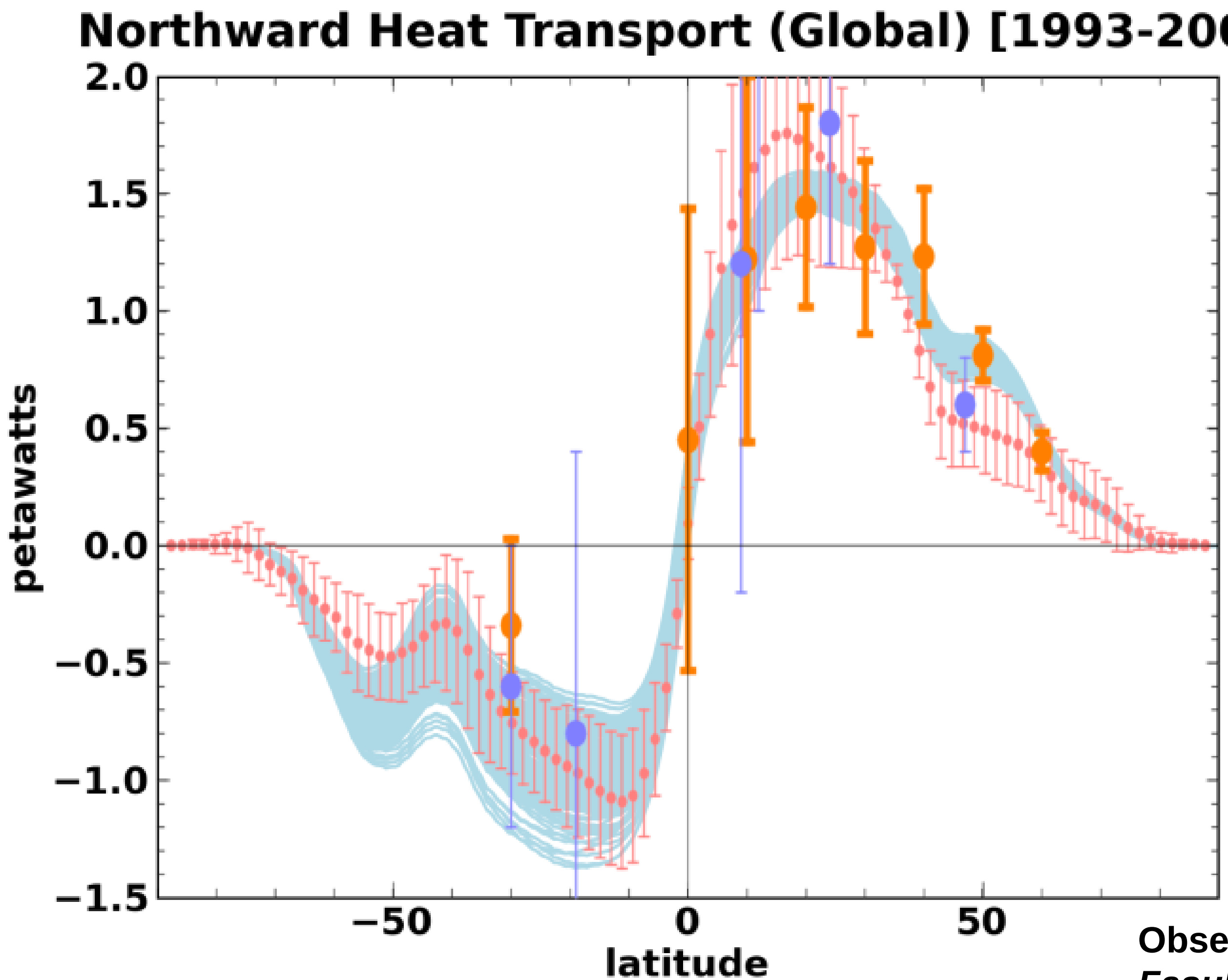
POP parameters used in the UQ study

#	Parameter Name	Range			Description	Namelist File	Namelist	Src*
		Low	Default	High				
1	vconst_1^ / _6^	0.3e7	0.6e7	1.2e7	Aeddy viscosity param. / #6 (cm^2/sec)	pop2_in	hmix_aniso	D/T
2	vconst_2	0.25	0.50	2.00	Aeddy/Beddy viscosity param.	pop2_in	hmix_aniso	D/T
3	vconst_3	0.16	0.16	0.20	Coefff. For Munk minimum viscosity	pop2_in	hmix_aniso	D/T
4	vconst_4	0.5e-8	2.0e-8	10.0e-8	Viscosity exponential decay param.? (1/cm)	pop2_in	hmix_aniso	D/T
5	vconst_5	2	3	5	# gridpts. from coast to apply Munk constraint	pop2_in	hmix_aniso	D/T
6	vconst_7	30.0	45.0	60.0	Latitude of tide-breaking viscosity (degrees)	pop2_in	hmix_aniso	D/T
7	ah^	2.0e7	3.0e7	4.0e7	Diffu. coeff. for Redi (rotated tensor) part (cm^2/s)	pop2_in	hmix_gm	D/T
7	ah_bkg_srfbl^				Bckgrd. horiz. diffusivity within surf. boundary layer	pop2_in	hmix_gm	D
8	ah_bolus	2.0e7	3.0e7	4.0e7	Diffu. coeff. for bolus (induced velocity) part (cm^2/s)	pop2_in	hmix_gm	D/T
9	slm_b^ / slm_r^	0.05	0.30	0.30	Maximum slope for bolus / Redi terms	pop2_in	hmix_gm	D
10	efficiency_factor	0.05	0.07	0.10	Efficiency factor for sub-mesoscale mixing	pop2_in	mix_submeso	D
11	tidal_mix_max	25.0	100.0	200.0	TBD?	pop2_in	tidal	D
12	vertical_decay_scale	250.0e2	500.0e2	2000.0e2	Vert. decay scale for tide-induced turbulence (cm)	pop2_in	tidal	D
13	convect_diff^	1000.0	10000.0	50000.0	Tracer mixing coeff. in diffu. option for convect.	pop2_in	vertical_mix	D/T
13	convect_visc^				Momentum mixing coeff. in diffu. option for convect.	pop2_in	vertical_mix	D/T
14	bckgrnd_vdc1	0.032	0.160	0.800	Base background vertical diffusivity (cm^2/s)	pop2_in	vmix_kpp	D/J/T
15	bckgrnd_vdc_ban	0.5	1.0	1.0	Banda Sea diffusivity (Gordon)	pop2_in	vmix_kpp	D
16	bckgrnd_vdc_eq	0.01	0.01	0.50	Equatorial diffusivity (Gregg)	pop2_in	vmix_kpp	D/J
17	bckgrnd_vdc_psim	0.10	0.13	0.50	Maximum PSI induced diffusivity (MacKinnon)	pop2_in	vmix_kpp	D/J
18	Prandtl	4.0	10.0	20.0	Prandtl #: Ratio of bckgrd. vert. viscosity & diffusivity	pop2_in	vmix_kpp	D

* Source => D:Danabasoglu, G; J:Jochum, M; T:Tokmakian, R

^ Values correlated; varied with identical values.

Ocean Heat Transport – Ensembles and Observations



Observations from
***Fasullo & Trenberth*, 2008**

Analysis of Failed POP Runs

- About 10% of our simulations failed

  540 simulations
  494 succeeded
  46 failed

- Lack of convergence
- What parameter combinations caused the failures?
- Can we predict (assign probabilities) future failures?

UQ Pipeline → Probabilistic Classifier → POP Ocean

***P*(fail) = 1 – *P*(success)**

Used SVMs to Train Probabilistic POP Classifiers

- 18 features
- 1 = fail, 0 = success
- cross validation
- bootstrapping to assess performance

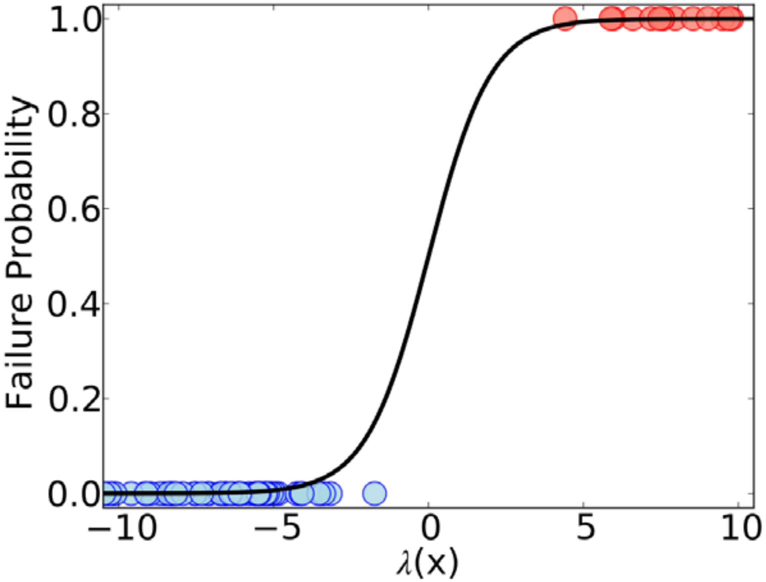
Failure Probability

- Binary classification problem
  $\mathcal{C}_f$ = simulation failure
  $\mathcal{C}_s$ = simulation success

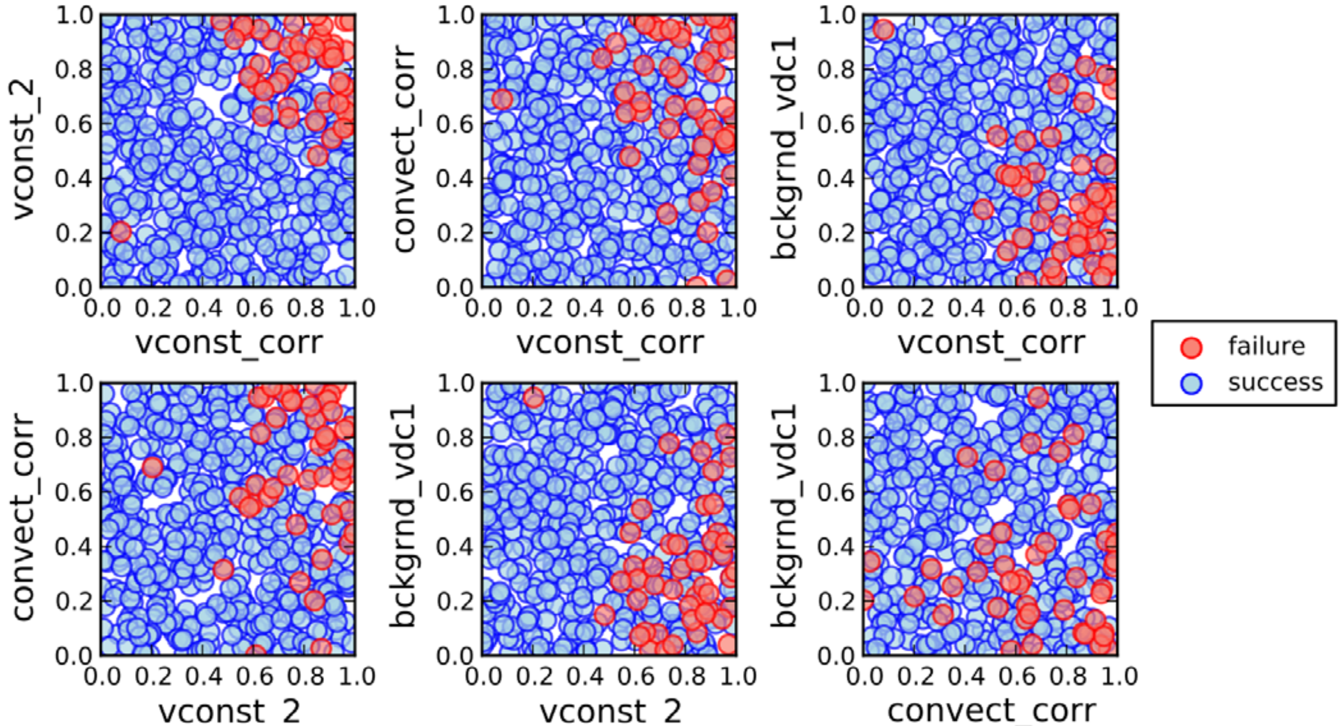
- Failure probability from Bayes' rule

$$\mathcal{P}(\mathcal{C}_f|\mathbf{x}) = \frac{1}{1+\exp(-\lambda(\mathbf{x}))}$$

  where $\mathbf{x}$ = model parameter values
  and λ = log(likelihood-odds ratio).

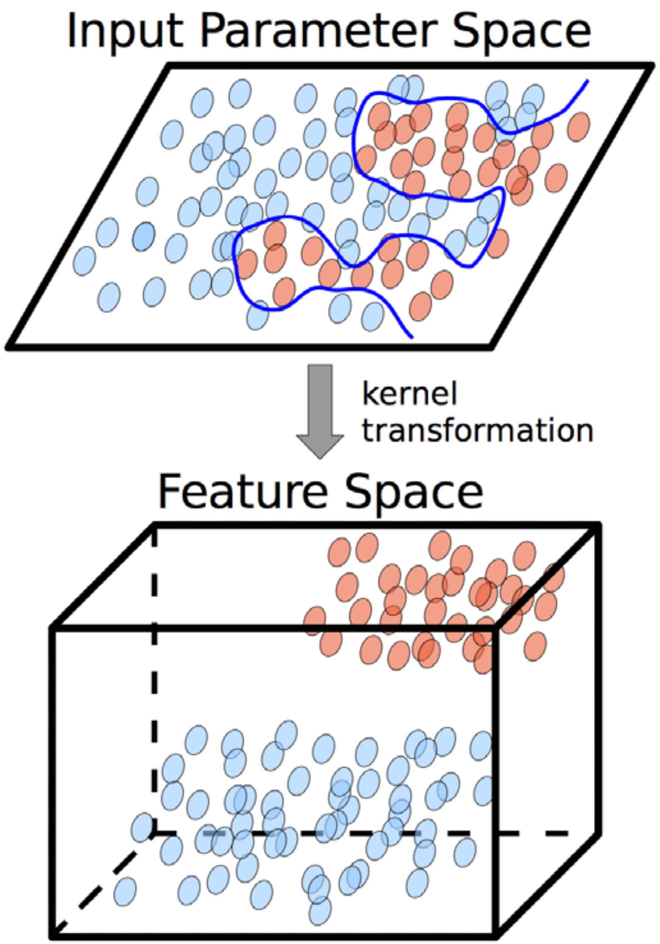


Descriptive Analysis



Scatter plots of 540 simulation outcomes versus pairs of normalized values of four parameters. Simulation failures strongly correlate with parameter values, but also overlap with many successful simulations. Advanced statistical methods are used to separate the overlaps.

SVM Classification



- Support Vector Machines (SVMs) are used to assign a simulation to $\mathcal{C}_f$ or $\mathcal{C}_s$ for input vector $\mathbf{x}$.
  - $\rightarrow$ effective for high dimensions
  - $\rightarrow$ nonlinear classification (see left)
- Use `LIBSVM` package (C-SVC, radial basis kernels, probability estimates)
- Committee of SVM classifiers through bootstrap aggregation ("*bagging*").

$$\mu_c = \frac{1}{N_b} \sum_{i=1}^{N_b} \mathcal{P}_i(\mathcal{C}_f|\mathbf{x})$$

$$\sigma_c^2 = \frac{1}{N_b} \sum_{i=1}^{N_b} [\mathcal{P}_i(\mathcal{C}_f|\mathbf{x}) - \mu_c]^2$$

Classifier Performance

- Studies 1 & 2 $\Rightarrow$ train SVM classifiers
  Study 3 $\Rightarrow$ independent validation
- Study 3 simulation outcomes predicted using three decision criteria $D \equiv$ variable $\geq$ threshold.

$$D_{avg} \equiv \mu_c \geq 0.5$$
$$D_{sum} \equiv \mu_c + \sigma_c \geq 0.5$$
$$D_{snr} \equiv \mu_c / \sigma_c \geq 3.53$$

- Results summarized in "confusion matrix" on the right.
- SVM classifiers successfully predict simulation failures (accuracy 96.7% and 97.8%).

		Actual	
		Failure	**Success**
Predicted	**Failure**	**True Positives** $D_{avg} = 9$ $D_{sum} = 11$ $D_{snr} = 12$	**False Positives** $D_{avg} = 1$ $D_{sum} = 3$ $D_{snr} = 2$
	Success	**False Negatives** $D_{avg} = 5$ $D_{sum} = 3$ $D_{snr} = 2$	**True Negatives** $D_{avg} = 165$ $D_{sum} = 163$ $D_{snr} = 164$
		14 actual failures	166 actual successes

Sensitivity Analysis of the Simulation Failures

Network Diagram of Sobol Indices

Total variance is decomposed:

$v_t = \Sigma v_i + \Sigma v_{ij} + \Sigma v_{ijk} + \ \ldots$, where

v_i = variations from parameter *i*

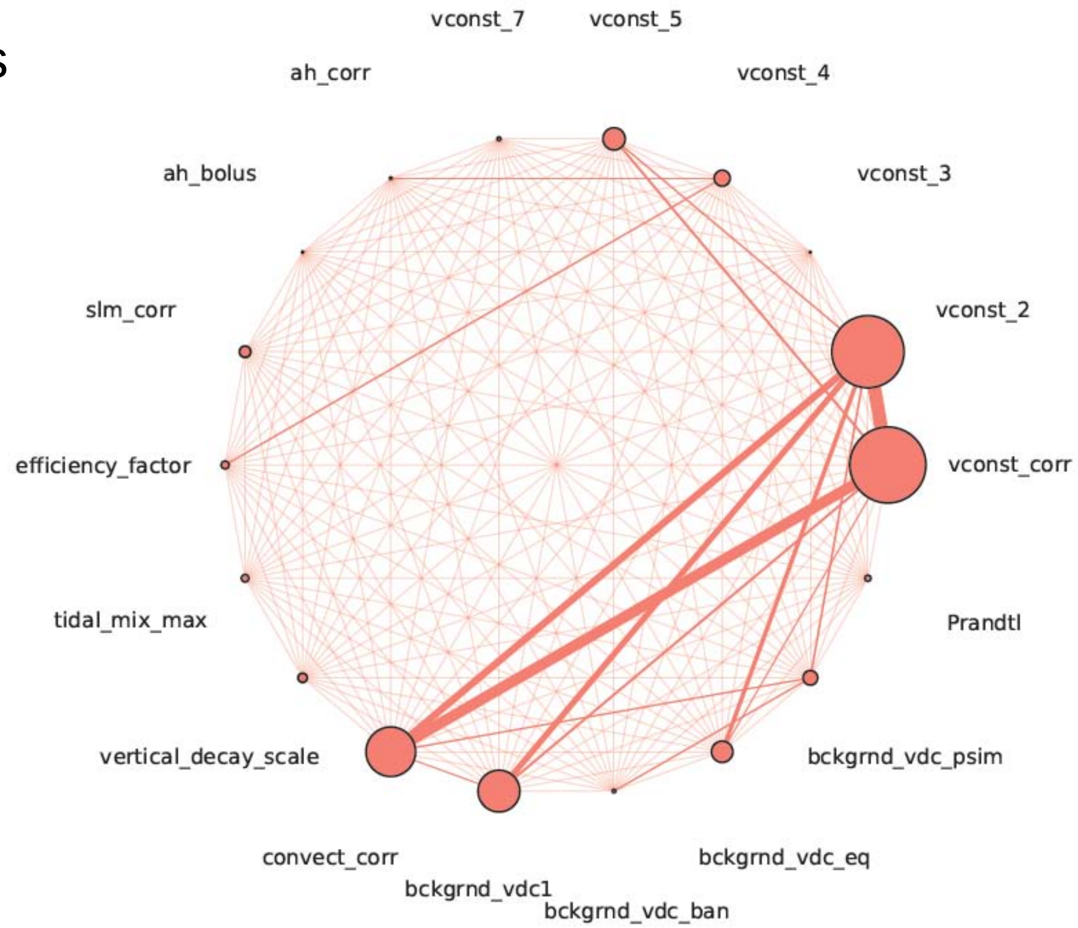
v_{ij} = co-variations from parameters *i* and *j*

Variance contributions on a network graph.

node diameter $\propto V_i / V_{tot}$ (main effects)

edge width $\propto V_{ij} / V_{tot}$ (interactions)

(higher orders can also be displayed on the same graph)



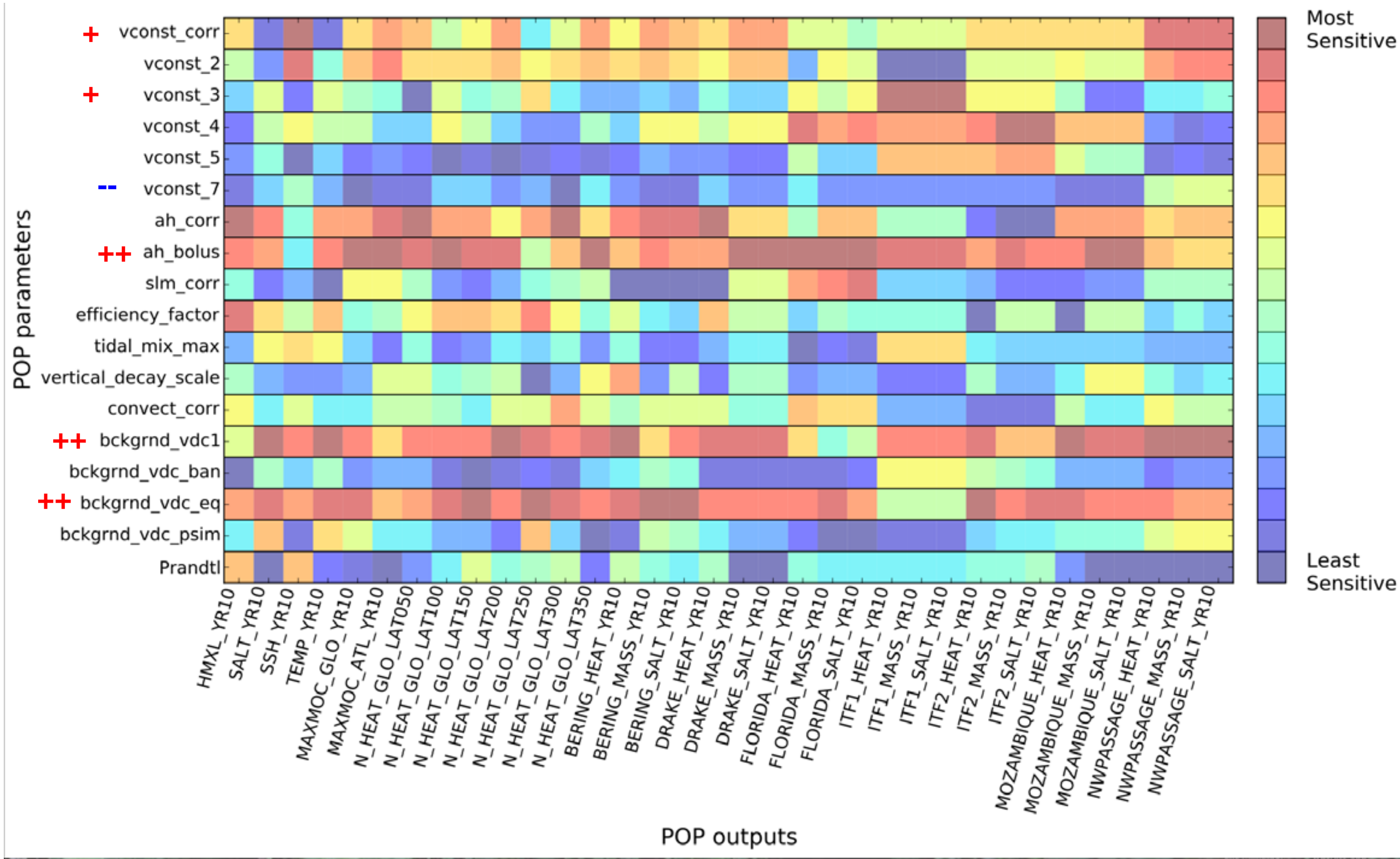
D. D. Lucas, R. Klein, J. Tannahill, D. Ivanova, S. Brandon, D. Domyancic, and Y. Zhang *"Failure Analysis of Parameter-Induced Simulation Crashes in Climate Models*" submitted in Geoscientific Model Development.

Computational POP Sensitivities

- **Sensitivity analysis methods in the UQ Pipeline were applied to the *POP***

- **Sensitivity measures are used to identify important model parameters**

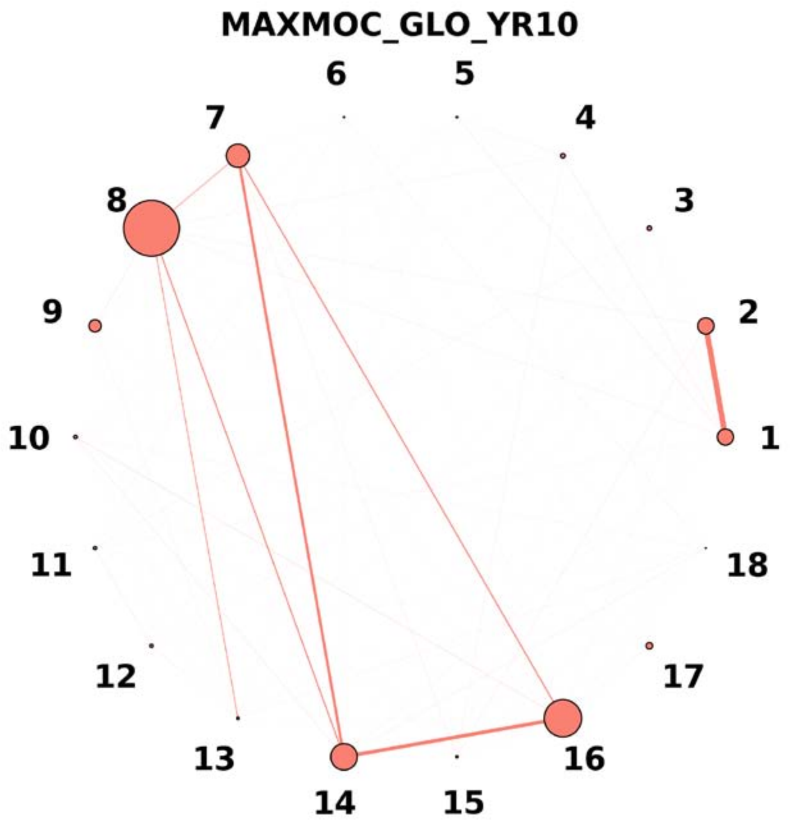
- **We ranked the importance of 18 uncertain parameters across 34 climate model outputs of interest**



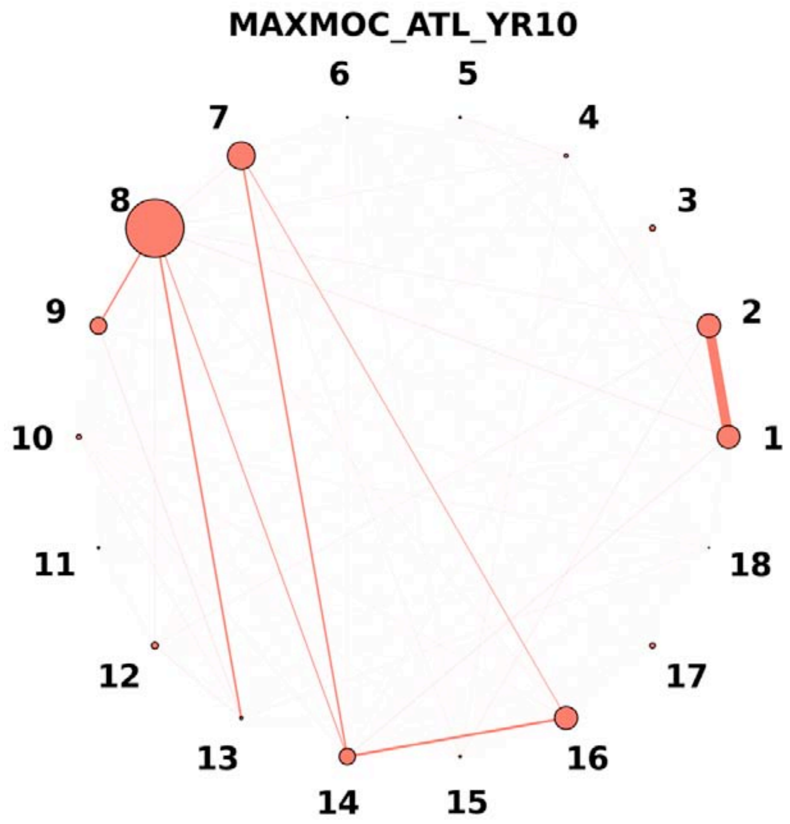
++ = important to many outputs **+ =** important to at least one output

POP MOC

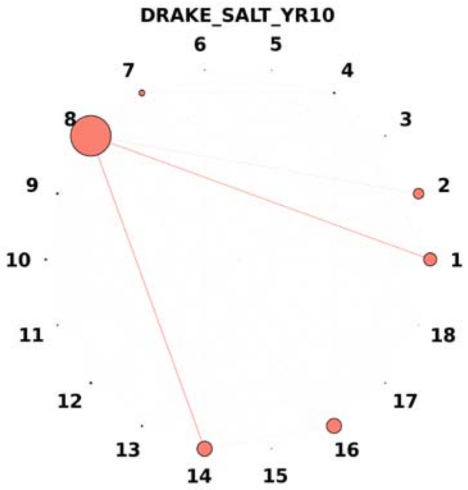
Global

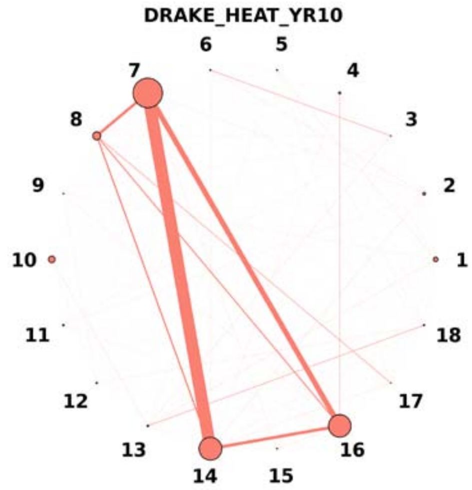


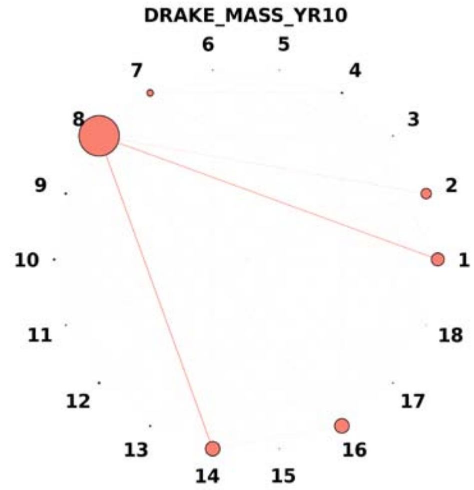
Atlantic



Drake Passage Transports







Conclusions

UQ technology potential:

- To use the probability classifiers in future planning of ensembles by prediction the model failure or success given a certain input parameters combination;
- To reduce the uncertainty of the input parameters;
- To study the model solution sensitivity to input parameters variations and their combinations across the different modules of the model component or the fully coupled climate system.

Future work

Data Archive @ LLNL

Contact: Don Lucas, lucas26@llnl.gov

Curt Covey, covey1@llnl.gov

Future Plans: Data available at LLNL ESG Portal

THANK YOU!

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