The Climate UQ Project at Lawrence Livermore National Laboratory

D. Lucas, G. Johannesson + many more

SAMSI Program on Uncertainty Quantification
Climate Modeling Workshop
Wednesday, August 31, 2011

This work performed under the auspices of the U.S. Department of Energy by
Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

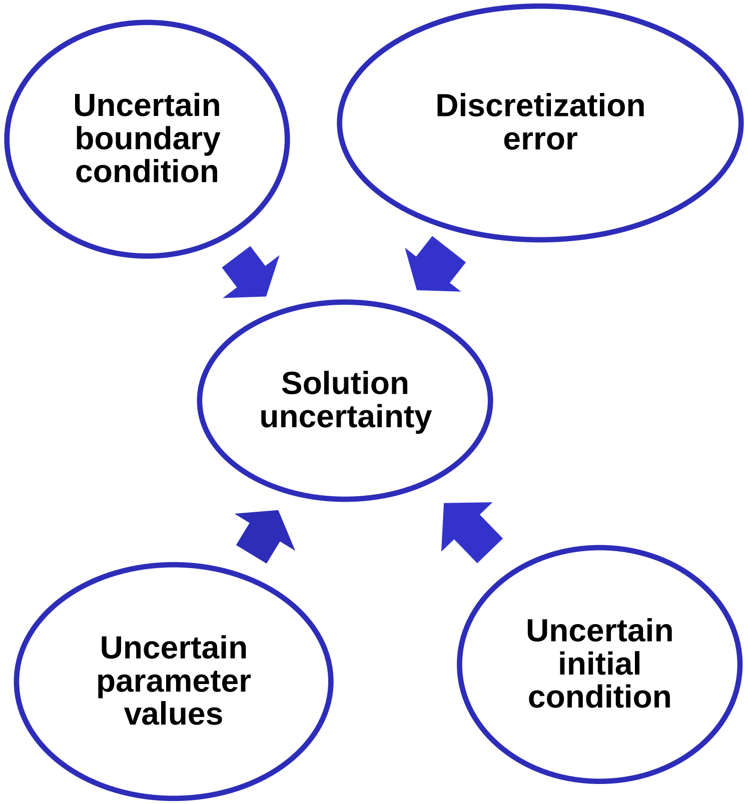
LLNL-PRES-492559

Advancing UQ Science: a Strategic Initiative at LLNL

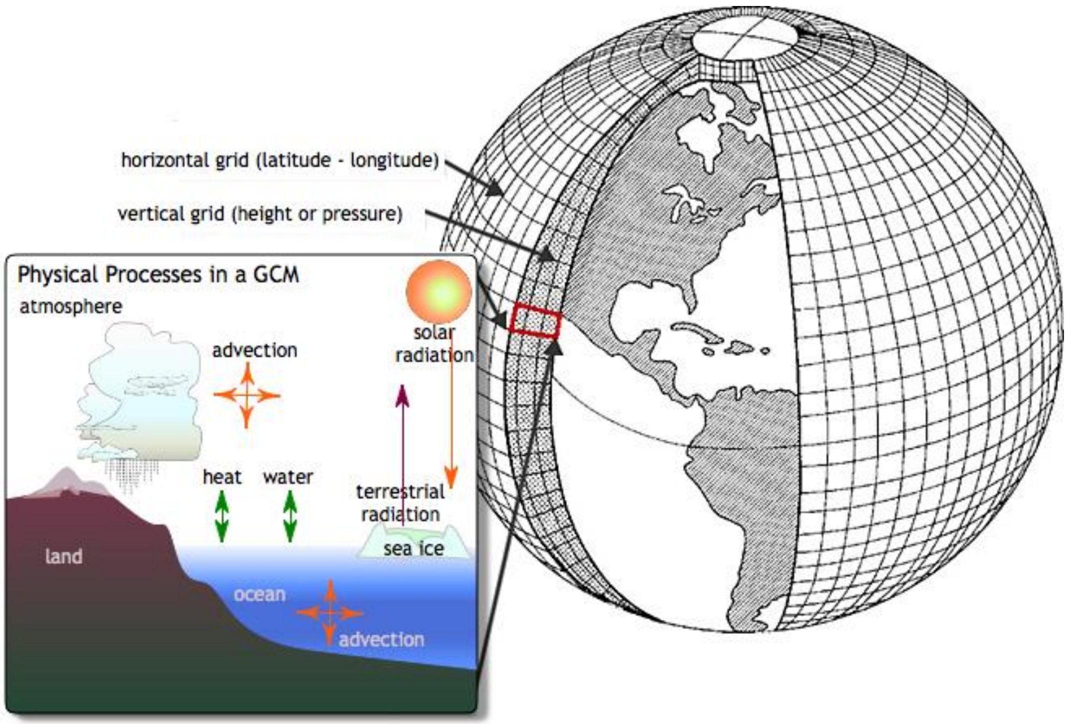
Creating an Advanced UQ Science Capability for Predictive Simulations

Four focus areas for building and testing a UQ computational engine for exascale computing

- **Error Estimation**
- **Curse of Dimensionality** (advanced statistical methods)
- **UQ Pipeline** (software development)
- **Climate Model**



Modeling the climate system

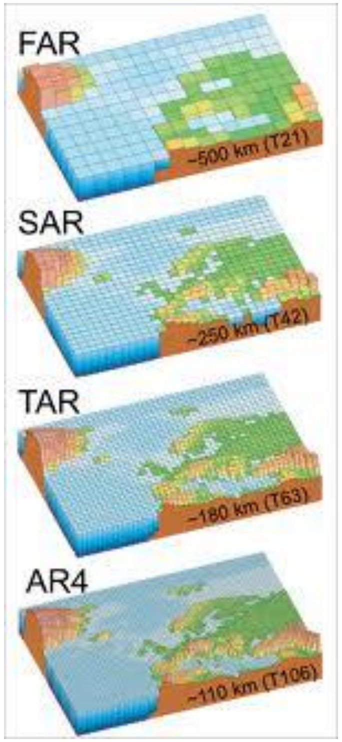


1990

1995

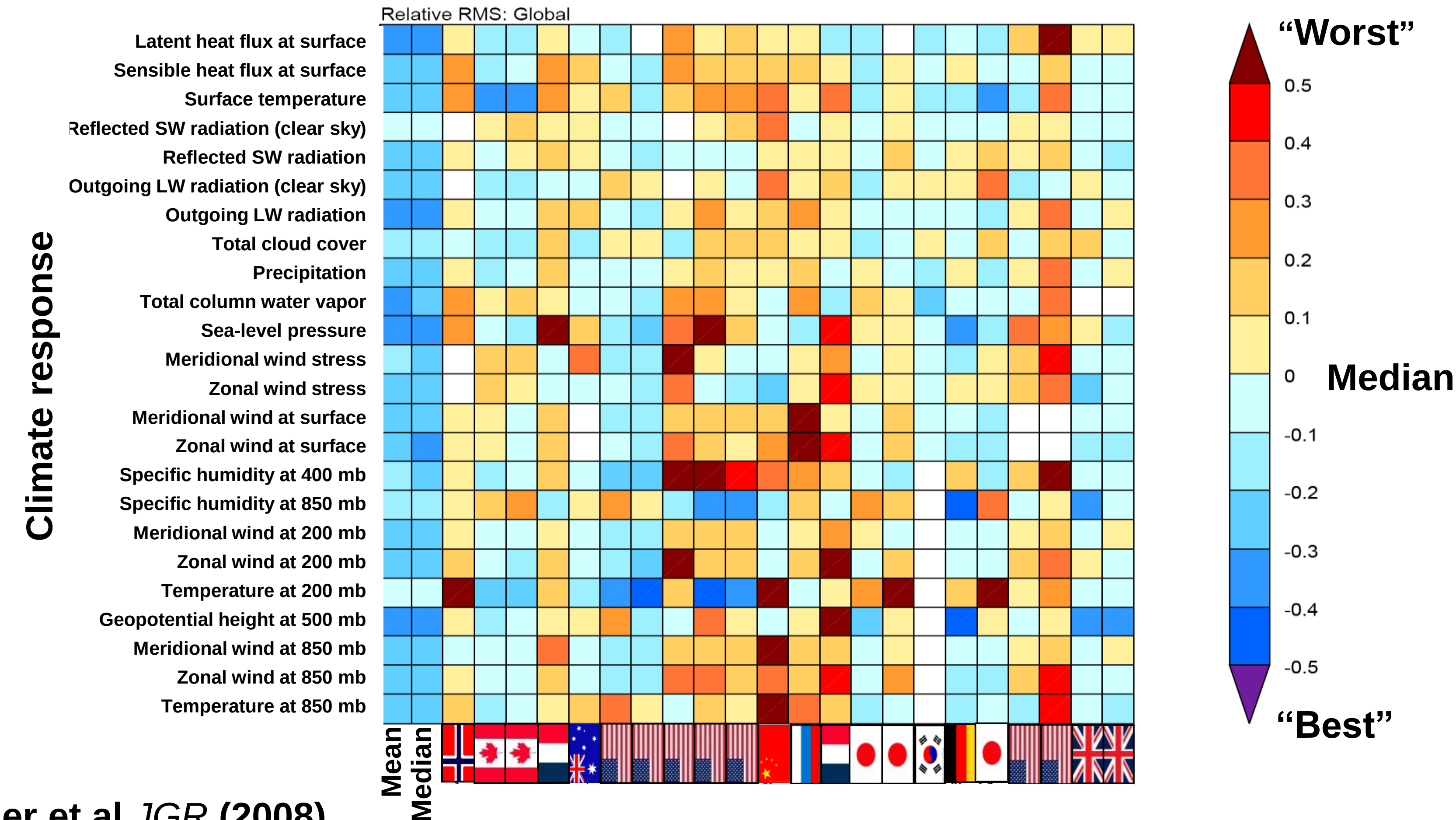
2001

2007



- **Climate models solve continuity equations for momentum, mass, energy and chemical constituents.**
- **Many processes occur at unresolved scales and require parameterizations (e.g. convection, cloud cover, rainfall, rough topography, urban centers)**

It is difficult to identify the sources of uncertainty in a multi-model assessment: example from PCMDI

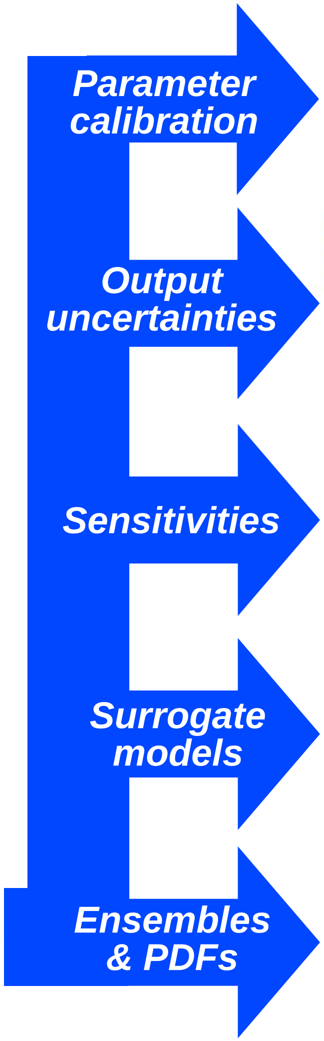


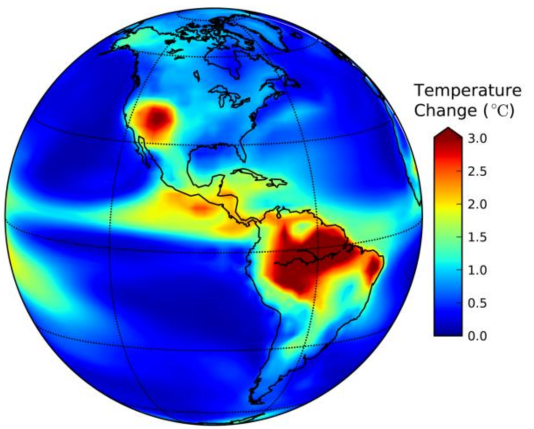
Gleckler et al *JGR* (2008)

Model used in IPCC Fourth Assessment

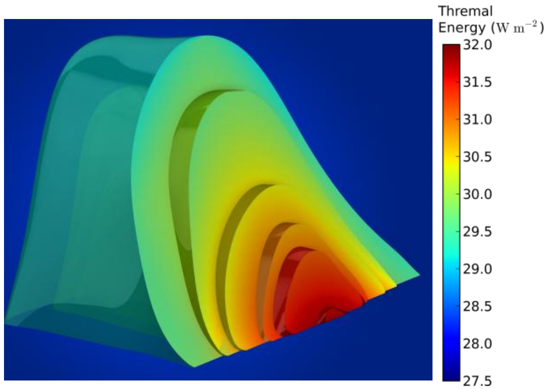
Assessing Climate Model Uncertainties using UQ

- Perturbed input parameter ensembles of the Community Earth System Model (CESM)
- Carry out sensitivity and uncertainty analysis of climate simulations
- Collect a comprehensive set of observations to use for UQ (emphasis on cloud-related observations)
- Calibrate input parameters using observations
- Calculate PDF of climate sensitivity
- Perform UQ analysis of climate change using coupled models and adaptive sampling refinement in LLNL's *UQ Pipeline*





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)

CESM configuration

- **Basic CESM configuration used:**
  - **CESM v1.0.1**
  - **E/F_2000 compsets**
  - **1.9x2.5° horizontal resolution**
  - **CAM4 physics**
  - **26 vertical levels**
  - **Finite-Volume dynamical core**

CESM namelist code modified to allow for up to 37 parameters of interest to be set.

CESM scripting system modified as needed.

Extensive Python script developed to insulate user from CESM specifics.

36 Uncertain Parameters Considered in Atmospheric (CAM) and Sea Ice (CICE) Components (part I)

#	Name	Low	Default	High	Description	Package
1	**rhminh^**	0.65	0.80	0.85	Threshold RH for fraction of high stable clouds	cloud_fraction
2	**rhminl^**	0.80	0.91	0.99	Threshold RH for fraction of low stable clouds	cloud_fraction
3	**rliqice**	8.4	14.0	19.6	Effective radius of liq. cloud droplets over sea ice	pkg_cldoptics
4	**rliqland**	4.8	8.0	11.2	Effective radius of liquid cloud droplets over land	pkg_cldoptics
5	**rliqocean**	8.4	14.0	19.6	Effective radius of liquid cloud droplets over ocean	pkg_cldoptics
6	**ice_stokes_fac^**	0.25	0.50	1.00	Scaling factor applied to ice fall velocity	pkg_cld_sediment
7	**capnc**	30.0	150.0	155.0	Cloud particle num. density over cold land/ocean	cldwat
8	**capnsi**	10.0	75.0	100.0	Cloud particle number density over sea ice	cldwat
9	**capnw**	150.0	400.0	500.0	Cloud particle number density over warm land	cldwat
10	**conke^**	2.0e-6	5.0e-6	10.0e-6	Evaporation efficiency of stratiform precipitation	cldwat
11	**icritc^**	2.0e-6	9.5e-6	18.0e-6	Threshold for autoconversion of cold ice	cldwat
12	**icritw^**	1.0e-4	2.0e-4	10.0e-4	Threshold for autoconversion of warm ice	cldwat
13	**r3lcrit**	5.0e-6	10.0e-6	14.0e-6	Critical radius at which autocon. becomes efficient	cldwat
14	**fac**	10.0	100.0	200.0	ustar parameter in PBL height diagnosis	hb_diff
15	**fak**	4.25	8.50	17.00	Constant in surface temperature excess	hb_diff
16	**ricr**	0.1	0.3	1.0	Critical Richardson number for boundary layer	hb_diff
17	**betamn**	0.02	0.10	0.30	Minimum overshoot parameter	hk_conv
18	**c0^**	0.3e-4	1.0e-4	2.0e-4	*Shallow* convection precipitation efficiency	hk_conv
19	**cmftau^**	900.0	1800.0	14400.0	Time scale for consumption rate of shallow CAPE	hk_conv
20	**sgh_scal_fac**	0.8	1.0	1.2	Land roughness scaling factor	physpkg

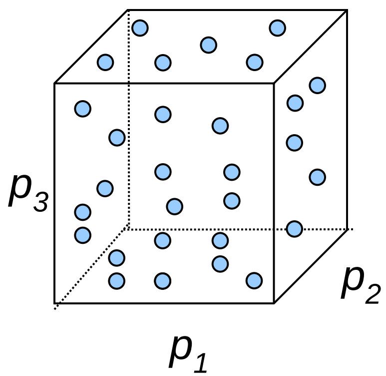
36 Uncertain Parameters Considered in Atmospheric (CAM) and Sea Ice (CICE) Components (part II)

#	Name	Low	Default	High	Description	Package
21	**alfa**	0.05	0.10	0.60	Initial cloud downdraft mass flux	zm_conv
22	**c0_lnd^**	1.0e-3	3.5e-3	6.0e-3	*Deep* convection precipitation efficiency over land	zm_conv
23	**c0_ocn^**	1.0e-3	3.5e-3	6.0e-3	*Deep* convec. precipitation efficiency over ocean	zm_conv
24	**capelmt**	20.0	70.0	200.0	Threshold value for CAPE for deep convection	zm_conv
25	**dmpdz**	-2.0e-3	-1.0e-3	-0.2e-3	Parcel fractional mass entrainment rate	zm_conv
26	**ke^**	0.5e-6	1.0e-6	10.0e-6	Environmental air entrainment rate	zm_conv
27	**tau**	1800.0	3600.0	28800.0	Time scale for consumption rate of deep CAPE	zm_conv
28	**cdn_scal_fac**	0.8	1.0	1.2	Ocean roughness scaling factor	shr_flux_mod
29	**z0m_scal_fac**	0.8	1.0	1.2	Mois. & heat resistance to vegetation scaling factor	Biogeophysics 1Mod
30	**dt_mlt_in^**	0.10	1.50	1.80	Temperature at which melt begins	ice_shortwave
31	**r_ice^**	-1.9	0.0	1.9	Sea ice tuning parameter	ice_shortwave
32	**r_pnd^**	-1.9	0.0	1.9	Ponded ice tuning parameter	ice_shortwave
33	**r_snw^**	-1.9	1.5	1.9	Snow tuning parameter	ice_shortwave
34	**rsnw_melt_in^**	500.0	1500.0	2000.0	Maximum snow grain radius	ice_shortwave
35	**Ksno**	0.10	0.30	0.35	Thermal conductivity of snow	ice_therm_vertical
36	**mu_rdg**	3.0	4.0	5.0	Gives e-folding scale of ridged ice	ice_mechred

Climate UQ Machinery

Hypercube Analysis

(global sensitivities, unfiltered uncertainties)



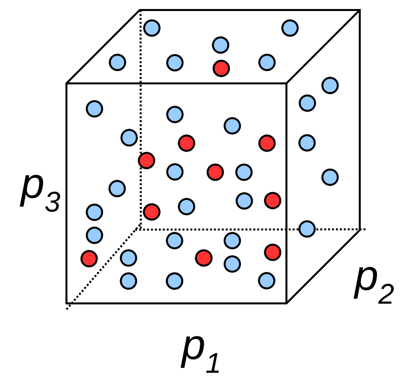
○ = simulations at sample points

(LHS & MOAT sampling)

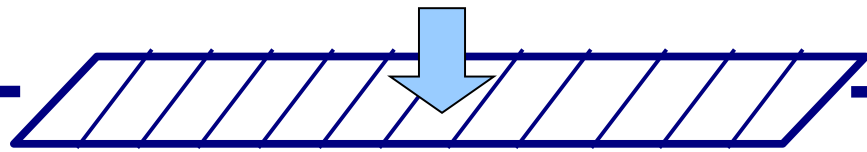
$R = f(p_1, p_2, p_3, \ldots)$

Surrogate Models

- Gaussian process models
- Polynomial chaos expansions
- Support Vector Regression
- Multivariate Adaptive Regression Splines (MARS)



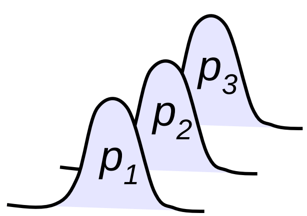
● = Surrogate predictions at new sample points



Observational constraint filter

Filtering Analysis

(parameter PDFs, response PDFs)



Filtering Methods

- Maximum likelihood parameter estimation
- Statistical filtering
  - sample *R* using LHS
  - calculate likelihoods
- Bayesian calibration using MCMC

Uncertainty Propagation

PDFs of present day climate quantities of interest

PDFs of future climate quantities of interest (*climate sensitivity*)

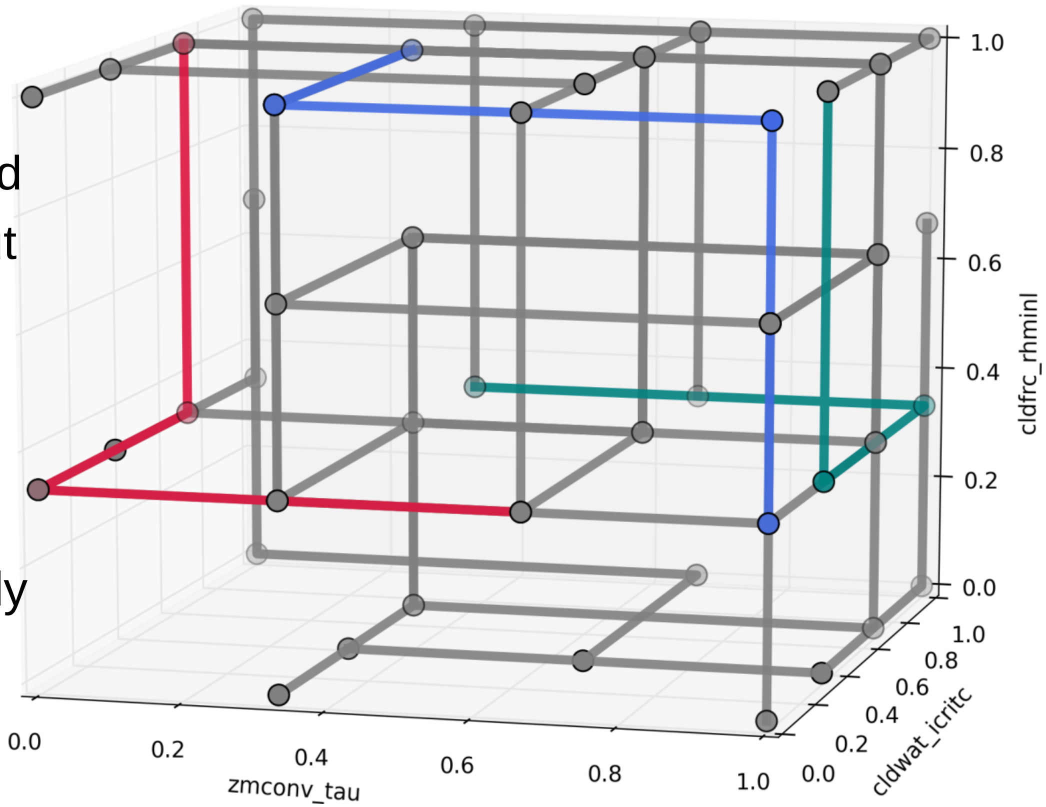
Summary of CESM UQ ensemble runs

Study Type	Ocean Mode	# Runs	Sim-Yrs/ Run	Sim-Yrs/ Study Type	Stored Size (TB)	Study Description
ics	prescribed	88	12	1,056	1.5	Six different Initial condition files
ldh	prescribed	3	12	36	0.0	Low/Default/High params
lhs	prescribed	110	12	1,320	1.6	Surrogate-based UQ
moat	prescribed	720	12	8,640	10.8	MOAT parameter screenings
nond	prescribed	1,850	12	22,200	26.3	Surrogate-based UQ
oat	prescribed	257	12	3,084	3.7	One At a Time analysis
vbd	prescribed	121	12	1,452	1.7	Surrogate-based UQ
ldh	som	17	36-60	728	1.4	Low/Default/High params
nond	som	226	30-40	7,840	15.8	Surrogate-based UQ
FY11 Subtotals =>		**1,772**		**26,916**	**38**	
TOTALS =>		**3,392**		**46,356**	**63**	

Over 18.4M cpu-hrs used on LLNL’s Atlas, more than 46,000 climate model years simulated, and 63TB of ensemble data generated

Analyzing Climate Model Sensitivities

- Morris (*Technometrics*, 1991)
- *M*ulti-path One-At-a-Time
  Sample along multiple paths and build up statistics of sensitivities throughout parameter space
- Easy to implement
- Relatively low computational cost
  $N_{\text{runs}} = M\,(N_{\text{p}} + 1)$
  M = number of MOAT paths (usually 10-20)
- *Screen* and *rank* important parameters with linear or non-linear effects
- Gridded sensitivities for no extra cost



20 MOAT paths in 3 of 21 dimensions

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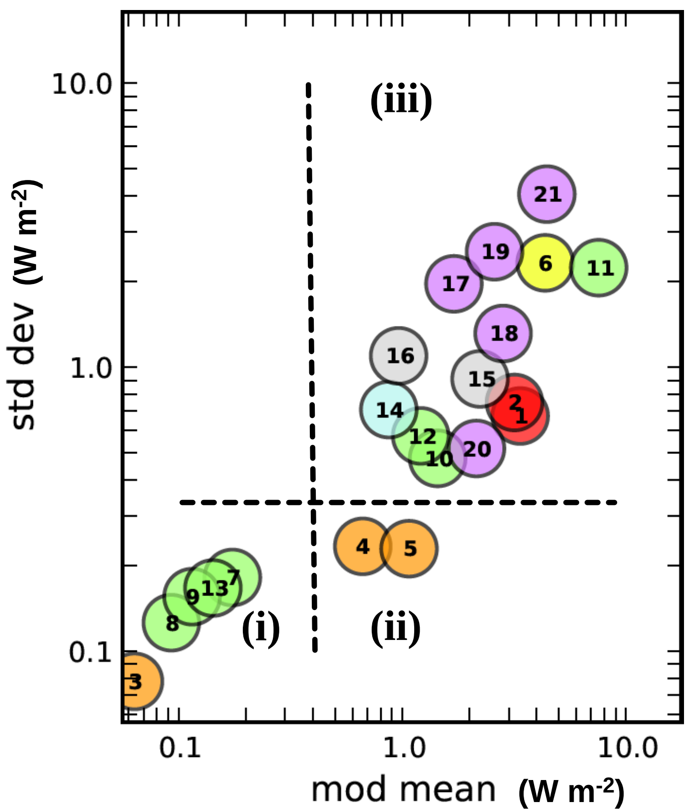
Example MOAT Screening Diagram



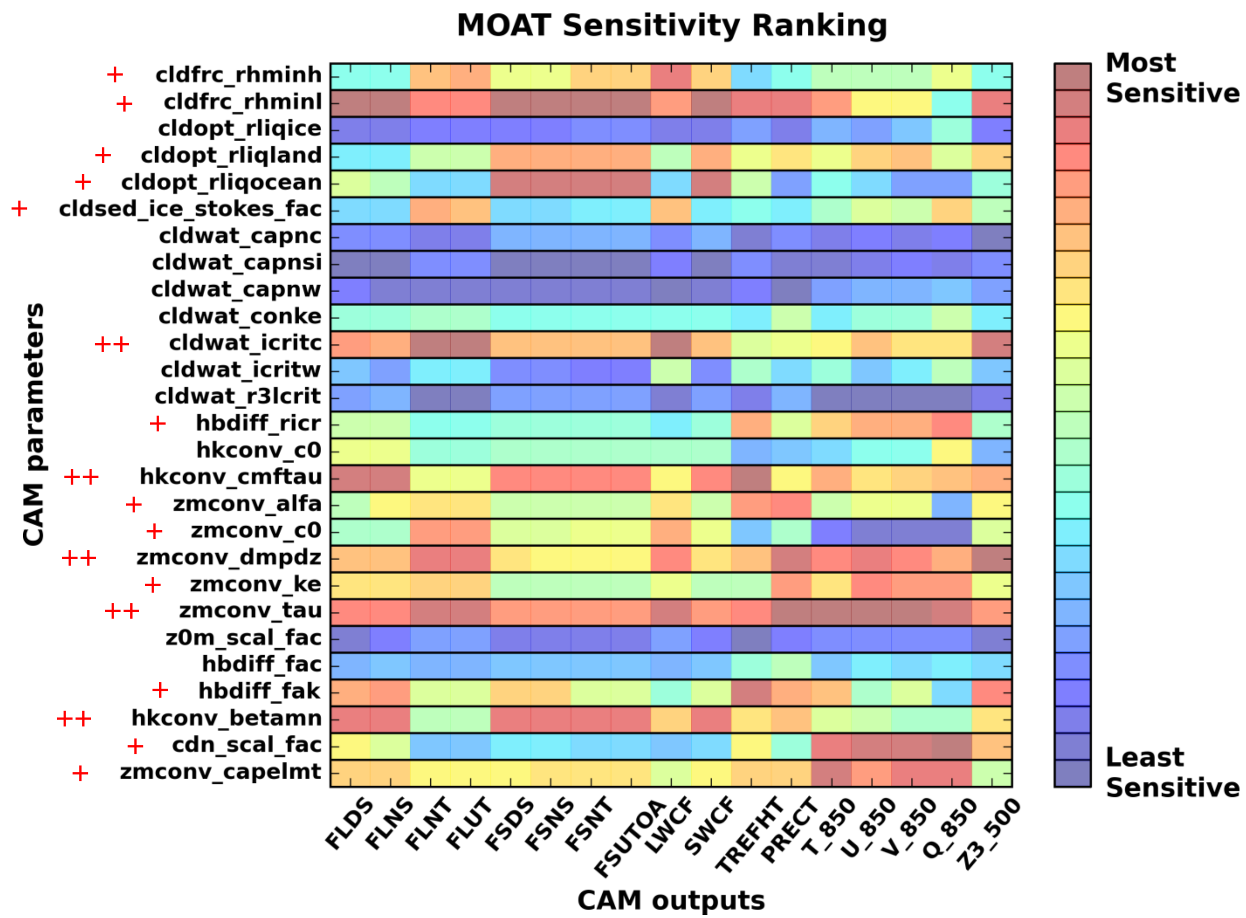
Sensitivity of the global average upwelling longwave flux (FLUT) at the top of model to 21 parameters in CAM3

Red cldfrc
Orange cldopt
Yellow cldsed
Green cldwat
Blue hbdiff
Gray hkconv
Violet zmconv

(i) Not important
(ii) Important and linear
(iii) Important and non-linear

Analyzing Climate Model Sensitivities

- Highly ranked parameters are targets for calibration.
- A sensitivity ranking for CAM4 using the Morris screening method is shown on the right
- 27 parameters are ranked across 17 outputs
  - A handful of parameters are important to many outputs (++)
  - Many parameters are important to at least one output (+)



Visualizing the Variance Decomposition of Climate Model Responses

Network Diagram of Sobol Indices

The total variance is expressed as:

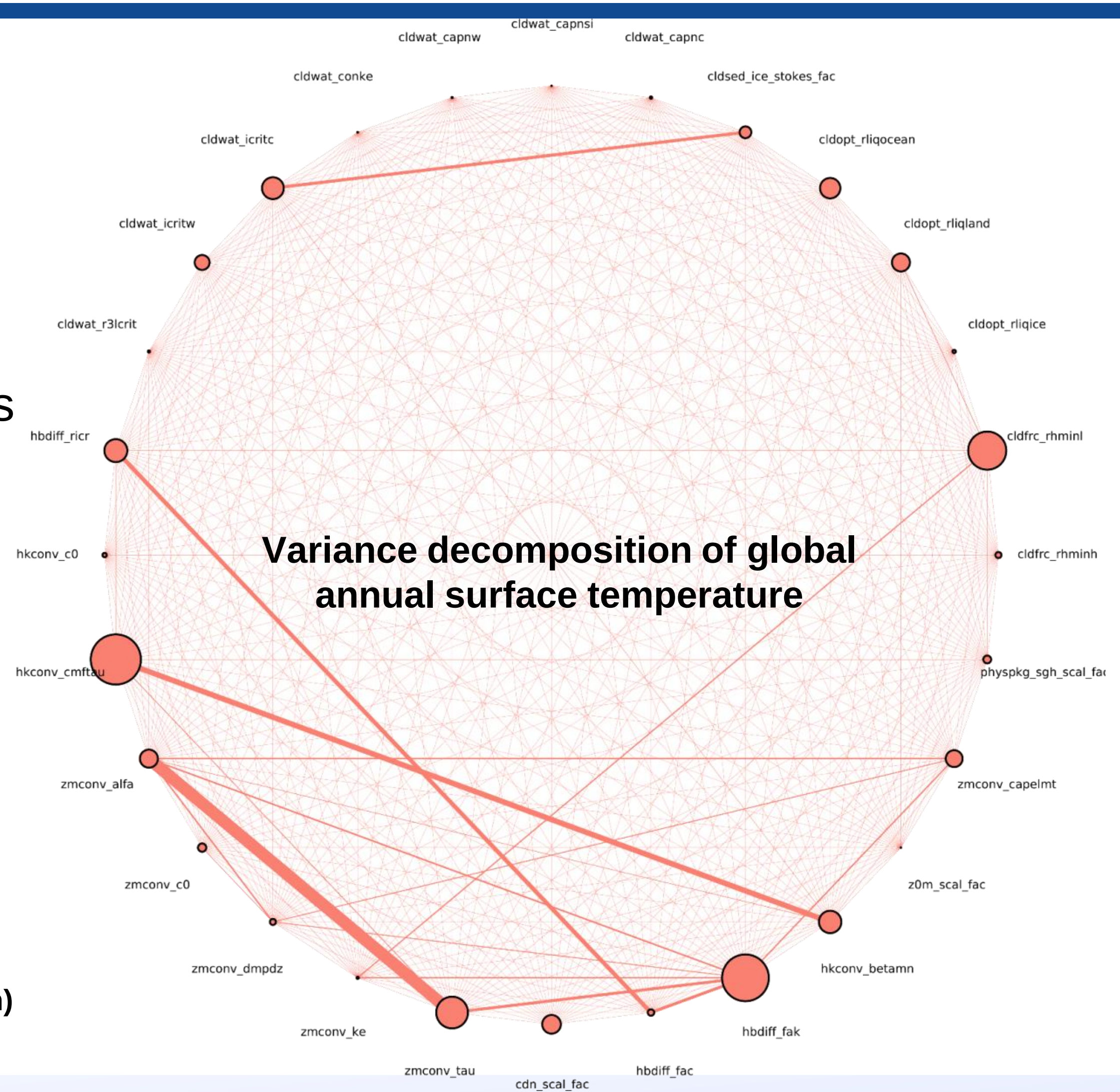
$v_t = \Sigma v_i + \Sigma v_{ij} + \Sigma v_{ijk} + \ldots$, where
v_i = variations from parameter *i*
v_{ij} = co-variations from parameters *i* and *j*

We represent the variance contributions on a network graph.

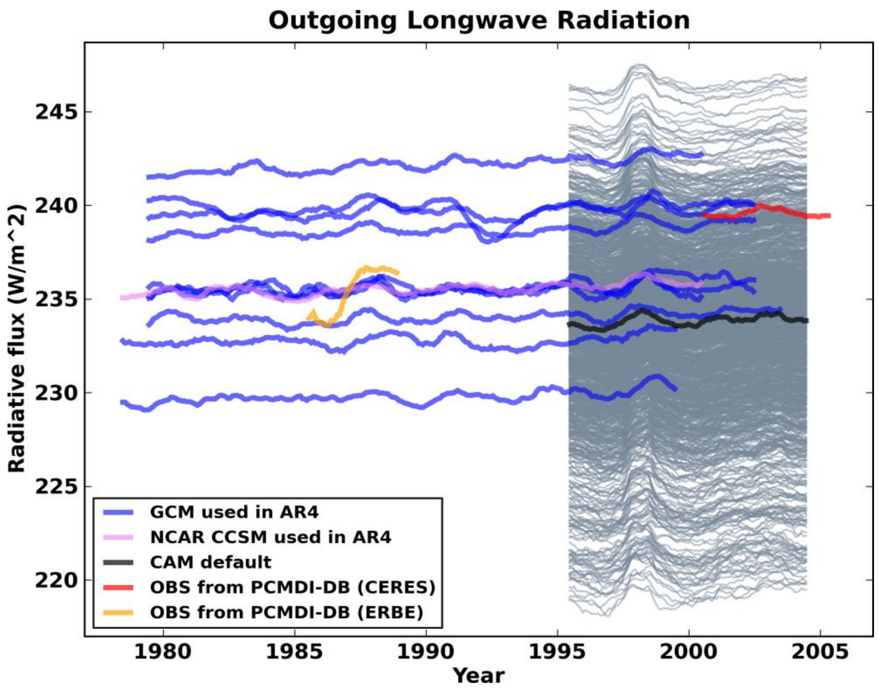
node diameter $\propto V_i / V_{tot}$ (main effects)

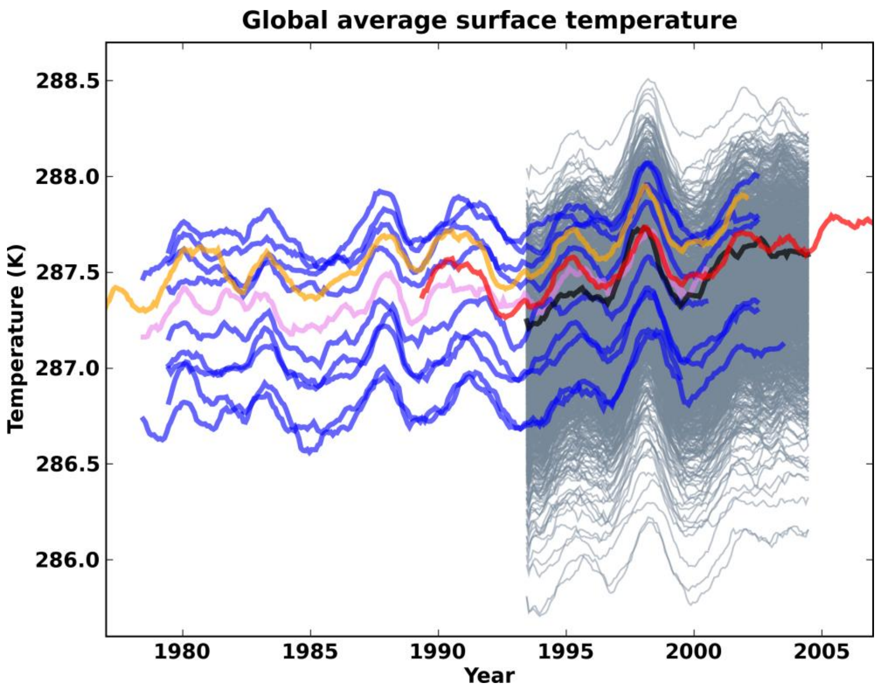
edge width $\propto V_{ij} / V_{tot}$ (interactions)

(only two-way interactions shown, but higher orders can also be displayed on the same graph)



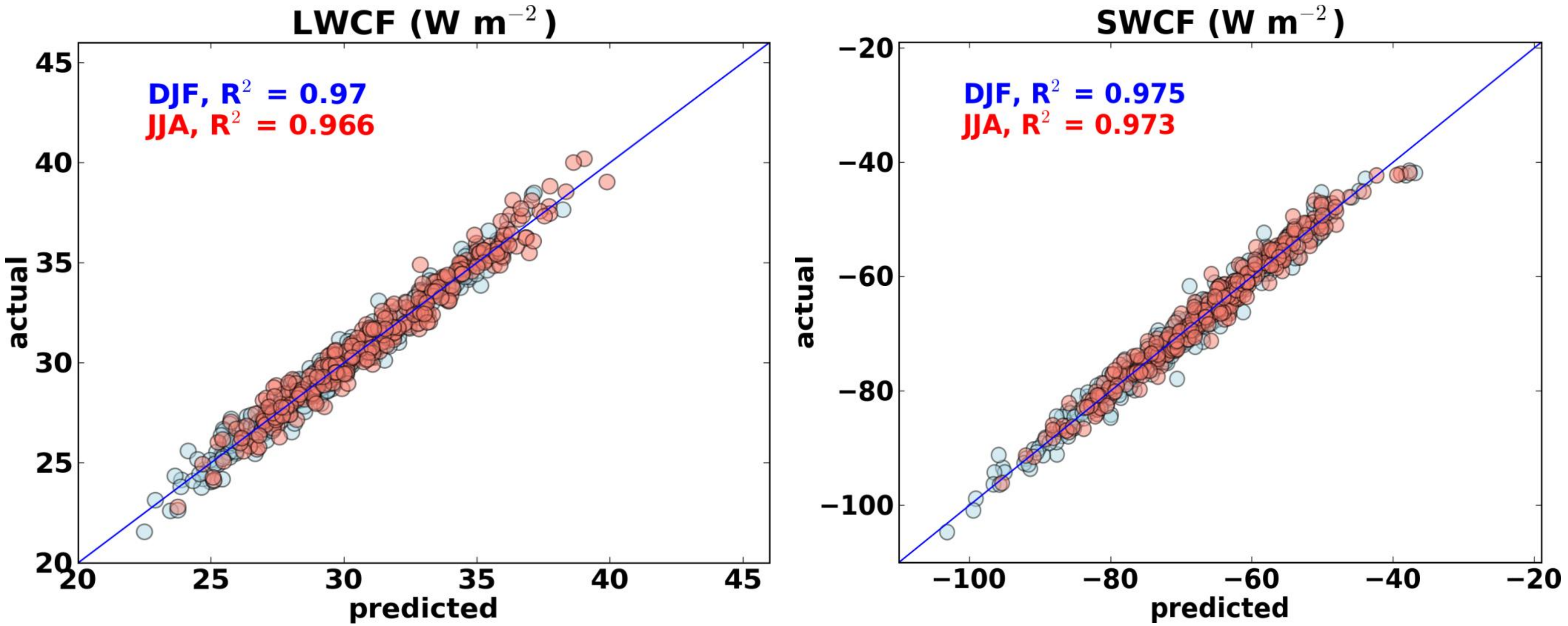
Examples of Unfiltered Ensembles





- Unfiltered ensembles consider only the *prior* parameter uncertainties
- *Filtering* is the process of constraining the ensembles with observations
- Having a large unfiltered ensemble spread facilitates the filtering process (i.e. it's easier to interpolate than extrapolate)

Surrogate Models



- Surrogate models are validated using independent data.
- Examples of the actual and predicted `LWCF` and `SWCF` responses are displayed above.
  - surrogates were derived using *Support Vector Regression* trained on over 1,000 CAM4 runs and tested on 300 independent runs.
- Surrogate model errors are important and factored in the UQ analysis.

Initial Bayesian calibration of CAM

Sample joint posterior distribution given prior information (uniform PDFs) and observational constraints (likelihoods).

$$\underbrace{P(\text{params} \mid \text{obs})}_{\text{posterior}} \propto \underbrace{P(\text{obs} \mid \text{params})}_{\text{likelihood}} \underbrace{P(\text{params})}_{\text{flat priors}}$$

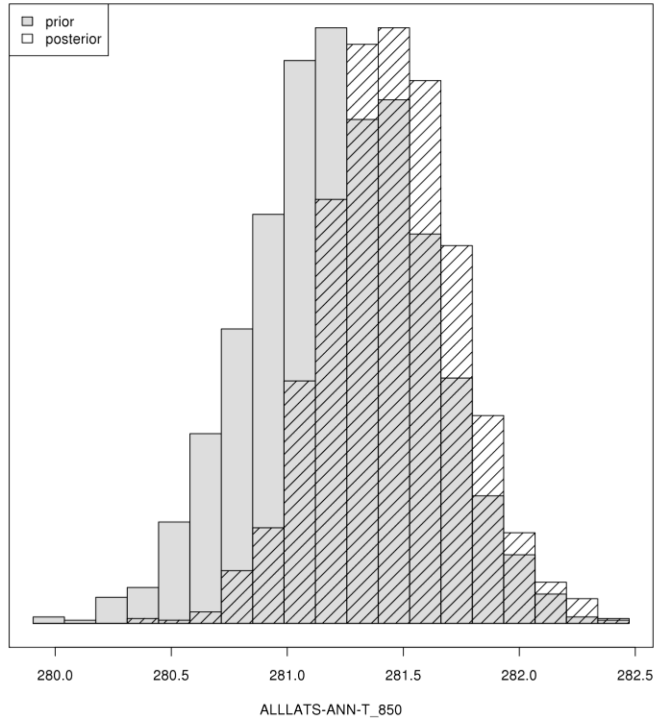
Trained and validated 24 Gaussian Process surrogate models on ~1,300 LHS CAM4 simulations: [`FLUT`, `FSUTOA`, `LWCF`, `PRECT`, `Q_850`, `SWCF`, `T_850`, `Z3_500`] x [ANN, DJF, JJA]

Observational constraints (w/ "loose" uncertainties): CERES (`FLUT`, `LWCF`, `SWCF`), GPCP (`PRECT`), NCEP (`Z3_500`)

Use a hierarchical Bayesian model

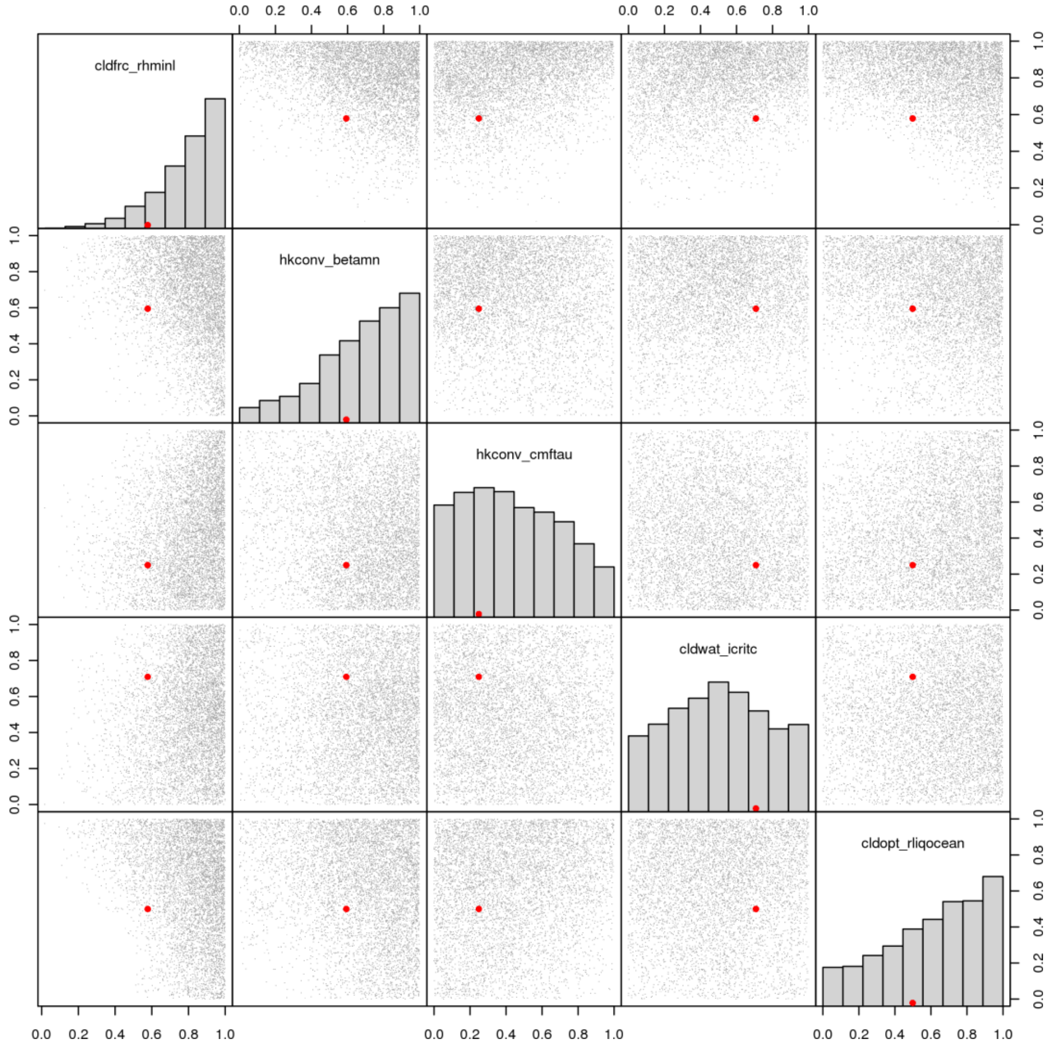
OBS = SYS + OBS_err
SYS = CAM4(p) + MOD_err
CAM4(p) = SURR(p) + SURR_err

MCMC used to sample the joint posterior distribution.



Above: prior and posterior PDFs for a response to which observational constraints were not applied

Parameter PDFs are not well constrained



Posterior Parameter PDFs

Diagonal shows the marginal posterior distribution of 5 selected input parameters (those most constrained by the observations)

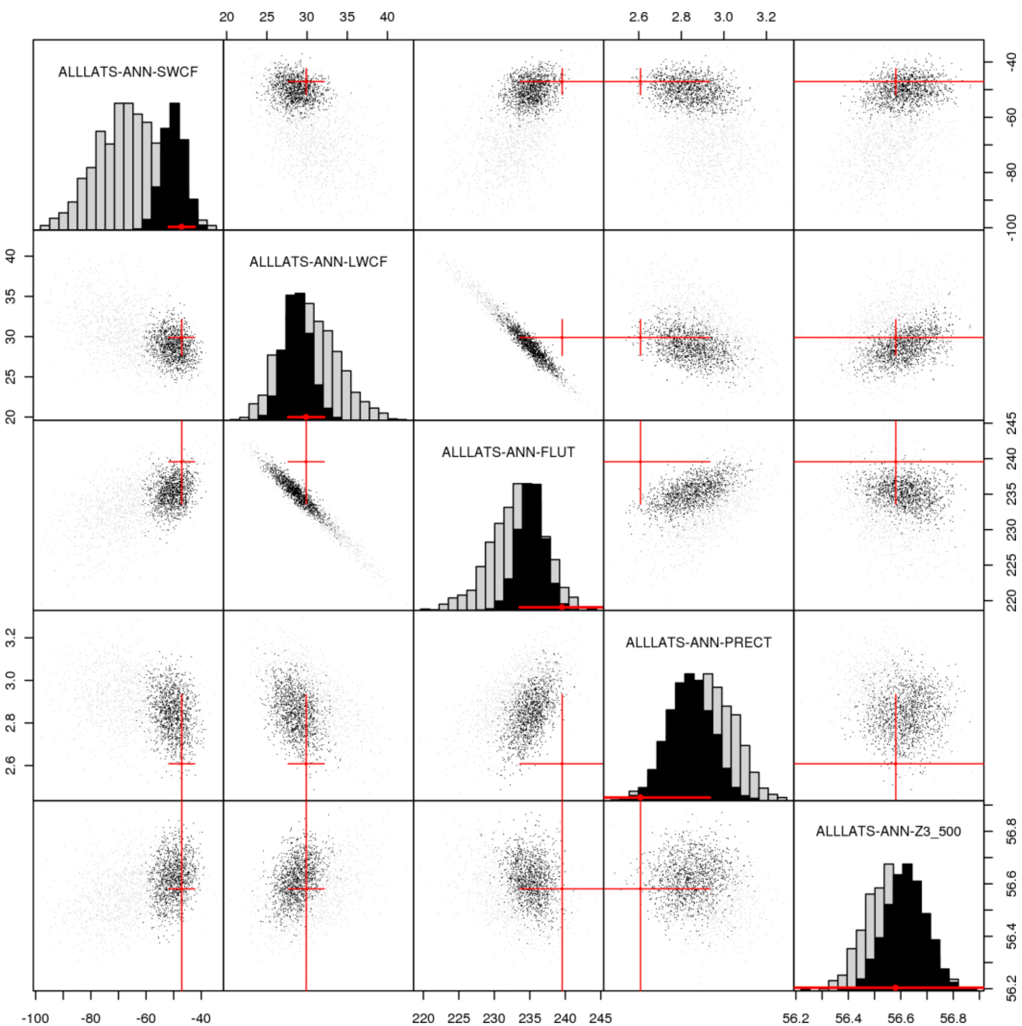
Off-diagonal shows posterior realizations (dots) from the bivariate distributions

Red dots show the default values

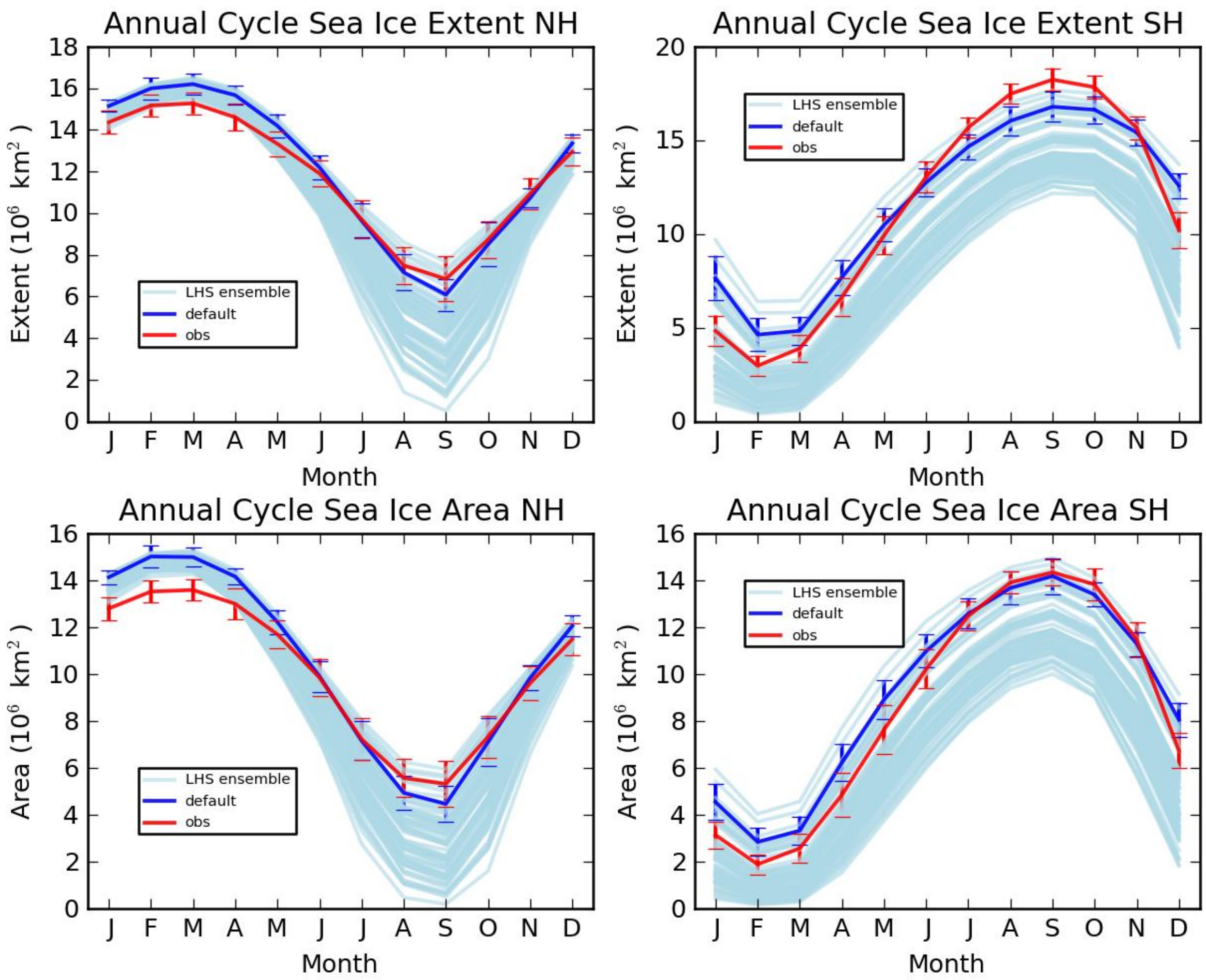
CAM responses are moderately well constrained

Posterior distribution of selected output variables

- Diagonal (marginal)
  - light-gray histograms show the prior (unfiltered) distributions
  - black histogram the posterior (filtered) distributions
  - red dots/bars show the observational constraints
- Off-diagonal (bivariate)
  - light-gray scatter plots show prior distributions
  - black scatter plots show posterior distributions
  - along with observations and error bars

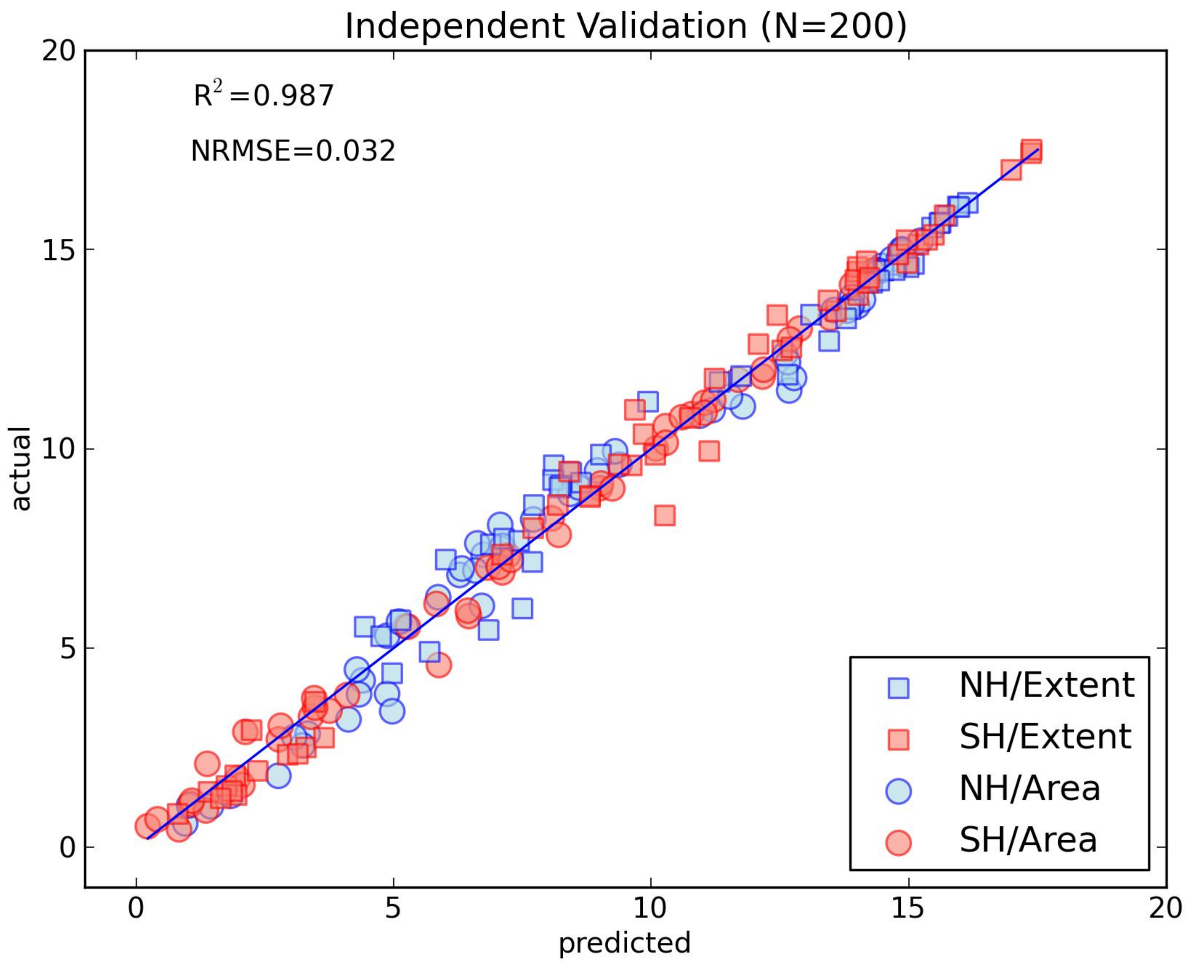


Moving on to Sea Ice Model Ensembles



- Coupled climate model configuration (CAM-CICE-Slab Ocean)
- More expensive model, longer integrations
- Sampled 7 parameters using 70 LHS runs
- Trained surrogate model on ensemble simulations
- Used surrogate model to perform statistical inference given observational data

Surrogate Model of Sea Ice Ensemble



Surrogate model using Support Vector Machine

fit single surrogate using hemisphere, month and quantity as predictors

$S = f(h, m, q, p_1, \ldots, p_7)$

Important difference with initial atmospheric calibration – used annual cycle information

Variance decomposition to select ice parameters for inference

Network Diagram of Sobol Indices

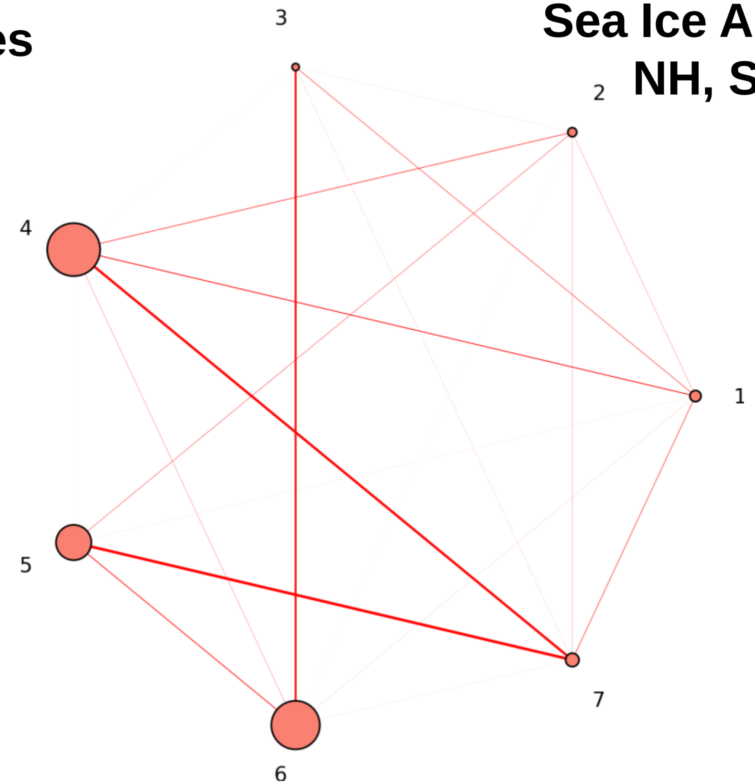
- Compute variance decomposition for each hemisphere, month and quantity
- Selection criterion
  keep parameter i if max(Vi/Vtot) > 5%
  keep parameters i,j if max(Vij/Vtot) > 5%
- Three parameters retained
  r_snw, rsnw_melt_in, ksno

node diameter ∝ V_i / V_{tot} (main effects)

edge width ∝ V_{ij} / V_{tot} (interactions)

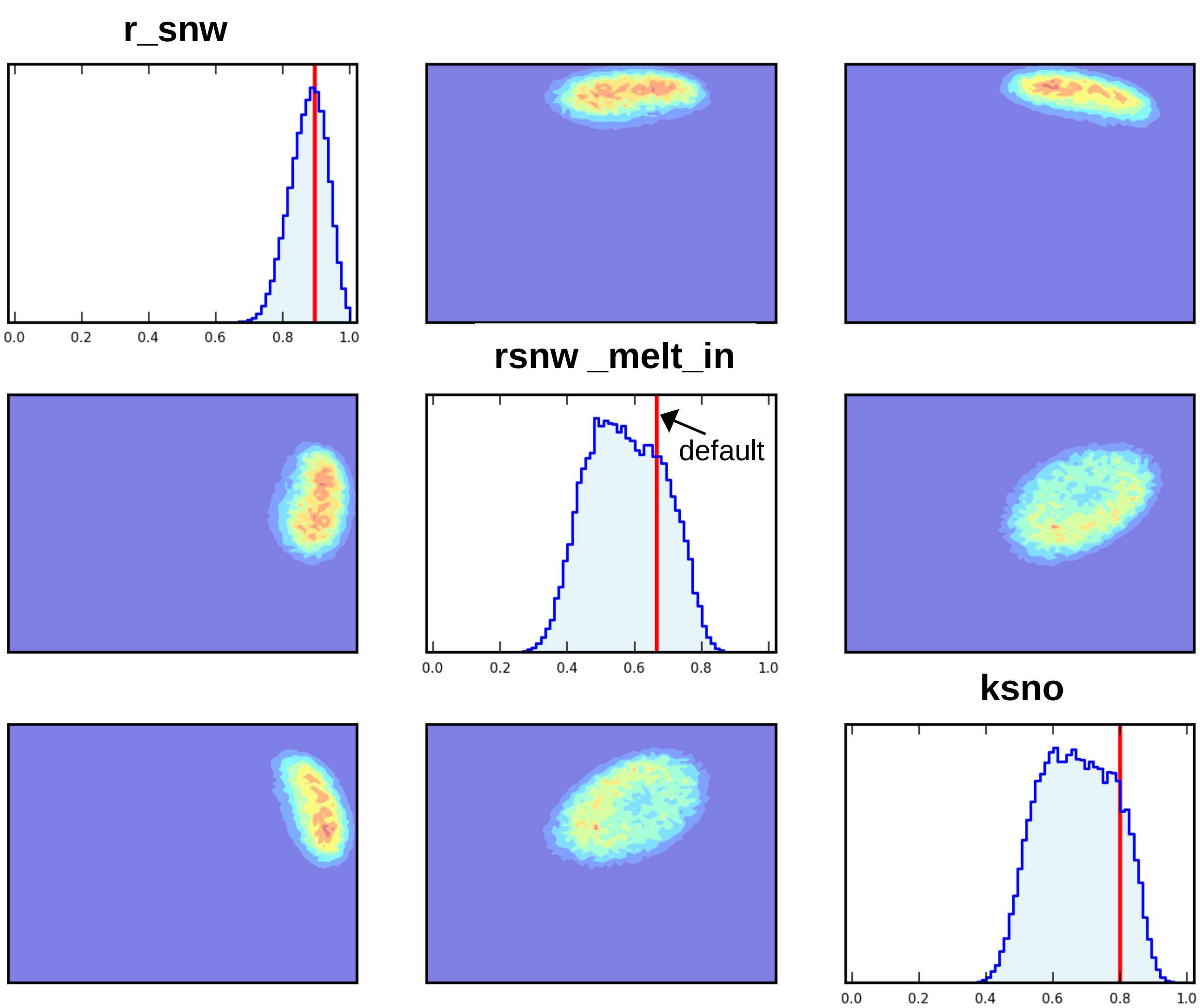
(only two-way interactions shown, but higher orders can also be displayed on the same graph)

Sea Ice Area
NH, SEP



1 = dt_mlt_in *temperature at which melt begins* (0.10, 1.50, 1.80)
2 = r_ice *sea ice tuning parameter* (-1.9, 0.0,1.9)
3 = r_pnd *ponded ice tuning parameter* (-1.9, 0.0, 1.9)
4 = r_snw *snow tuning parameter* (-1.9, 1.5, 1.9)
5 = rsnw_melt_in *maximum snow grain radius* (500, 1500, 2000)
6 = ksno *thermal conductivity of snow* (0.10, 0.30, 0.35)
7 = mu_rdg *e-folding scale of ridged ice* (3, 4, 5)

Posterior Sea Ice Parameter PDFs

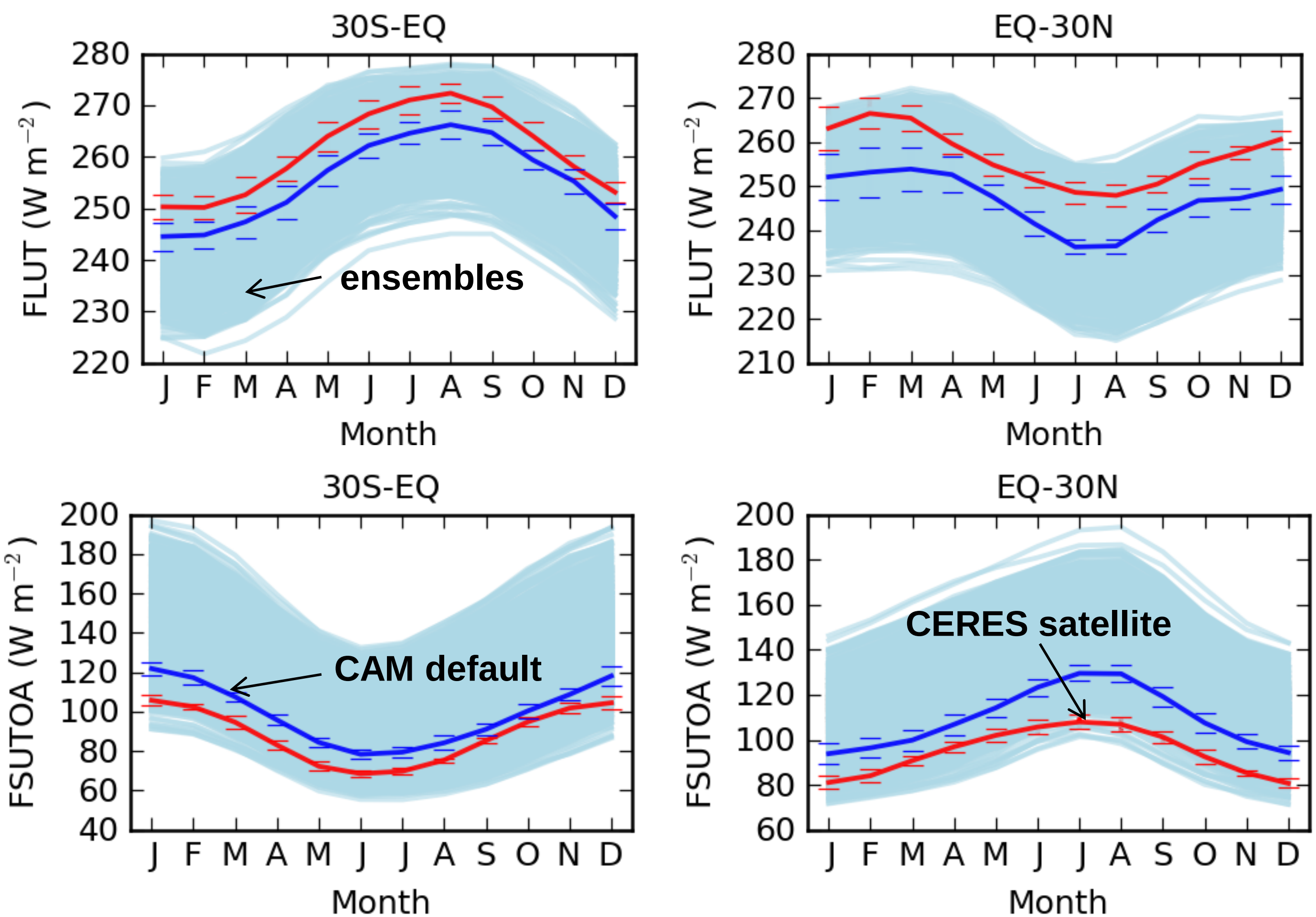


Diagonals are marginals; off-diagonals are bivariates

Ice parameters are well constrained.

Samples from the posteriors will serve as the basis for climate change ensembles

Revisited CAM calibration using annual cycles of energy fluxes from satellite data



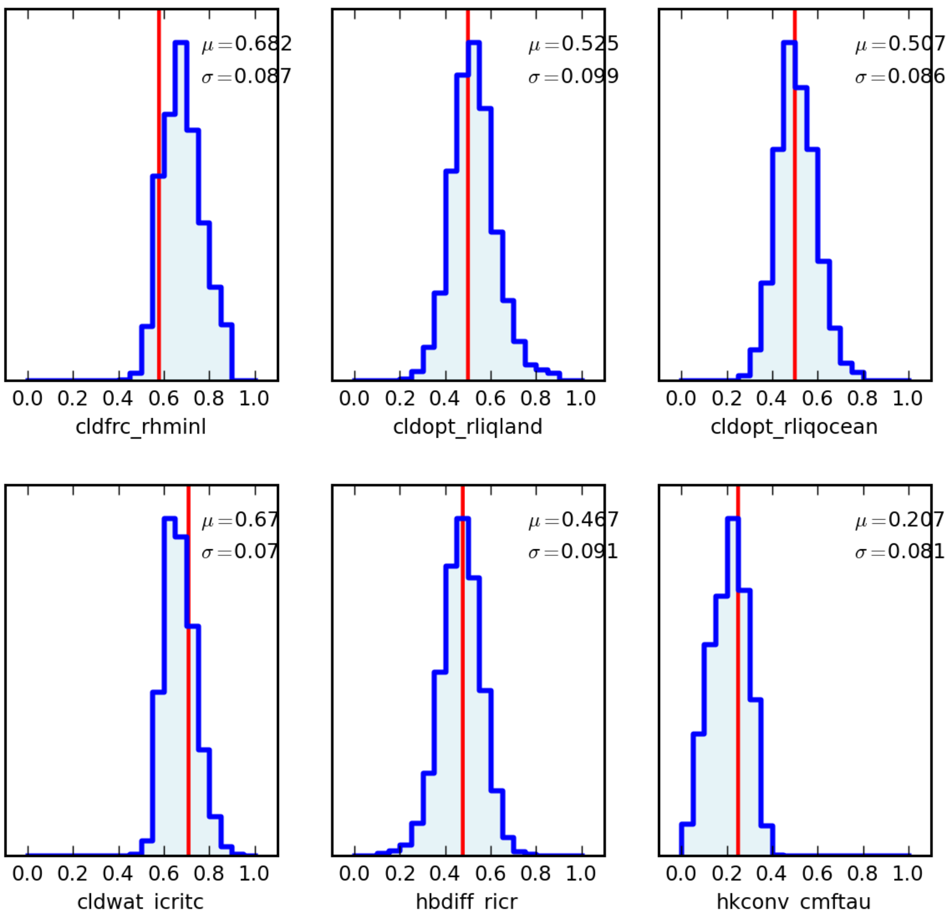
Given the success with the CICE calibration, we are revisiting CAM constraining with annual cycles of energy fluxes

Upper row: out-going longwave radiation

Lower row: out-going shortwave radiation

Parameter PDFs using annual cycles of energy fluxes are well constrained

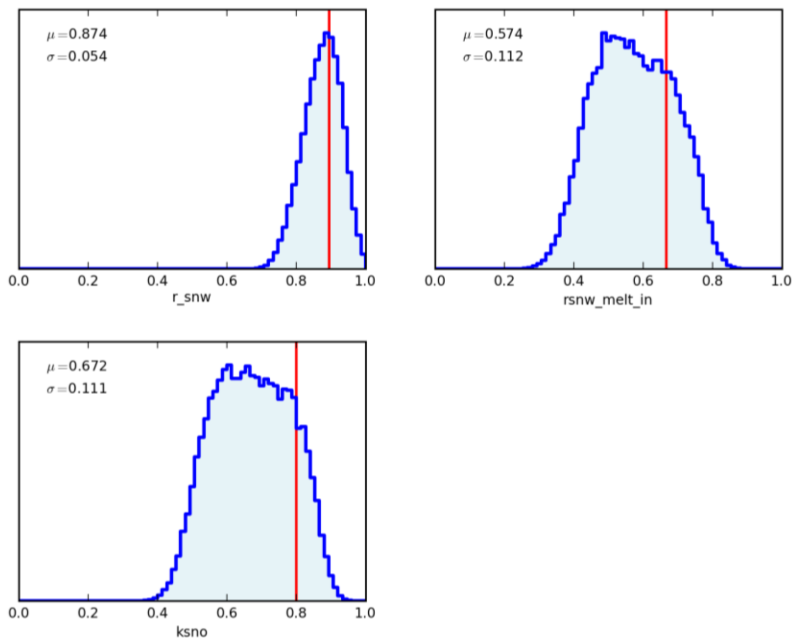
CAM posterior parameter PDFs



and more …

+

CICE posterior parameter PDFs



Forward UQ: The posterior parameter PDFs from the atmospheric and sea ice models serve as a basis for propagating model uncertainties through CO_2 change ensembles

Iterative Ensemble-based Climate UQ

- Start with simulations according to a given design

  LHS-based ensemble to train statistical output emulators
  MOAT-based design for sensitivity analysis (no emulator)

- Initial analysis, but too inaccurate due to few simulations

- Next runs to improve the accuracy of the analysis?

  Q: global and/or local improvements?

  - Improve prediction accuracy of emulators globally (e.g. global sensitivity analysis)
  - Improve emulators in a region of the input space (e.g. statistical calibration)

- Iterate between analysis and sampling until the accuracy of the results are satisfactory

Sequential and Adaptive Sampling

And The Aggregation of Those

Multiple objectives

- Want to understand the response of multiple output variables of interest to variation in uncertain inputs
- What uncertain parameters drive the variation in a given output?
- Constrain the input uncertainty using observations (go from prior input uncertainty to posterior input uncertainty)

Multiple methods for sequential and adaptive sampling

- Such methods are often driven by single output quantity of interest (QoI)

Examples:

- Improve the prediction accuracy of a statistical emulator for a QoI
- Input-space filling and response-shape driven designs

Aggregate the feedback from multiple adaptive sampling strategies

- Adaptive sampling and aggregation strategies are being studied at LLNL

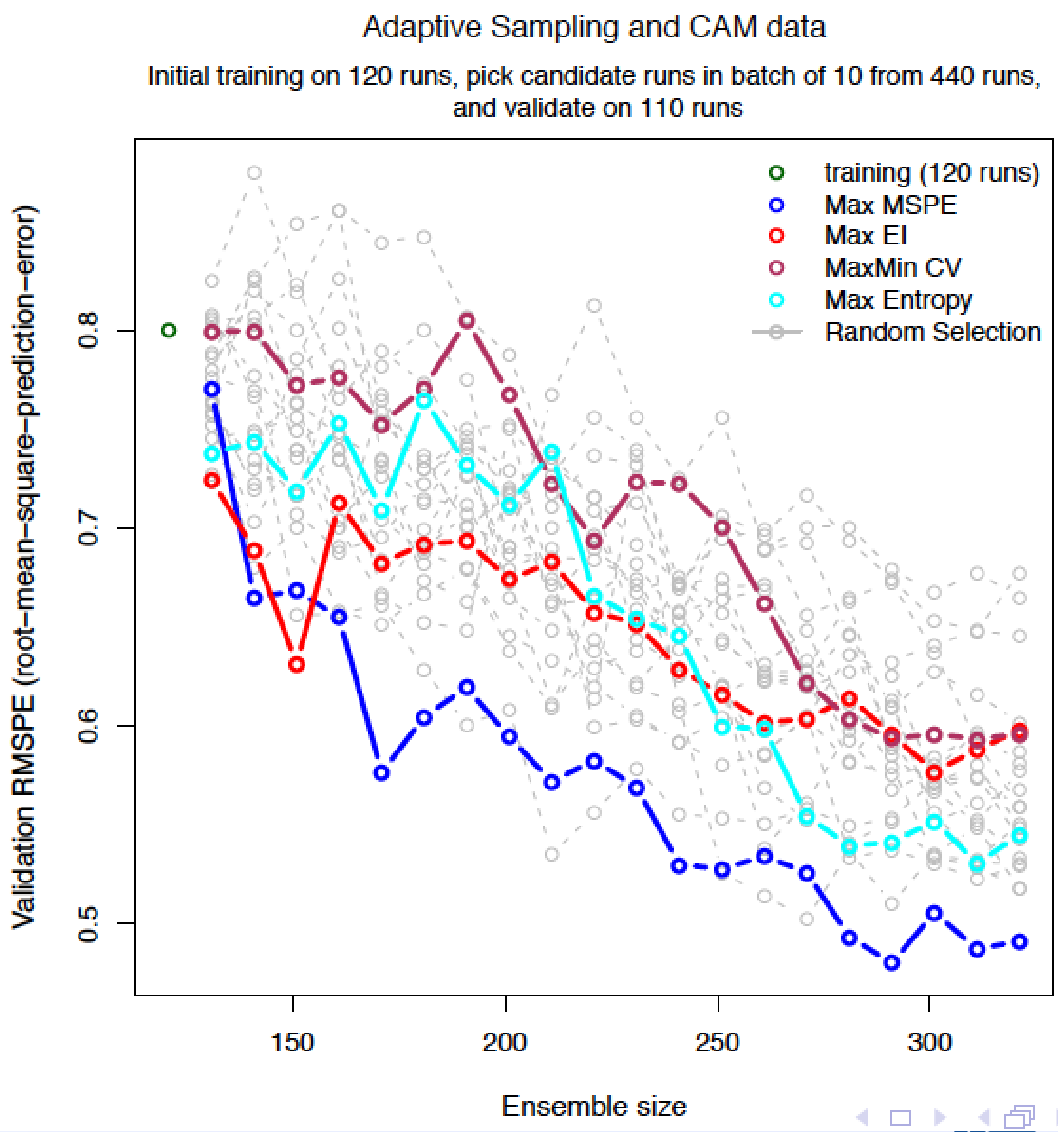
Example: Case Study of Adaptive Sampling of 21 Uncertain CAM Input Parameters

Goal: Compare different adaptive sampling strategies to select new CAM simulations

Setup: three sets of LHS-designed ensembles of size 110, 120, and 440

Study:

- Train a GP emulator on 120 simulations to predict a scalar QoI and then validate on 110 runs
- Select additional runs, in batches of 10, from the existing ensemble of 440 simulations using four different adaptive sampling criteria



Summary

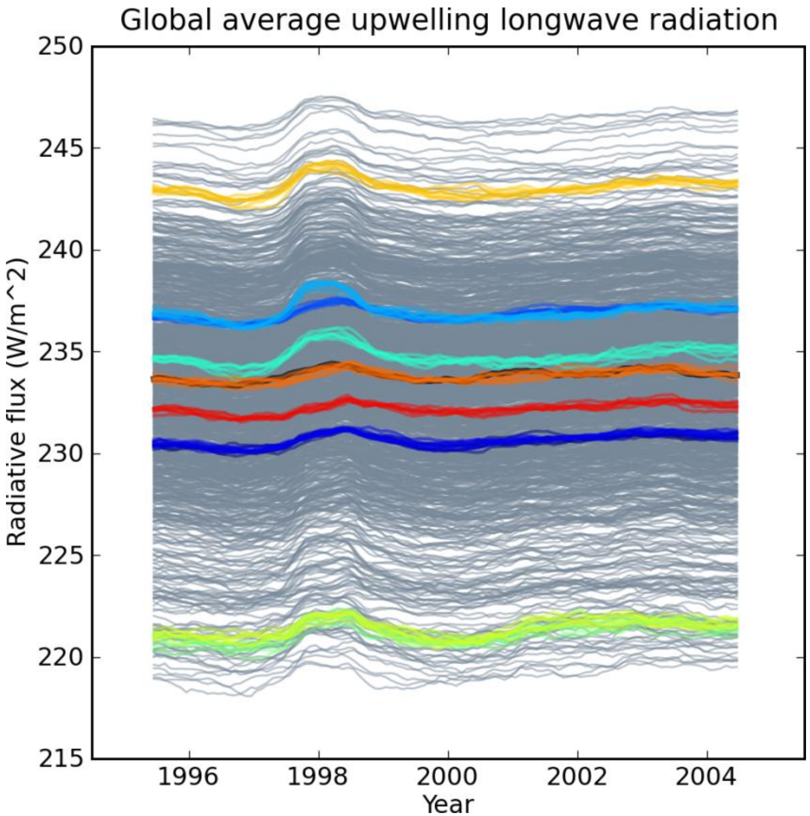
- **We have performed UQ analysis on the CESM using:**
  - the *UQ Pipeline* to generate a large database of ensemble runs
  - surrogate models as inexpensive proxies for the actual models
  - multiple methods for combining observations and ensembles

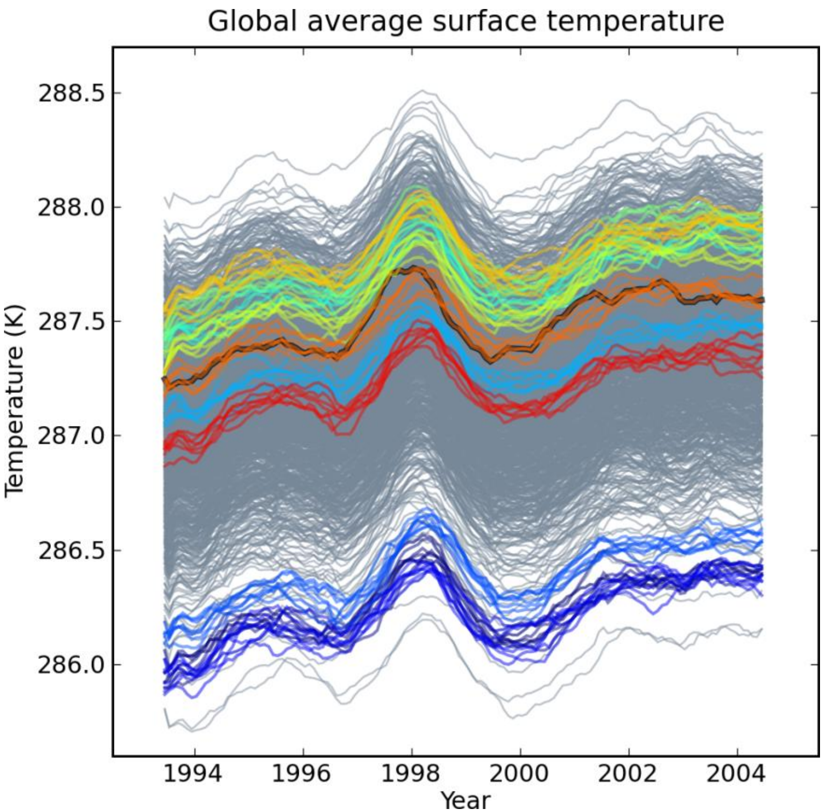
- **Calibrating the CAM and CICE models depends critically on the observations and metrics**
  - Using surrogate models provides an efficient way to quantify the assumptions made during ensemble filtering. (e.g. What observations should we use? How should we combine the data and ensembles?)

- **Using the information from the present-day calibration to propagate uncertainties through climate change simulations**
  - Equilibrium climate sensitivity using CAM + CICE + SOM (expensive)
  - Transient climate change using CAM + CICE + POP (very expensive)
  - Adaptive and sequential sampling guides the climate change ensembles

Extra slides

Perturbed Parameters vs. Initial Conditions





- Gray lines = perturbed parameters
- Colored bands = 10 different initial conditions for fix parameter set

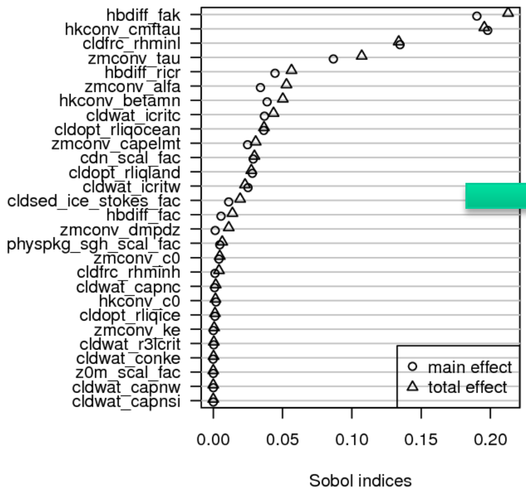
Example: Case Study of Using Variable Selection and Statistical Filtering to Design a Batch of CAM-SOM Runs

Goal: use prior knowledge from CAM3/CAM4 runs to design the batches of CAM4+SOM runs

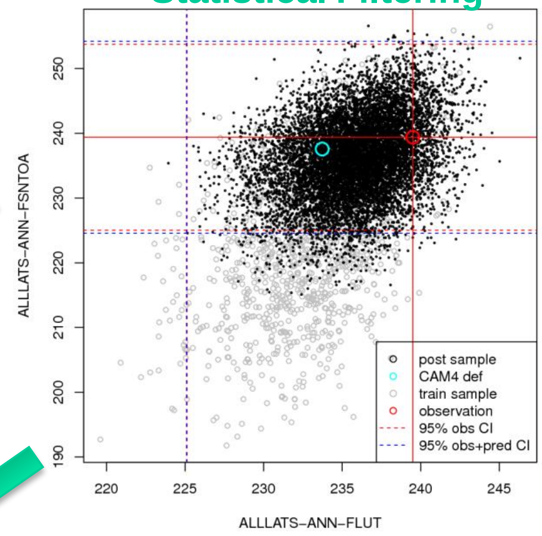
One Approach:

- Use *variable selection* to reduce the number of input CAM parameters considered
- Carry out a conservative statistical filtering to generate a large candidate set of points
- Thin the large candidate set of points down to a design set of points using, for example, a distance-based criterion

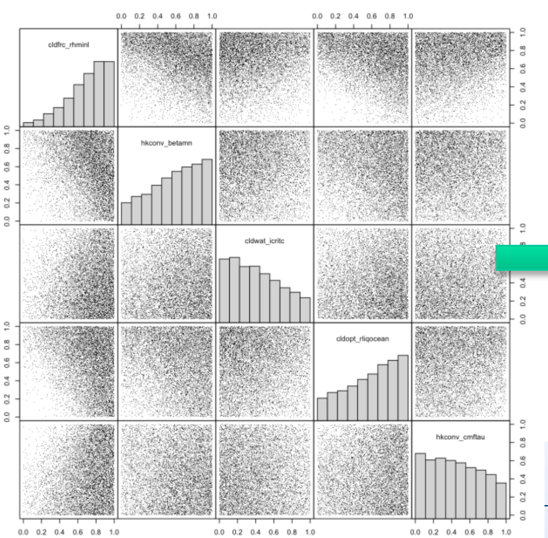
Variable Selection



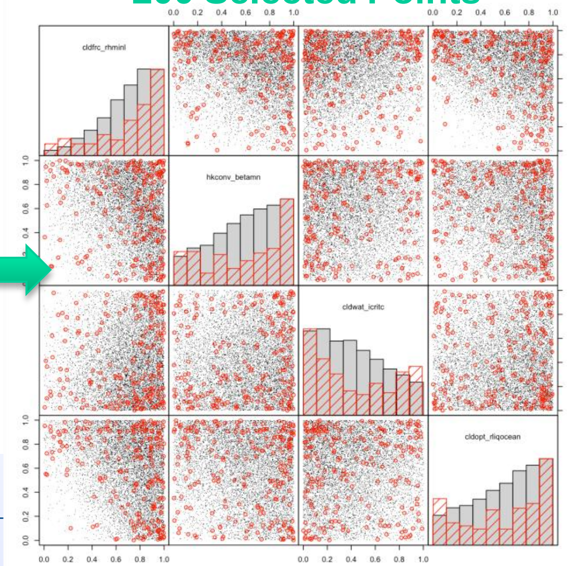
Statistical Filtering



Posterior Sample



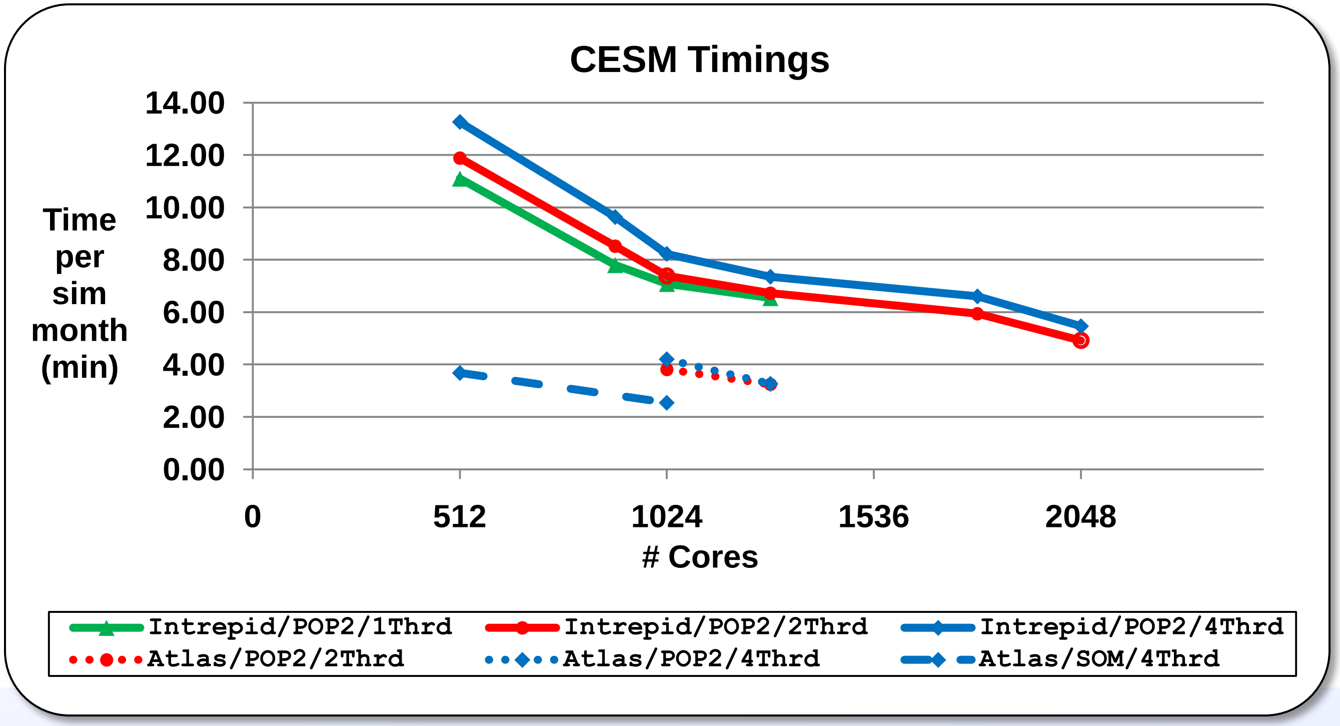
200 Selected Points



Moving to fully coupled climate UQ ensembles

"Prepare for coupled ocean-atmosphere UQ"

FY11	**FY12**
Atmosphere (CAM)	Atmosphere (CAM) +
+ Sea Ice (CICE)	Sea Ice (CICE) +
+ Slab Ocean Model (SOM)	***Full Ocean Model (POP2)***
For equilibrium climate change UQ	***Realistic time-evolving climate UQ***

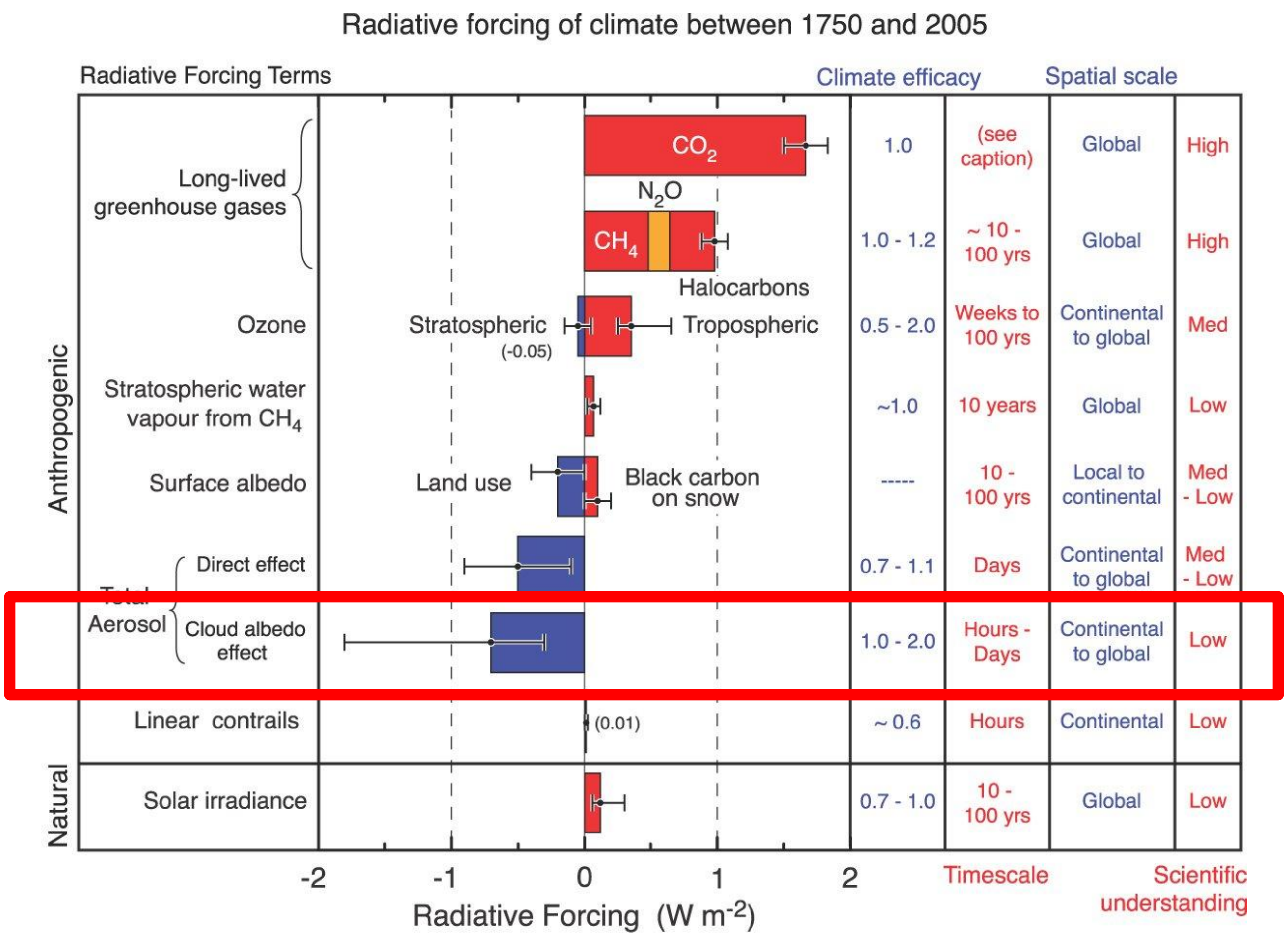


- **Performed extensive timings of the full atmosphere-ocean-ice CESM model on LLNL's *Atlas* and ANL's *Intrepid***
- **Used timing results to design coupled climate UQ experiments**
  - **Variation of CMIP5 exp 1.2**
  - **30-yr hindcast** for calibration and model selection (about 1000 ensemble members)
  - **30-yr forecast** for climate change UQ (about 150 ensemble members)
  - **Submitted proposal to INCITE** for 50M cpu-hr allocation

Uncertainties in radiative forcing

"A Watt per meter squared"

Thanks S. Schwartz!



Largest uncertainties are due to the aerosol-cloud interactions