The Community Terrestrial Systems Model (CTSM) Parameter Perturbation Experiment (PPE)

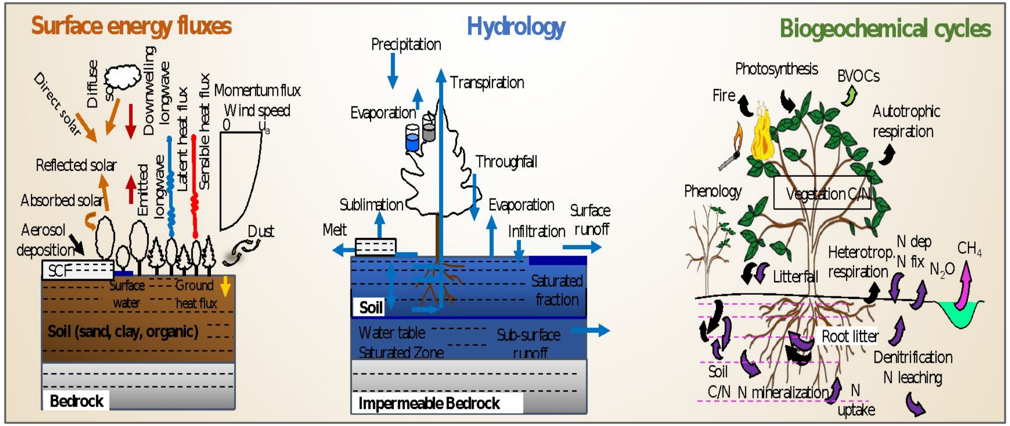
Quantifying parametric uncertainty and working towards systematic land model calibration

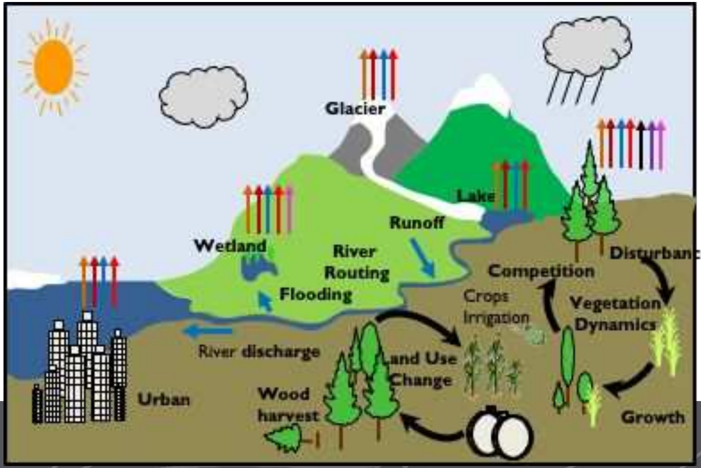
Dave Lawrence, Daniel Kennedy, Katie Dagon
and the CTSM-PPE working group (and soon, LEAP)

This material is based upon work supported by the National Center for Atmospheric Research, which is a major facility sponsored by the National Science Foundation under Cooperative Agreement No. 1852977.

Motivation for the CTSM PPE Project

- Growing complexity and comprehensiveness of land models → increasing # of uncertain parameters





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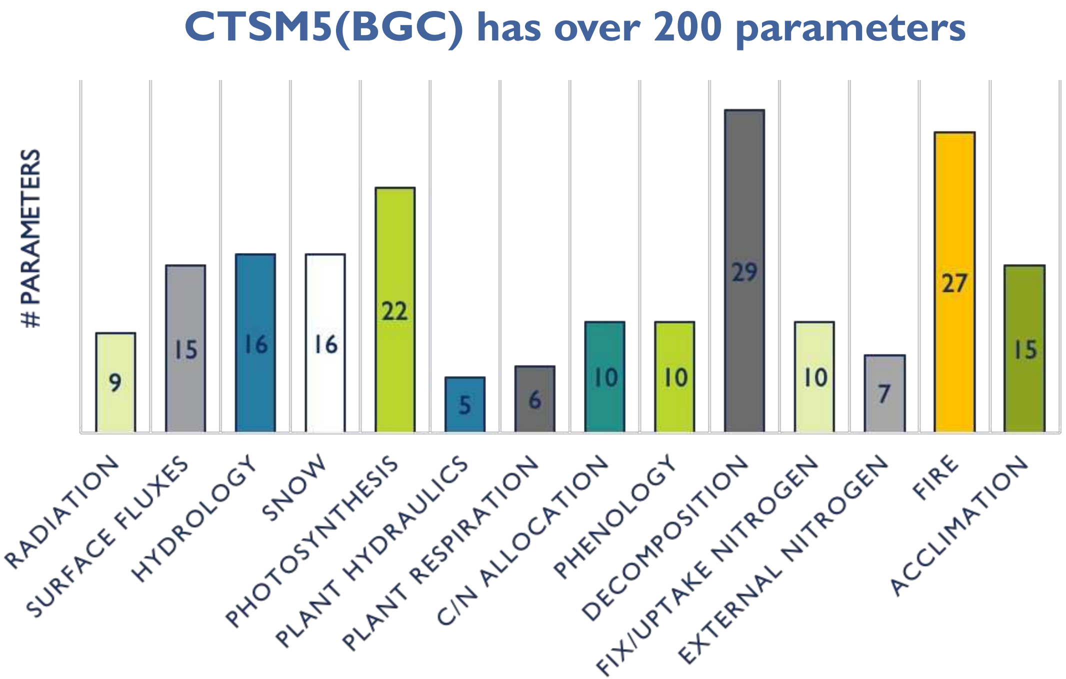


Motivation for the CTSM PPE Project

- Growing complexity and comprehensiveness of land models → increasing # of uncertain parameters

Drawbacks of hand tuning

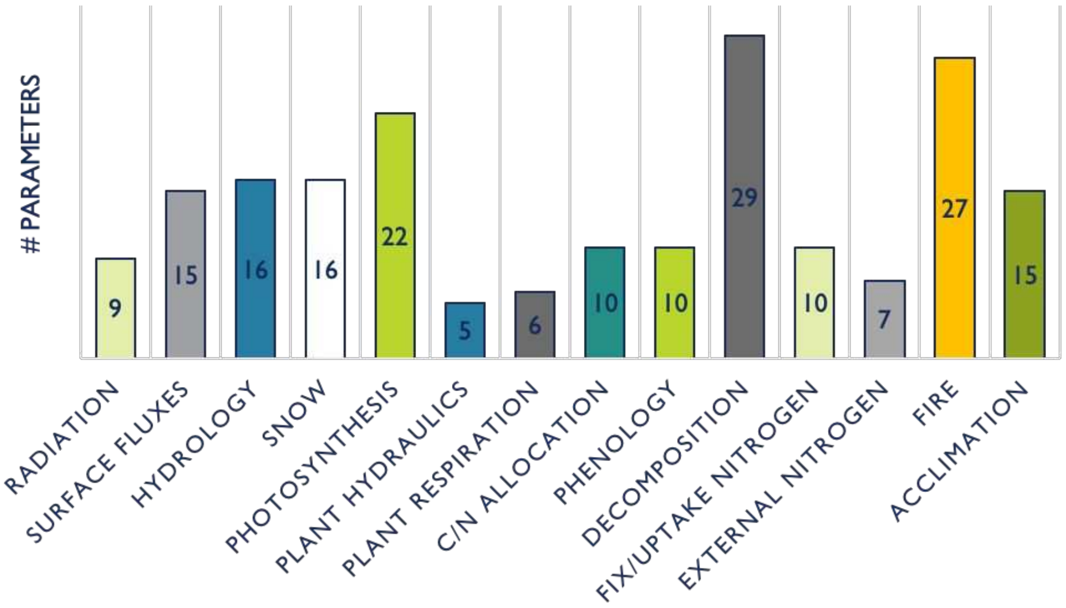
- Difficult to diagnose structural improvements

- Challenging to incorporate new parameterizations

- Impractical requisite knowledge base

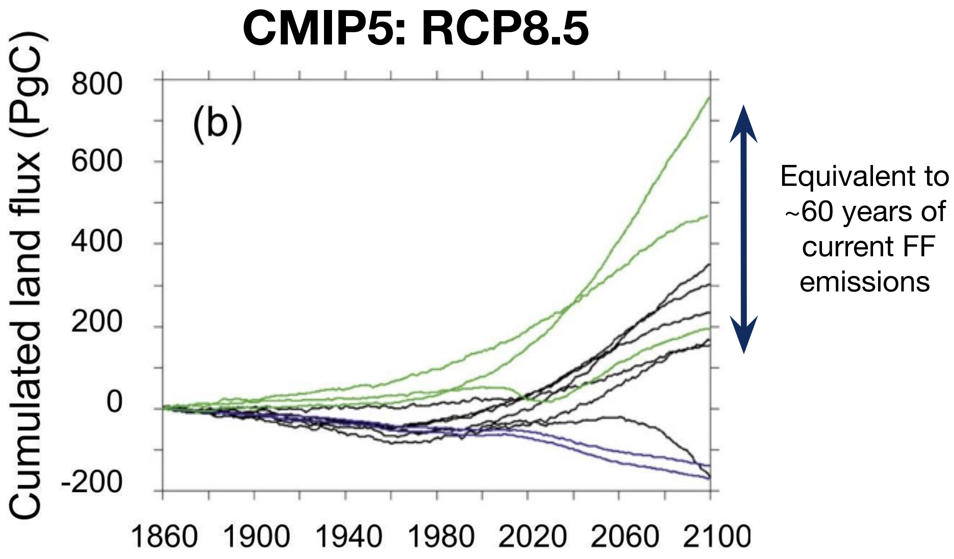
- Doesn't scale well with increasing complexity

CTSM5(BGC) has over 200 parameters



Motivation for the CTSM PPE Project

- Growing complexity and comprehensiveness of land models → increasing # of uncertain parameters (CTSM5 has over 200 parameters)
- Contribution of parameter uncertainty to total uncertainty expected to be large, but largely unquantified



Emissions driven RCP8.5: 795 to 1140 ppm CO_2

→ ±1.2C uncertainty on top of 3.7C projected change

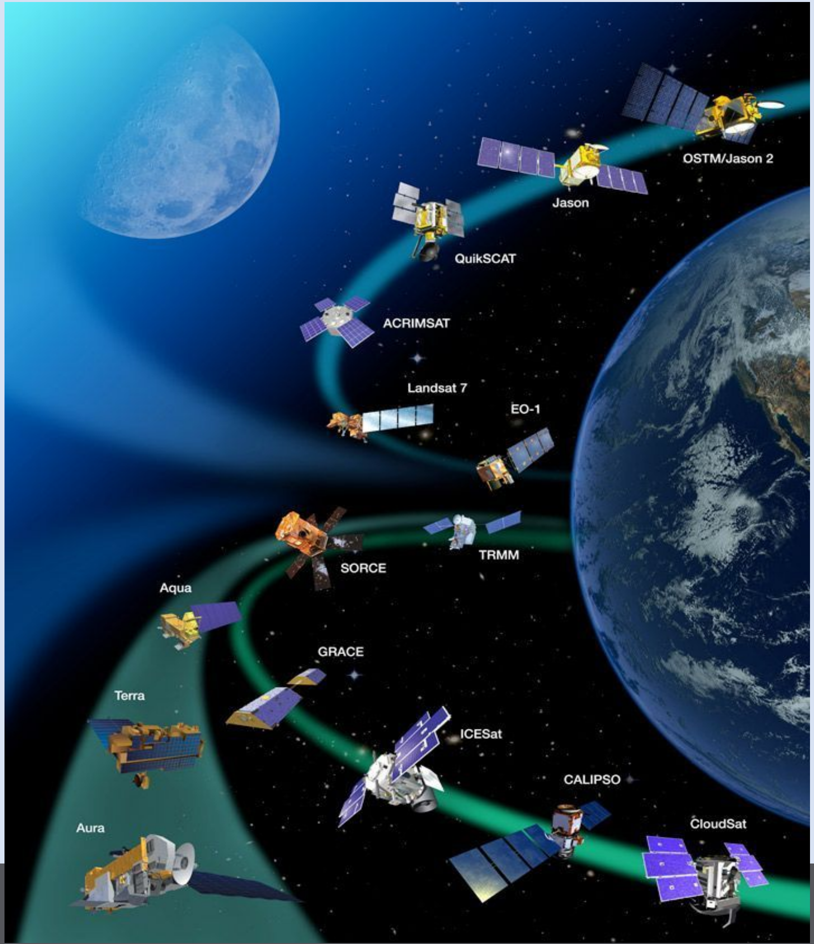
Motivation for the CTSM PPE Project

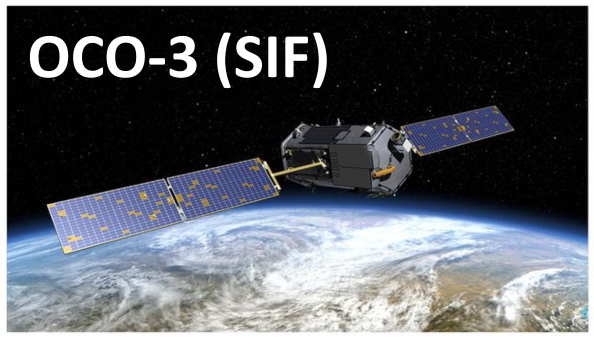
- Growing complexity and comprehensiveness of land models → increasing # of uncertain parameters (CTSM5 has over 200 parameters)
- Contribution of parameter uncertainty to total uncertainty expected to be large, but largely unquantified
- Systematic parameter calibration will enhance accuracy of simulations, and increase suitability and accessibility of CTSM for actionable science

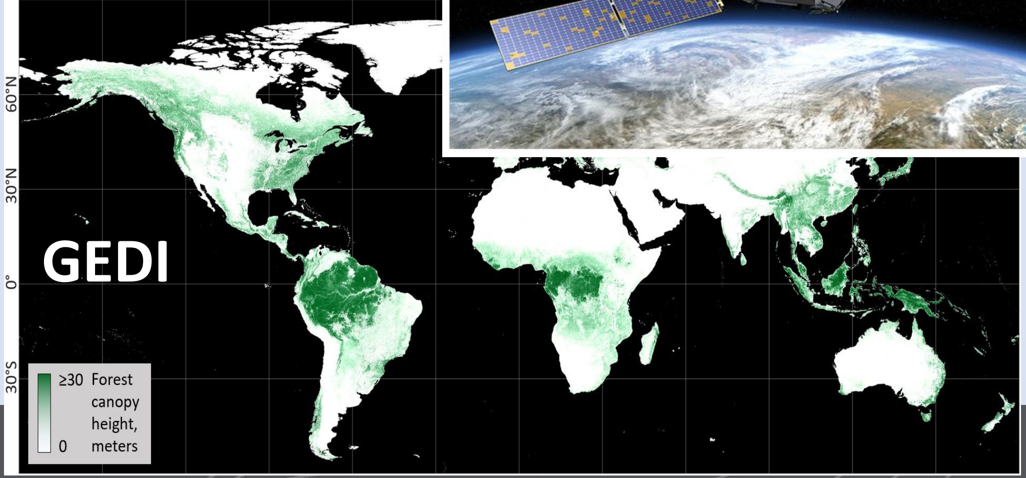
- Ecosystem vulnerability and impacts on carbon cycle and ecosystem services
- Water and food security in context of climate change, climate variability, and extreme weather
- Ecological, hydrological, and Earth system prediction
- Terrestrial contribution to Net Zero emissions goals

Unprecedented availability of Earth Observations

Unprecedented availability of Earth Observations

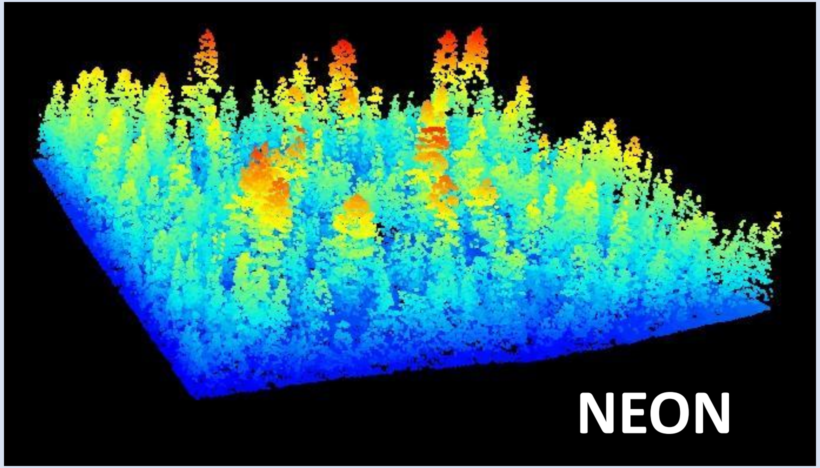




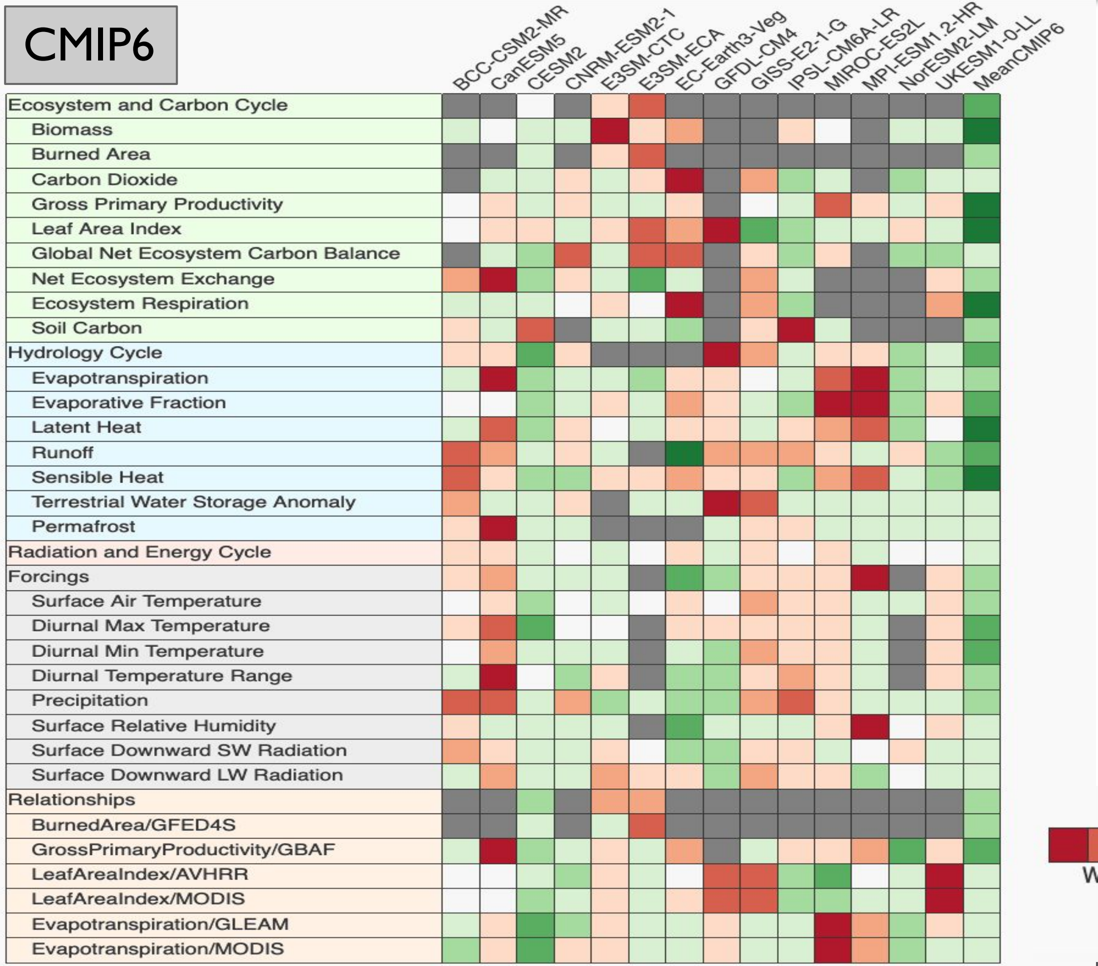


Unprecedented availability of Earth Observations

Flux tower networks like NEON, Ameriflux, FluxNet



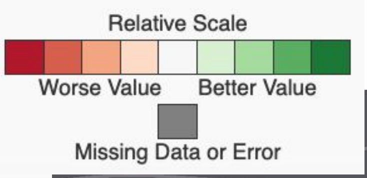
And new integrated metrics packages



International Land Model Benchmarking (ILAMB) project

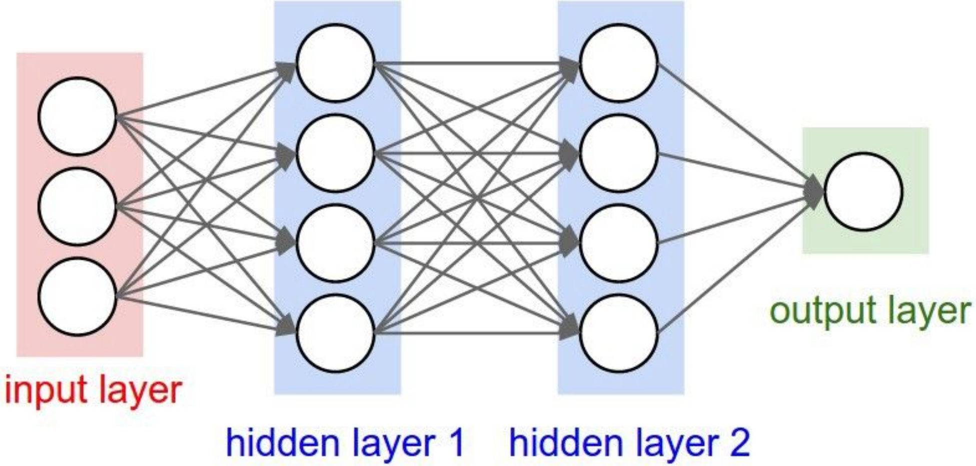
- Integrates analysis of ~30 variables against 70+ global, regional, and site-level observational datasets
- Graphics and scoring system for
  - RMSE
  - bias
  - seasonal cycle phase
  - spatial patterns
  - interannual variability
  - variable-to-variable relationships

DOE, NCAR, University collaboration



RUBISCO

Can we use machine learning to calibrate land model parameters?



Can we use machine learning to calibrate land model parameters?

But most prior efforts have focused on small number of sites and on one or two variables.

And, there is a lot of 'reinventing the wheel' (identify important params, param ranges, build an emulator, optimization methods)

Yes!

SIAM/ASA J. UNCERTAINTY QUANTIFICATION
Vol. 3, pp. 199–233

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Bayesian Calibration of the Community Land Model Using Surrogates*

J. Ray†, Z. Hou‡, M. Huang‡, K. Sargsyan†, and L. Swiler§

JGR Biogeosciences

Research Article | Free Access

Estimation of Community Land Model parameters for an improved assessment of net carbon fluxes at European sites

Hanna Post, Jasper A. Vrugt, Andrew Fox, Harry Vereecken, Harrie-Jan Hendricks Franssen

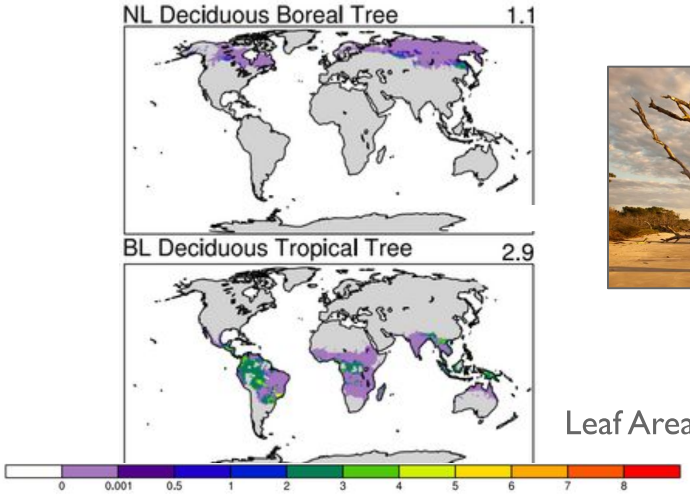
First published: 02 February 2017 | https://doi.org/10.1002/2015JG003297 | Citations: 20

Final stages of CLM5 development

The CLM development team successfully integrated the pile of CLM5 developments from the research community

… but many new uncertain parameters and a growing realization that in some parts of the parameter space, plants do not survive through spinup … and the model freeze date was rapidly approaching

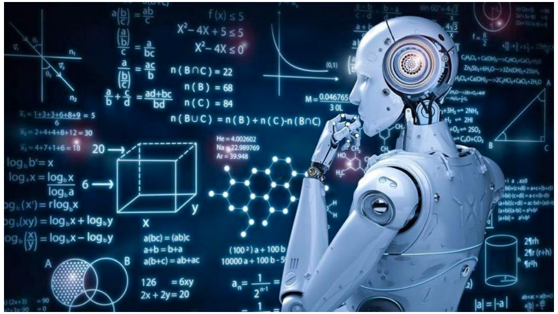
"The Dead Plant Problem"



Leaf Area Index

Solving the Dead Plant Problem

Global parameter optimization via machine learning!



many attempts, mostly dead

… meanwhile, the rest of the team focused on painstaking 'hand-tuning' of parameters

... and I ran interference with the CESM Chief Scientist Jean-Francois

January 25, 2017 (a reenactment)

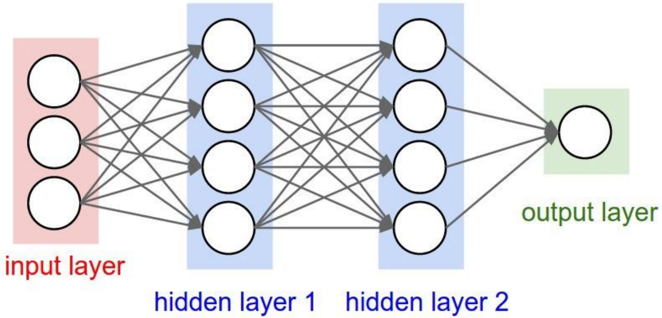
The scene: We were desperately trying to finalize CESM2 in order to take advantage of the Cheyenne / Yellowstone overlap to run CMIP6 simulations. After multiple extensions, Jean-Francois gave us one last weekend to sort out our parameter problems or revert to CLM4.5. On Friday, Keith Oleson set off two CLM spinups, one with latest (of many) machine-learning calibrated parameter set and one with our best hand-tuned parameters.

6:45am Monday morning: Keith comes into my office and shows me the ML calibrated parameter results – mainly dead plants.
Dave – "ok, that's not unexpected, check the other parameter set."

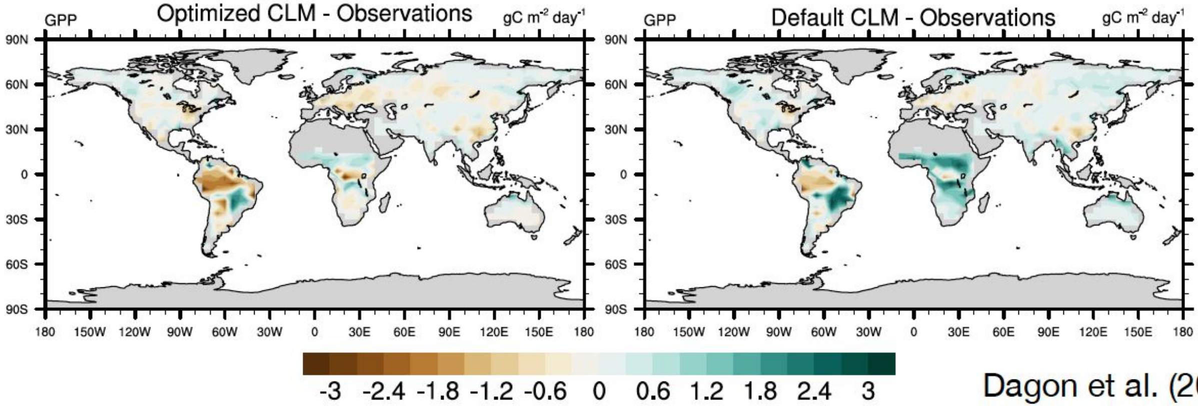
10 minutes later: email from Keith – "Plants in backup hand-tuned parameter set are not surviving either. Uh-oh."

Another 30 minutes later: another email from Keith – "Scratch that. Bug in my code. Backup parameter set results look great! My bad."

Can we use machine learning to calibrate land model parameters?



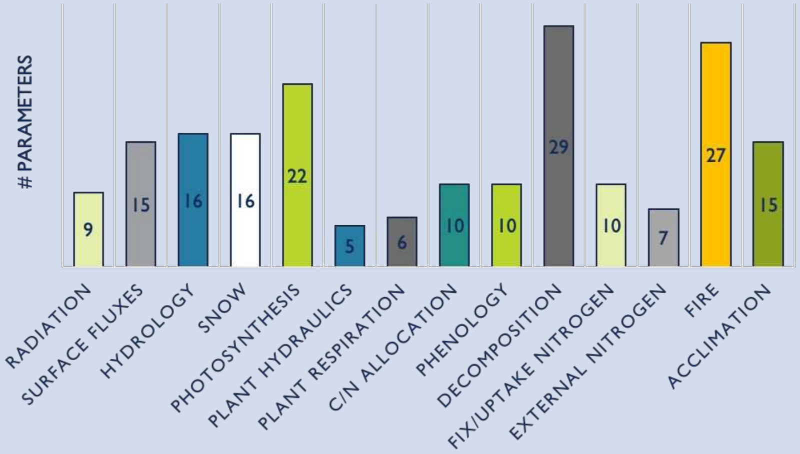
Dagon, K., B.M. Sanderson, R.A. Fisher, D.M. Lawrence (2020), *Adv. Stat. Clim. Meteorol. Oceanogr.*, 6, 223-244, doi:10.5194/ascmo-6-223-2020.



Dagon et al. (2020)

CTSM Perturbed Parameter Experiment (PPE) Project

- **Phase 0:** Infrastructure development (fast spinup, expose parameters, identify parameter ranges, ensemble and analysis scripting)



Parameter ranges

CLM5 Parameter List

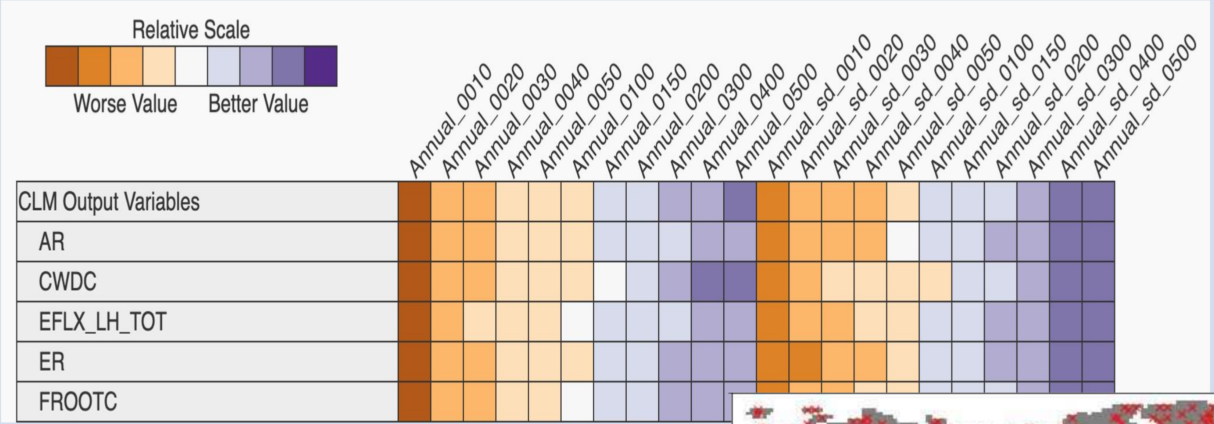
File Edit View Insert Format Data Tools Add-ons Help Last edit was made 4 days ago by Keith Oleson

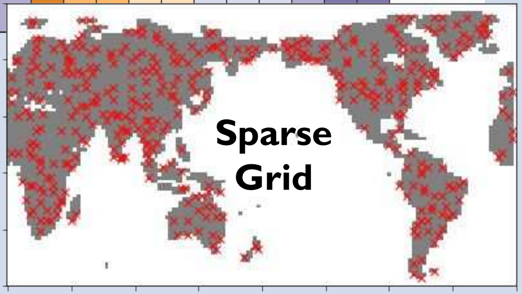
name	min	max	comments?	Description
should match the name on paramfile or namelist	low side perturbation	high side perturbation	feel free to add any comments below **ok, to write XXpercent, in lieu of absolute range**	this and the columns farther right not currently essential, but of course feel free to peruse and/or add information
Photosynthetic capacity (LUNA)				
slatop	pft	pft		specific leaf area at the canopy top
jmaxb0	0.01	0.05		the baseline proportion of nitrogen allocated for electron transport (J)
jmaxb1	0.05	0.25	This is Jmaxb1 in the code (note the capital J)	the baseline proportion of nitrogen allocated for electron transport (J)
Plant hydraulics				
kmax	pft	pft	see https://github.com/ESCOMP/CTSM/issues/1162 for how I chose kmax/krmax	Plant segment max conductance
krmax	pft	pft		Root segment max conductance
psi50	30percent	30percent		Water potential at 50% loss of conductance

CTSM PPE Project

- **Phase 0:** Infrastructure development (fast spinup, expose parameters, identify parameter ranges, ensemble and analysis scripting)

Use ILAMB to assess reconstructed output against 2º simulation 'truth'





Until recently, it has been computationally prohibitive to attempt to calibrate global CTSM(BGC)

- Cluster analysis → reasonably replicate global simulation results with 400 gridcells (Hoffman et al., 2013)
- Matrix solution to C/N states decreases spinup timescale by >10X (Lu et al., 2020)
- **1 million pe-hrs = ~2000 parameter perturbation simulations, inc. spinup**

CTSM PPE Project

- **Phase 0:** Infrastructure development (fast spinup, expose parameters, identify parameter ranges, ensemble and analysis scripting)

1. Spinup model to equilibrium with default params
2. From previous spinup, perturb parameter
3. 20 years Accelerated Decomposition (AD) spinup - provides good initial estimate of NPP
4. 80 years Semi-Analytical Spin-Up (SASU, “Step 3”)
5. 40 years Native Dynamics

140 total years;
- Compares to 445 years for cnmatrix step 0-4 spinup sequence
- Compares to ~1500 years for AD/pAD

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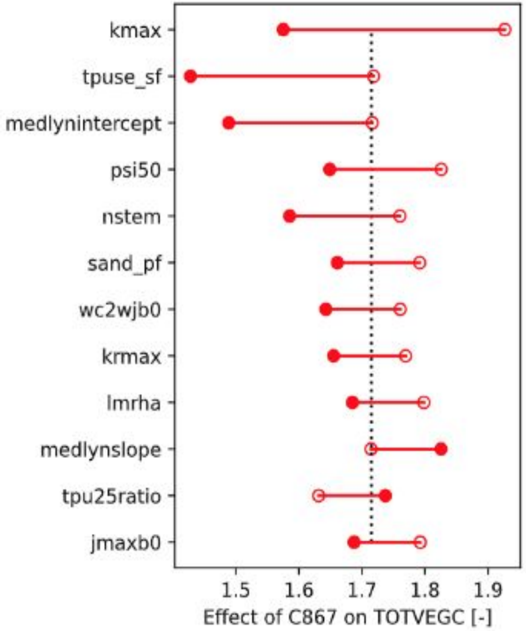
CTSM PPE Project

- **Phase 0:** Infrastructure development (fast spinup, expose parameters, identify parameter ranges, ensemble and analysis scripting)
- **Phase 1:** One-at-a-time parameter ensembles under range of environmental perturbations
  - Present-day control conditions
  - Climate: 1850 and SSP3-7 CESM2 climate
  - CO_2: 1850 and SSP3-7
  - N-dep: +5 gN/m2/yr
  - *Last Glacial Maximum conditions*
  - Restrict parameter ranges again if low-side environmental perturbation doesn't pass reasonableness checks

Top 12 params regulating CO_2 fertilization effect on global vegetation carbon

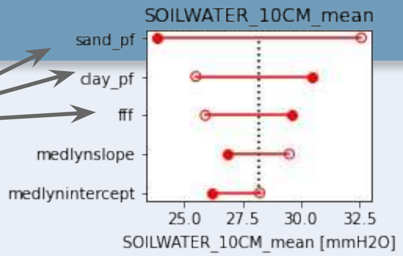


Which parameters control SOILWATER_10CM?

Exploring parameter sensitivity

Which parameters control SOILWATER_10CM?

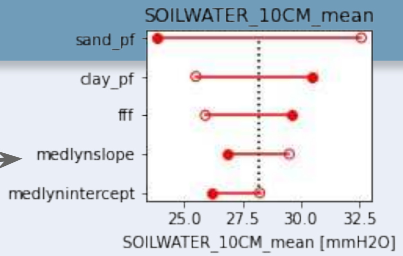
hydrology params



Exploring parameter sensitivity

Which parameters control SOILWATER_10CM?

plant params



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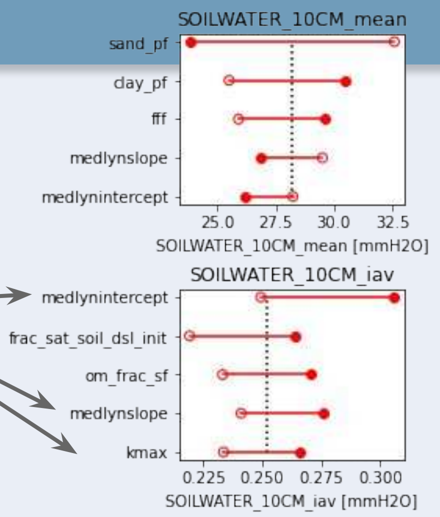

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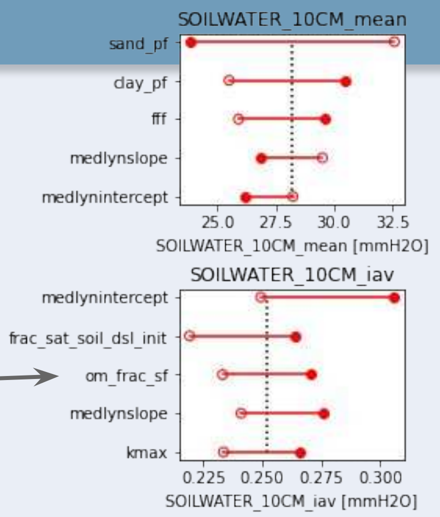
soil evap

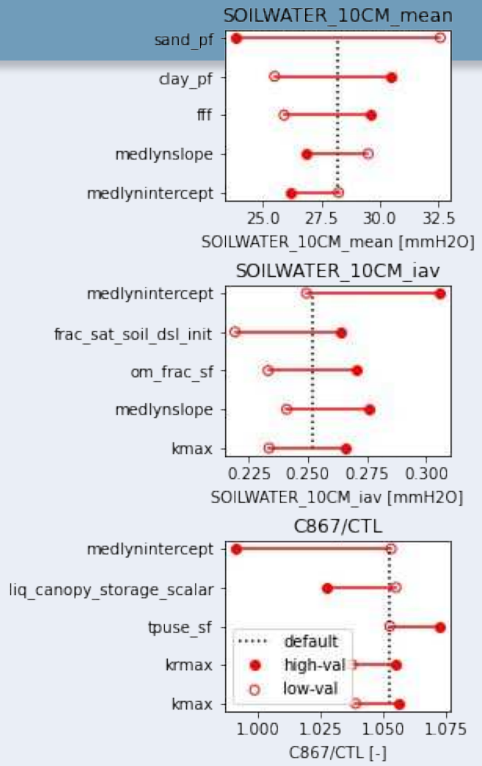
soil org. matter



Exploring parameter sensitivity

Which parameters control SOILWATER_10CM?

it's the plants!



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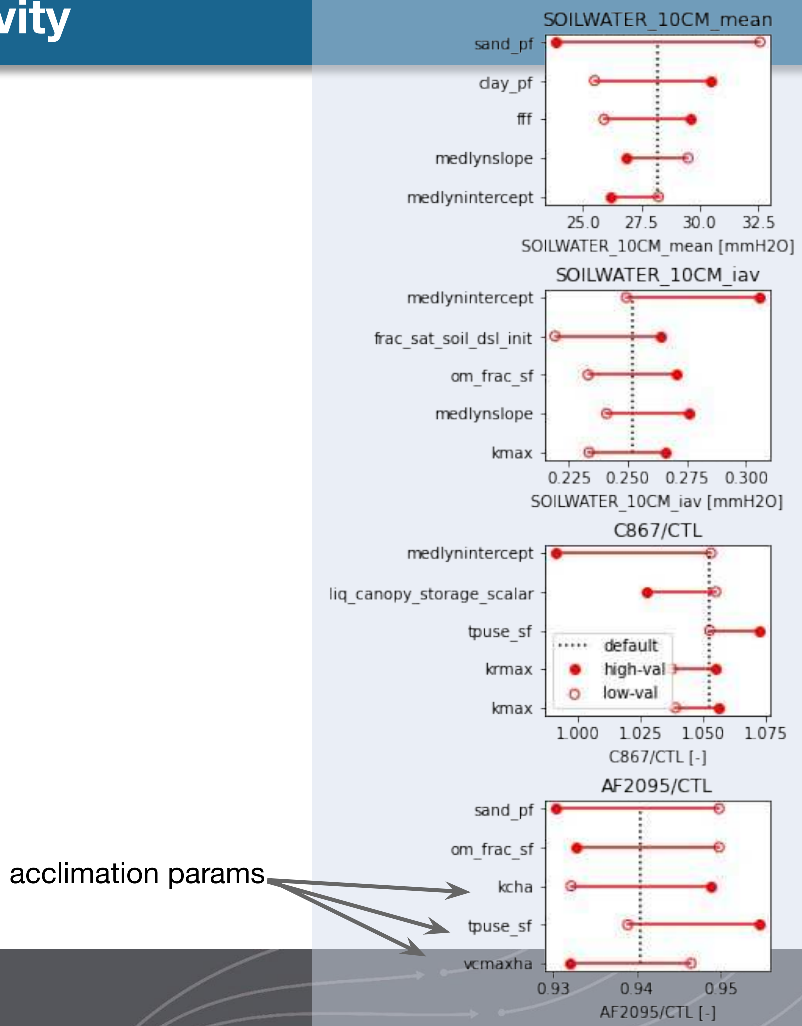
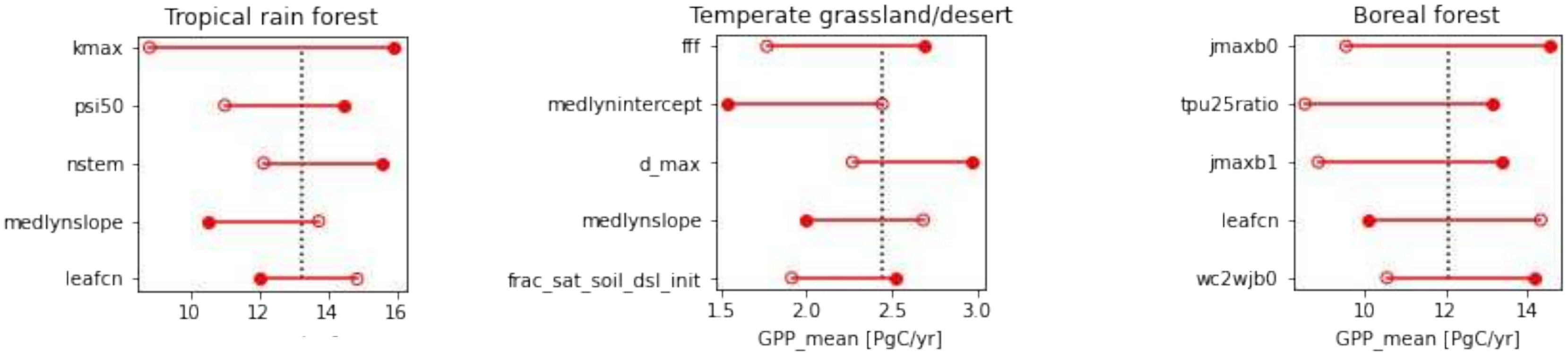


Most sensitive parameters differ across biomes

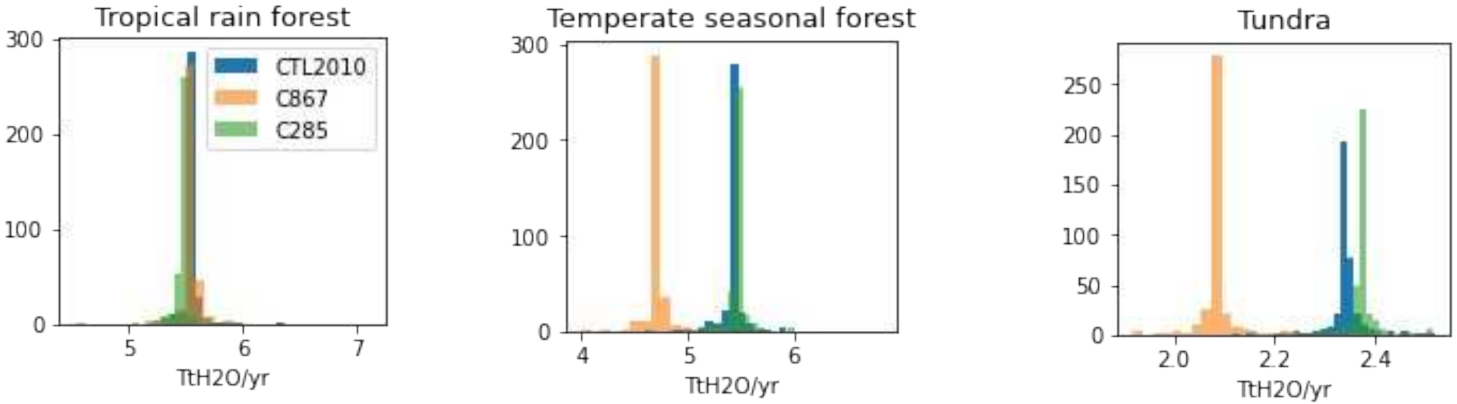


Plant water use

Soil water availability

Light use efficiency

CO_2 fertilization effect on ET varies by biome



CLM5 PPE Project

- **Phase 0:** Infrastructure development (fast spinup, expose parameters, identify parameter ranges, ensemble and analysis scripting)
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CTSM PPE Spinoff Projects

- Land-atmosphere interactions (Univ Washington)
- NEON site calibration (Auburn Univ)
- ET recession timescales (Oregon State)
- Arctic river flow (RAL)
- Land influence on drought (CGD)
- Hydrologic sensitivity (Cornell Univ)
- Tropical carbon cycle interannual variability (JPL)
- GPP response to permafrost thaw (Northern Arizona Univ)

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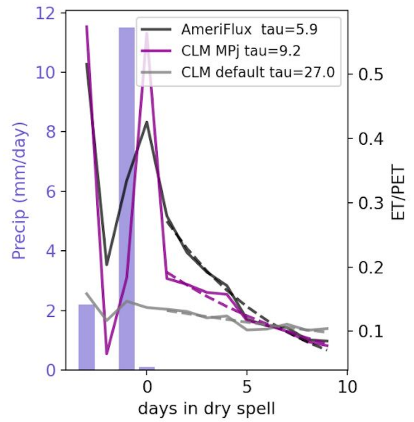

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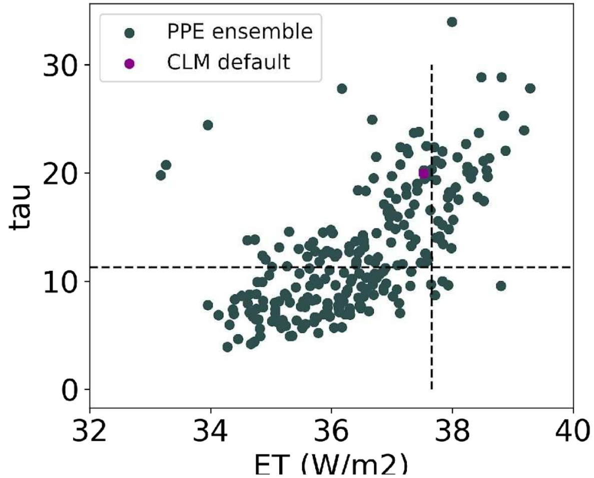

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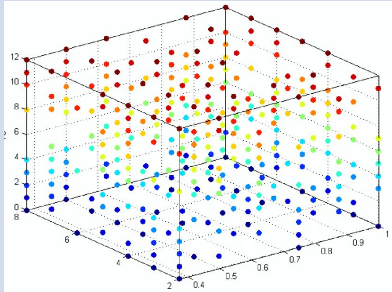
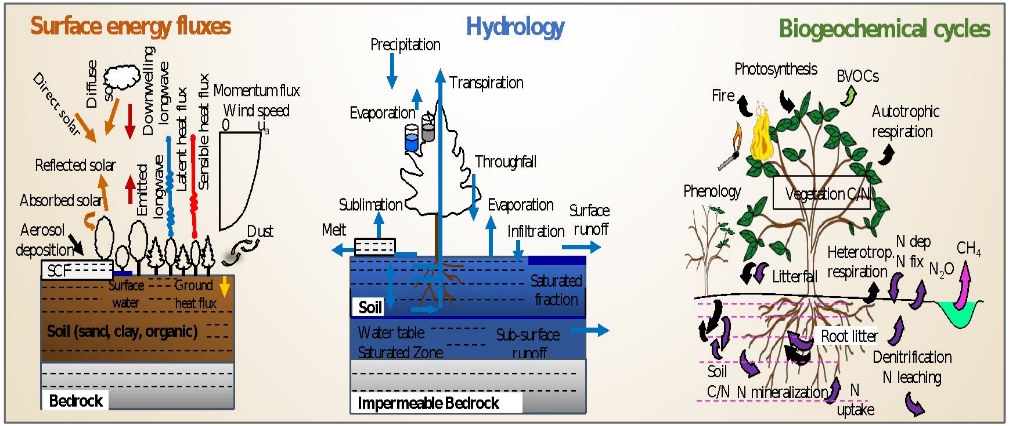
- **Phase 1:** One-at-a-time parameter ensembles under range of environmental perturbations (low/high CO_2, PI and future climate, N-dep)
- **Phase 2:** Parameter interactions
  - Latin-hypercube ensemble with most 'important' parameters
  - Neural network to emulate CLM output with parameters as input



NSF STC: Learning the Earth with Artificial intelligence and Physics

What are you calibrating for?

Twelve key variables
Leaf Area Index
Soil moisture
Soil temperature
Gross primary productivity
Latent Heat Flux
Sensible Heat Flux
Albedo
Ecosystem respiration
Vegetation carbon
Soil carbon
Burned area
Total Water Storage

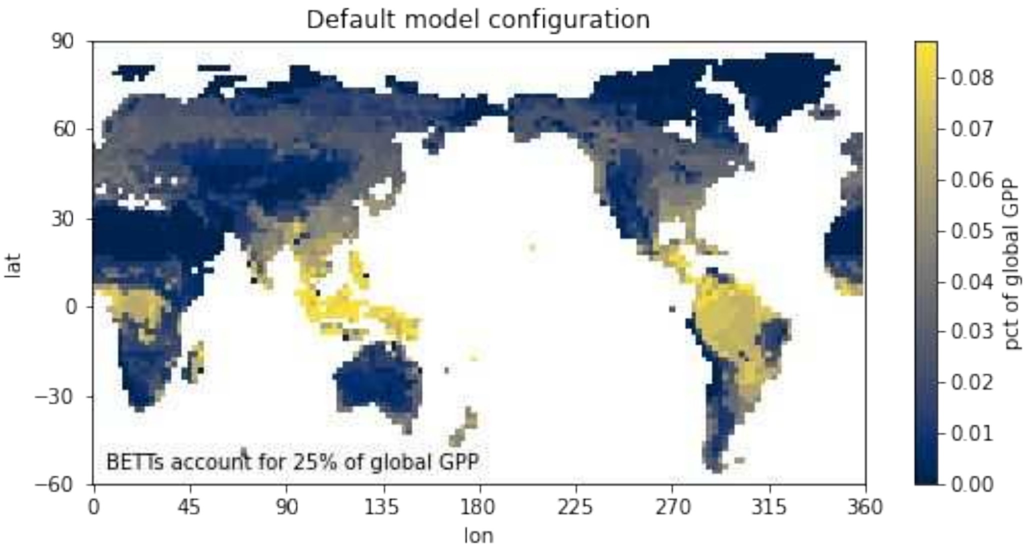


What are most important parameters for:
Global Mean
Global Interannual Variability
Diurnal Cycle
Biome-level Mean
Response to perturbations (CO, climate, Ndep)
…

CAVEAT #1: Avoid tropical bias

Which are the most important parameters?

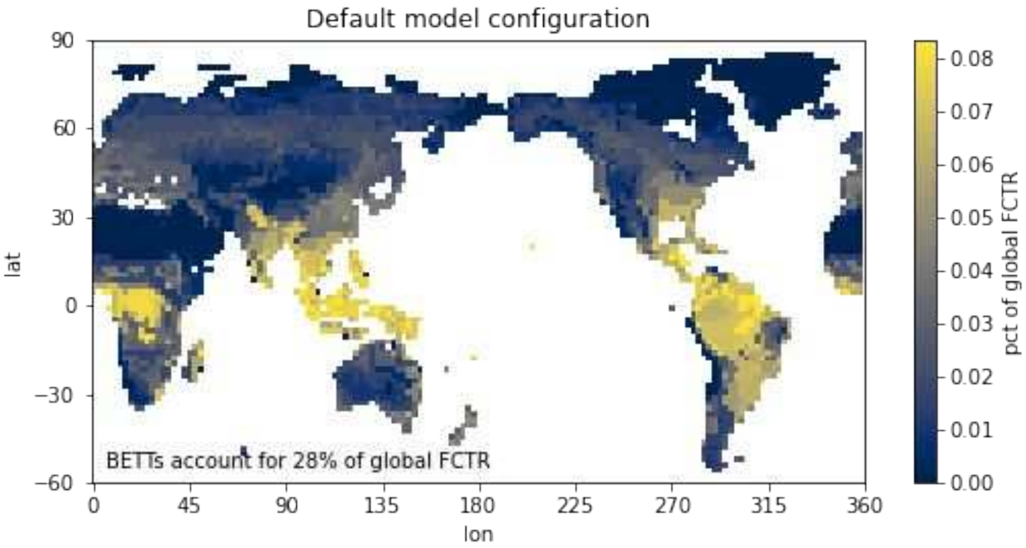
GPP



can we define a framework for reducing from 200→50?

Which are the most important parameters?

Transpiration



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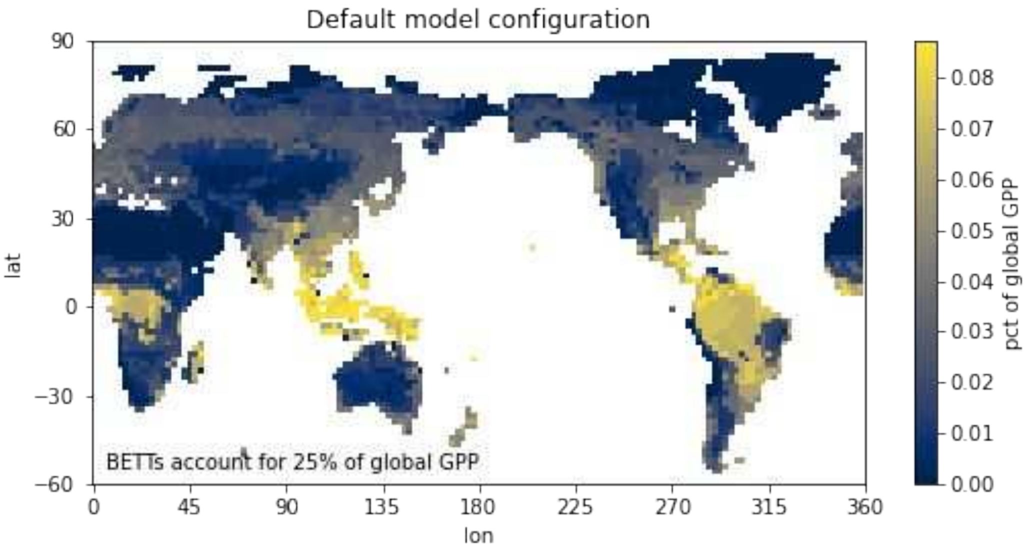
GPP

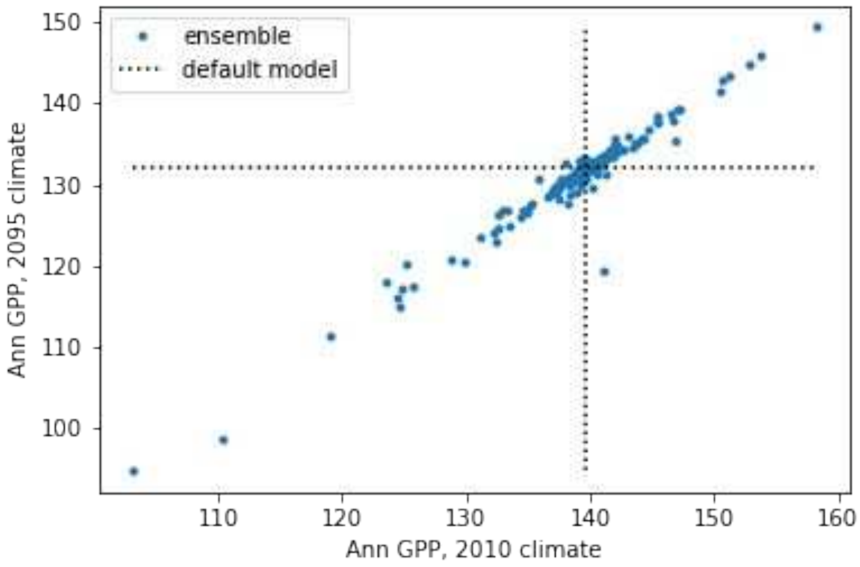


tropical trees dominate global fluxes

can we define a framework for reducing from 200→50?

CAVEAT #2: Survive spinup, capture climate response

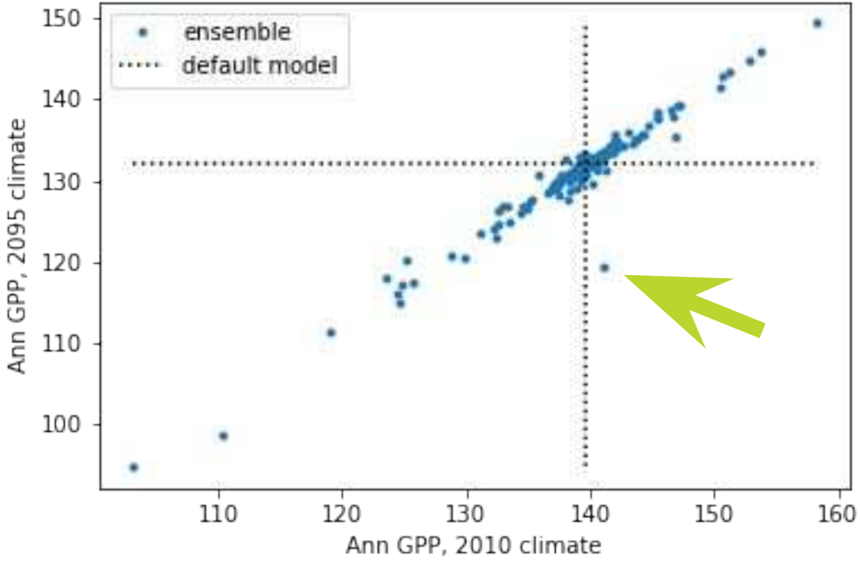
Should include parameters that affect present day climate, but also past/future climate



can we define a framework for reducing from 200→50?

Should include parameters that affect present day climate, but also past/future climate

tpu acclimation parameter
- small effect on present-day GPP
- big effect on warm-climate GPP



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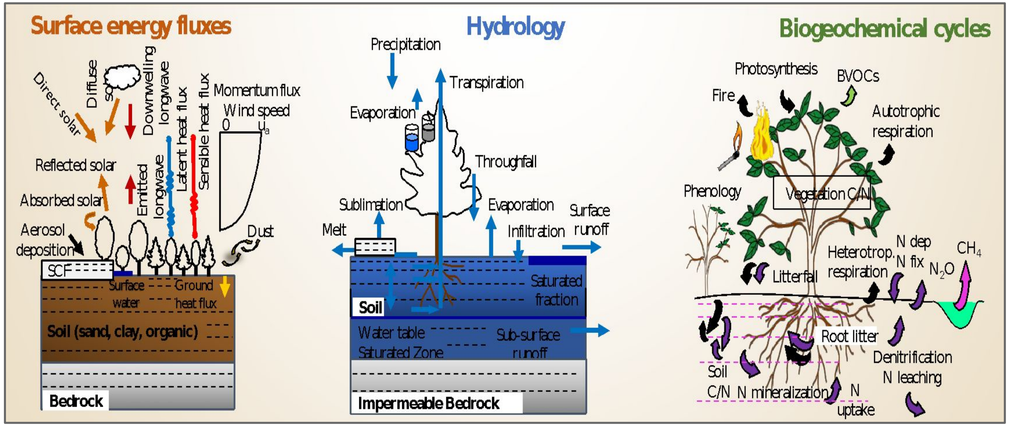

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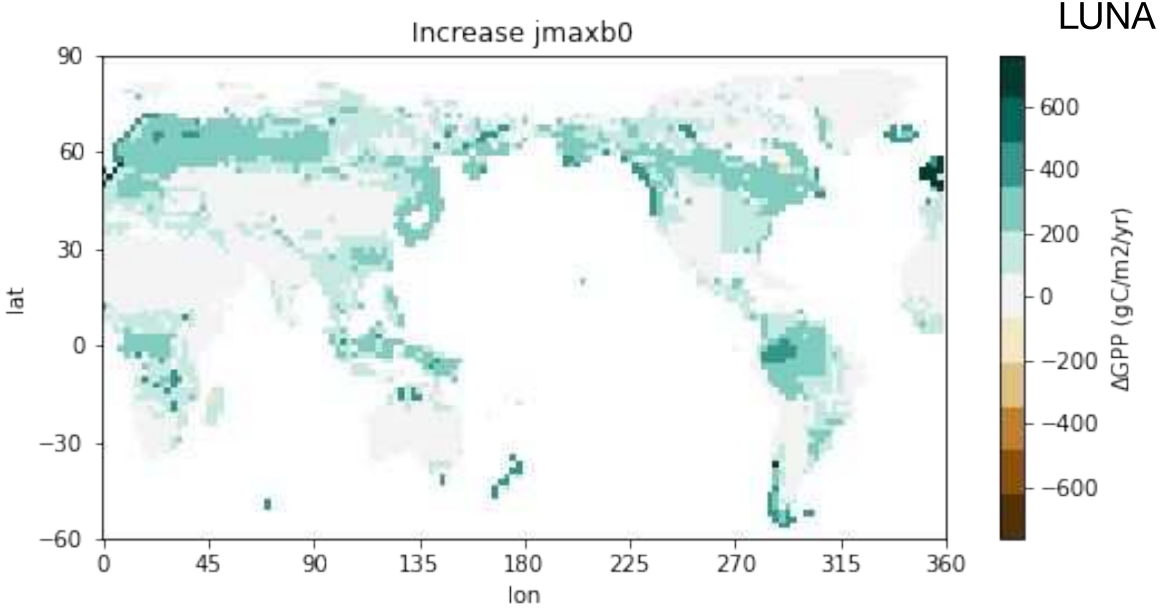
Response to perturbations (CO, climate, Ndep)

‘Good’ calibration requires regional levers



jmaxb0 is a global photosynthesis parameter:
LUNA param with strong control on jmax

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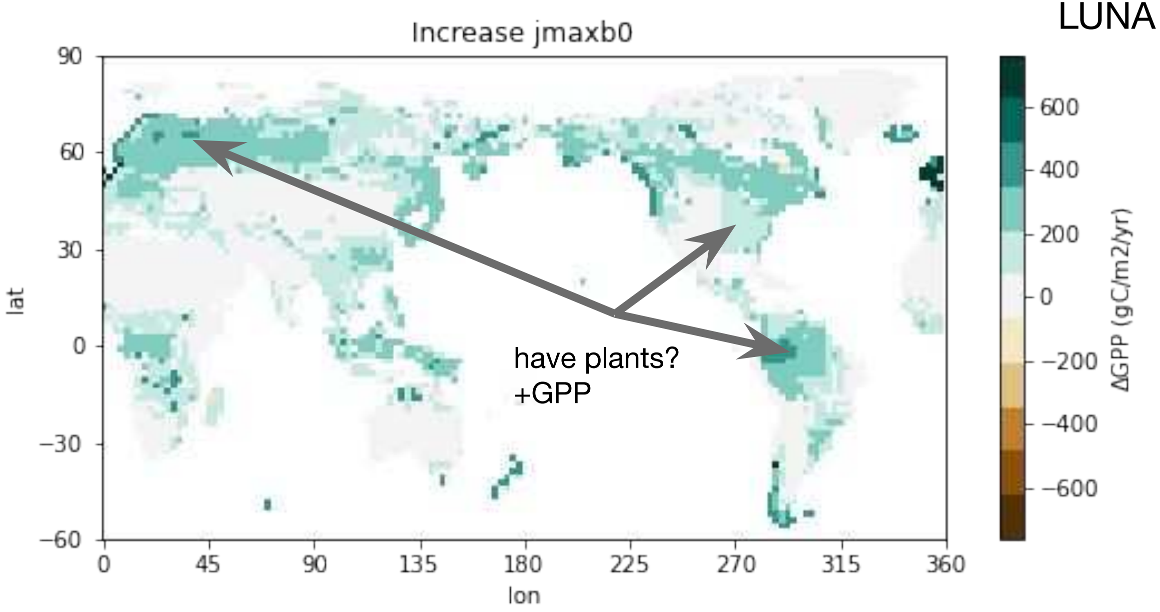

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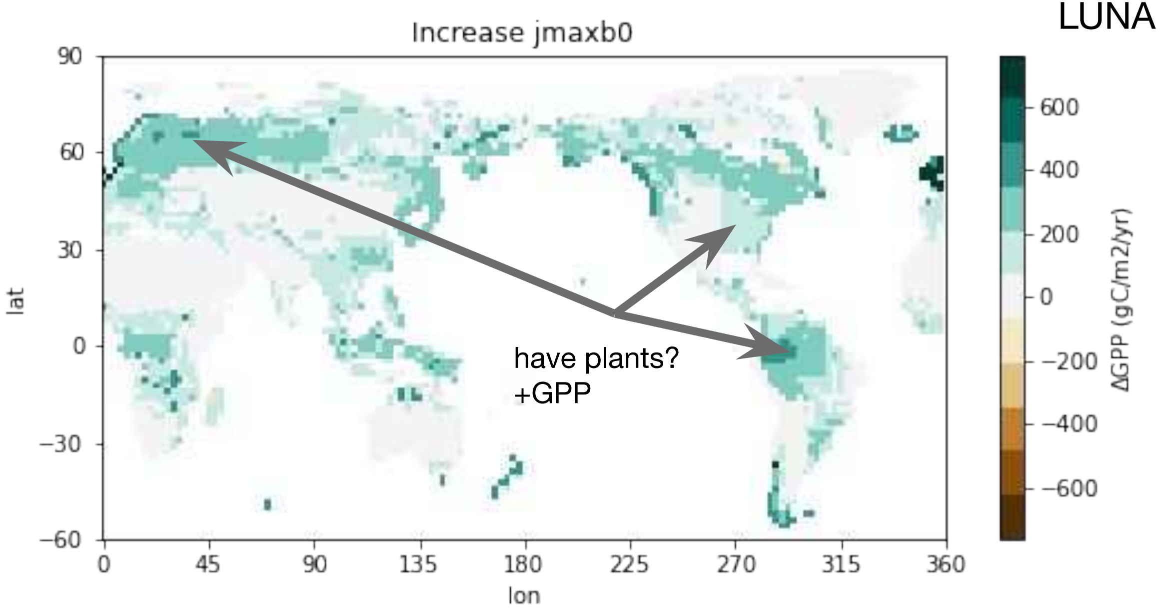
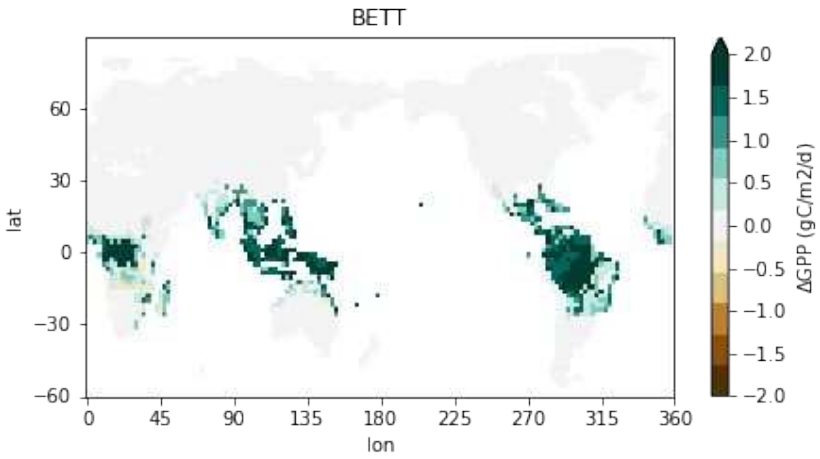


CAN PFT PARAMS HELP?

PFT example: medlynslope

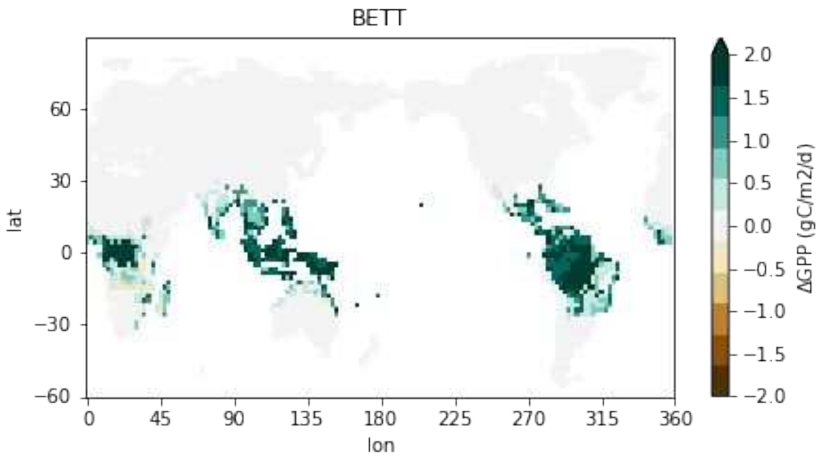


Reducing medlynslope for

Broadleaf Evergreen Tropical Trees

has a clear regional signature

PFT example: medlynslope



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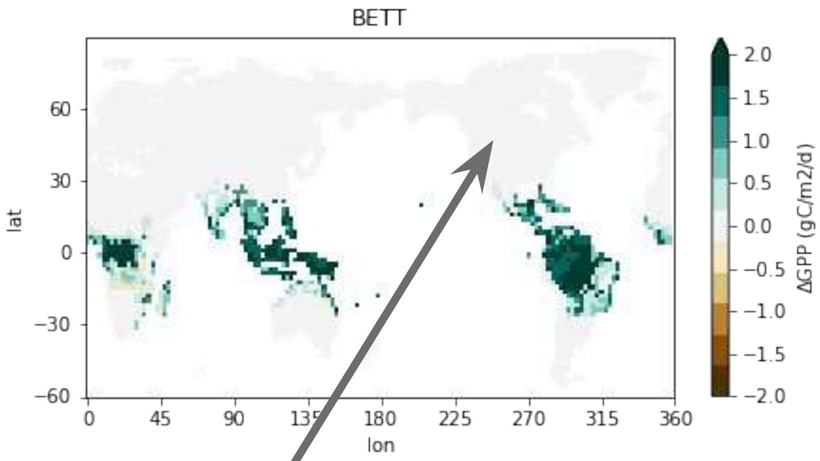
Broadleaf Evergreen Tropical Trees

has a clear regional signature

CLM5 has 16 natural vegetation PFTs

- if we perturb them all at once, we can't discern regional hydrology levers
- costly to perturb them all independently

PFT example: medlynslope



everywhere that is gray
we are essentially re-running
the default simulation

Reducing medlynslope for

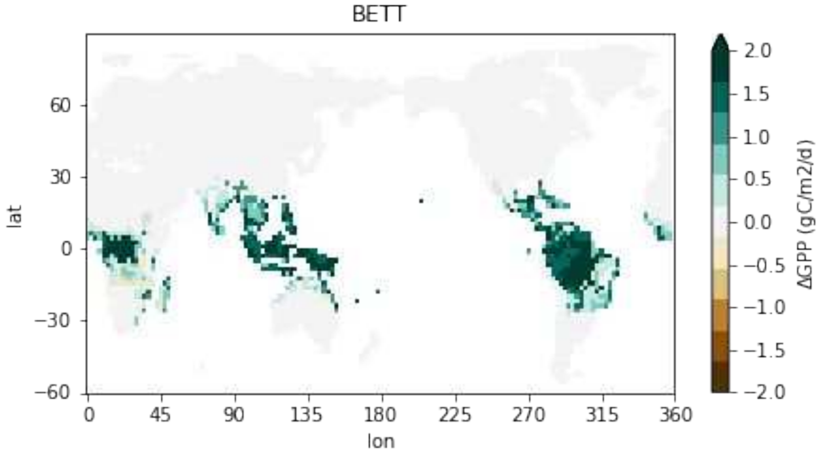
Broadleaf Evergreen Tropical Trees

has a clear regional signature

CLM5 has 16 natural vegetation PFTs

- if we perturb them all at once, we can't discern regional levers
- costly to perturb them all independently

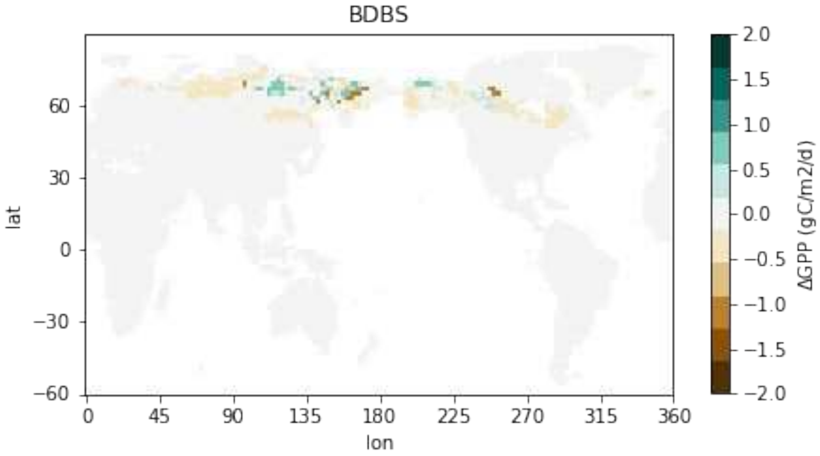
Varying medlynslope



can we find groups of PFTs that

- minimize spatial PFT interactions
- maximize information

3 groups looks ideal, so this means we effectively treat selected PFT parameter as 3 parameters in Latin Hypercube



What are you calibrating for?

Twelve key variables

Leaf Area Index
Soil moisture
Soil temperature
Gross primary productivity
Latent Heat Flux
Sensible Heat Flux
Albedo
Ecosystem respiration
Vegetation carbon
Soil carbon
Burned area
Total Water Storage

Which parameters control?

Global Mean
Global Interannual Variability
Biome-level Mean
Response to perturbations
(CO, climate, Ndep)

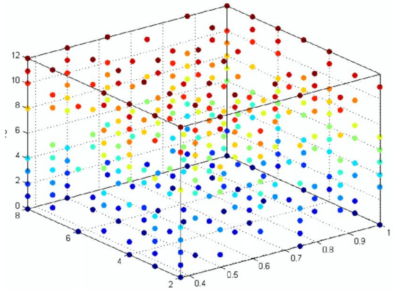
Leaf Area Index

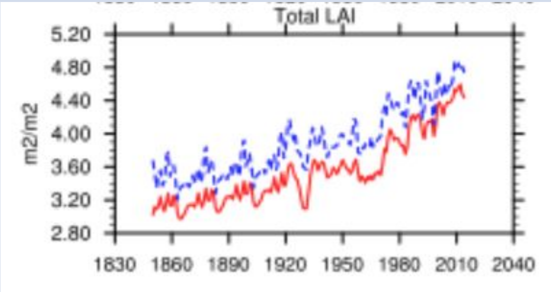
Parameter	Param type
jmaxb0	Photosynthesis
jmaxb1	
wc2wjb0	
theta_cj	
leafcn (PFT)	
jmaxha	
tpu25ratio	
hksat_sf	Soil hydrology
fff	
sucsat_sf	
d_max	
kmax (PFT)	Plant water use
medlynslope (PFT)	
medlynintercept (PFT)	
crit_dayl	Phenology
soilpsi_off	
leaf_long (PFT)	Leaf physiology
slatop (PFT)	
lmr_intercept_atkin	Respiration
lmrha	
froot_leaf (PFT)	Allocation
FUN_fracfixers (PFT)	Nitrogen uptake
pc	Snow

Parameter Selection

22 parameters, 3 PFT level = 28 effective params * 15 =

420 simulations

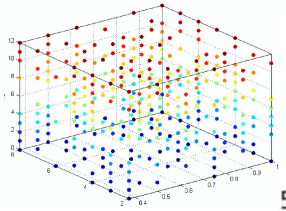


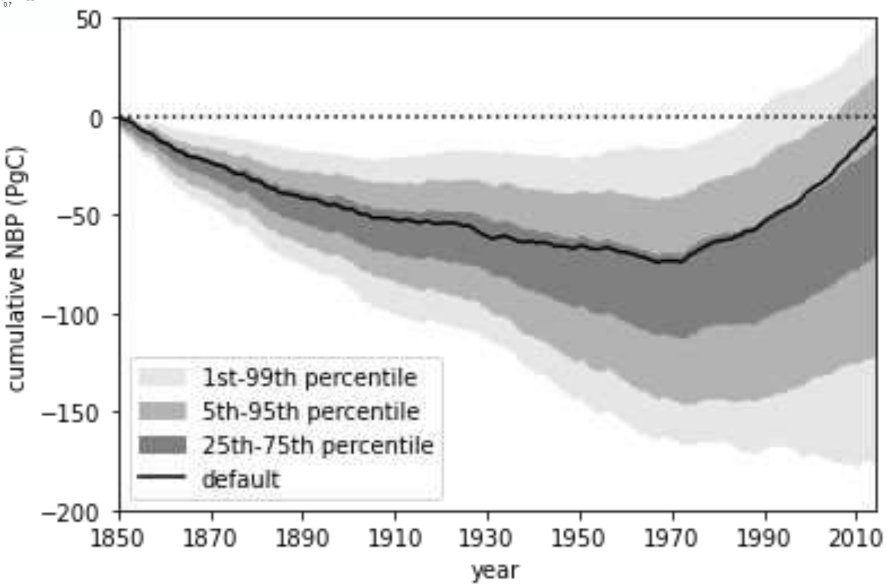


To best enable comparison to present-day observations, each simulation run over historical period

Leaf Area Index	
Parameter	**Param type**
jmaxb0 jmaxb1 wc2wjb0 theta_cj leafcn (PFT) jmaxha tpu25ratio	Photosynthesis
hksat_sf fff sucsat_sf d_max	Soil hydrology
kmax (PFT) medlynslope (PFT) medlynintercept (PFT)	Plant water use
crit_dayl soilpsi_off	Phenology
leaf_long (PFT) slatop (PFT)	Leaf physiology
lmr_intercept_atkin lmrha	Respiration
froot_leaf (PFT)	Allocation
FUN_fracfixers (PFT)	Nitrogen uptake
pc	Snow

Parameter Selection





Leaf Area Index	
Parameter	**Param type**
jmaxb0	Photosynthesis
jmaxb1	
wc2wjb0	
theta_cj	
leafcn (PFT)	
jmaxha	
tpu25ratio	
hksat_sf	Soil hydrology
fff	
sucsat_sf	
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kmax (PFT)	Plant water use
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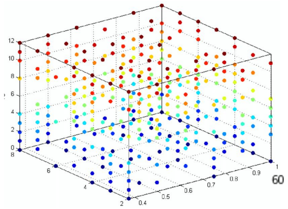
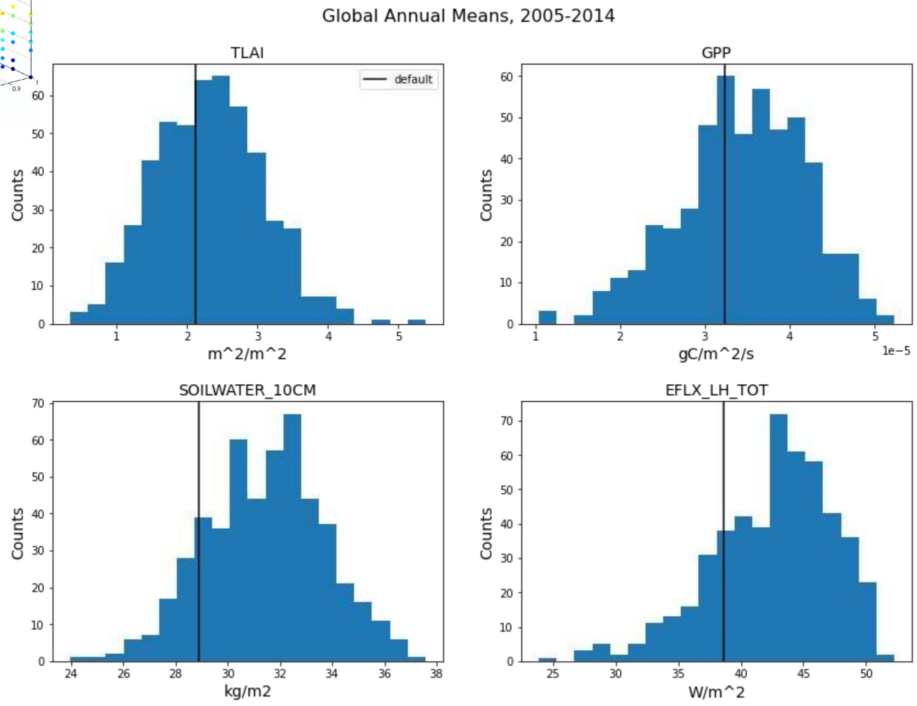
Parameter Selection





Leaf Area Index	
Parameter	**Param type**
jmaxb0	Photosynthesis
jmaxb1	
wc2wjb0	
theta_cj	
leafcn (PFT)	
jmaxha	
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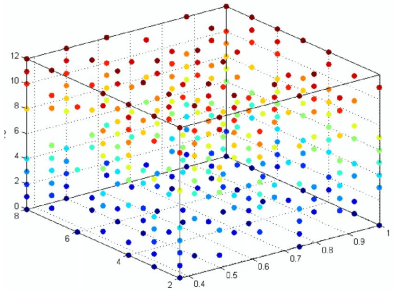
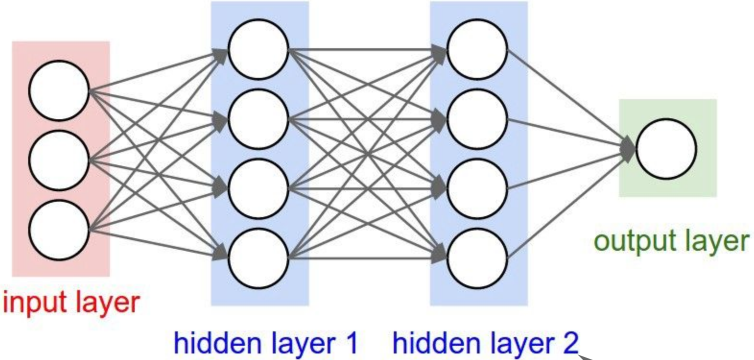
Neural Networks as Land Model Emulators

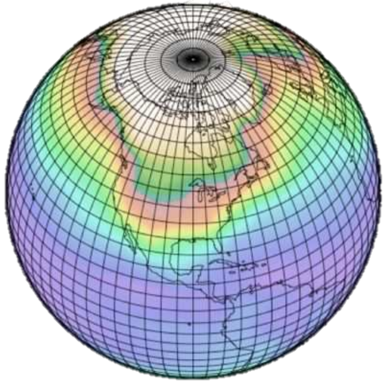
Input: land model parameter values



Neural network emulator



Output: land model predictions



A machine learning algorithm is trained to predict land model output, given parameter values as input.

Network image: http://cs231n.github.io/neural-networks-1/

CTSM PPE Project

- **Phase 3:** Develop tools to identify optimized parameter *sets*
  - multi-objective calibration targets (mean, variability, response to perturbation, spatial distribution for carbon, water, energy fluxes and states)

$$J(p) = \sum_{v=1}^{2} \left[\sum_{m=1}^{3} \lambda_{v,m} \left(\frac{\hat{U}_{v,m}(p) - U_{obs,v,m}}{\sigma(U_{obs*,v,m})} \right)^2 \right]$$

Sum over output variables *v*

Sum over modes *m* for each term, weighting by % variance

Emulator predictions for parameters *p*

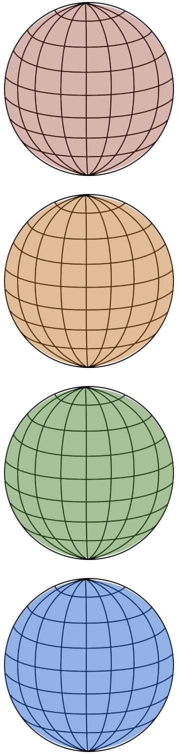
Normalize by standard deviation in observations

Observations

NSF STC: Learning the Earth with Artificial intelligence and Physics

- Calibrated parameter sets for CESM3 or for specific actionable science projects
- Goal: Quantify carbon and water projection uncertainty due to parametric uncertainty (~200 member ensemble of global historical and projection period land-only simulations)

Summary



- We are able to run large ensembles of global CLM
  - 2000+ simulations with full BGC version of model
  - Taking advantage of sparse grid and CN-Matrix spinup
  - note that SP mode is even cheaper!
- OAAT ensemble dataset provides valuable insight into model behavior
  - available on Cheyenne
  - analysis template available via github
  - will put dataset on the cloud (LEAP-Pangeo)
- Making progress towards open-source parameter estimation tools
  - Supports parameter uncertainty quantification
  - Model calibration for actionable science
- PPE working group meets ~monthly
  - email dlawren@ucar.edu to join the list

github.com/djk2120/ppe_tools

djk2120@ucar.edu